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SCHIFF BASE COMPLEXES OF CO(II) AND NI(II) DERIVED FROM 2-AMINOPYRIMIDINE AND 2-HYDROXYNAPHTHALDEHYDE: SYNTHESIS, SPECTRAL CHARACTERIZATION, AND BIOLOGICAL SIGNIFICANCE

Chemistry

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ABSTRACT

A new series of Co(II), Ni(II) complexes of tridentate Schiff base derived from condensation of 2-aminopyrimidine with 2-hydroxynaphthaldehyde were synthesized in a 2:1 molar ratio. Physical (magnetic measurements, molar conductance), spectral (IR, UV-Vis and Mass) and analytical data have established the structures of synthesized Schiff base and its metal complexes. The elemental analysis data suggest the stoichiometry to be 2:1 (L: M). Infra-red spectral data indicate the coordination between the ligand and the central metal ion through deprotonated phenolic oxygen, pyrimidine nitrogen and azomethine nitrogen atoms. Spectral studies and magnetic susceptibility measurements suggest an octahedral geometry for the complexes. The ligand and its complexes were tested / screened for their antibacterial activity against two Gram-positive bacteria species Staphylococcus aureus and Lactobacillus and two Gram-negative species Escherichia coli and Pseudomonas aeruginosa. It is observed that the ligand as well as the complexes showed good activity against all microbes.

KEYWORDS

Schiff base, metal complex, ligand, stoichiometry, geometry, pharmacological activities, antibacterial activity

INTRODUCTION

Schiff bases, first introduced by Hugo Schiff in 1864, are a class of organic compounds containing a functional group characterized by a carbon-nitrogen double bond (C=N), formed through the condensation of primary amines with carbonyl compounds (aldehydes or ketones) [1]. These compounds are of great interest in both synthetic and biological chemistry due to their structural versatility and diverse reactivity, making them valuable intermediates in organic synthesis and essential ligands in coordination chemistry [2-4].

In this paper, a Schiff base was synthesized from 2-aminopyrimidine and 2-hydroxynaphthaldehyde. The resulting Schiff base (3-((pyrimidin-2-ylimino)methyl)naphthalene-2-ol exhibit a variety of structural configurations depending on the substituents attached to the nitrogen and carbon atoms. This Schiff base, due to its ability to chelate metal ions was then used to form complexes with Co(II) and Ni(II) metal ions. The coordination of these metal ions to the Schiff base ligand significantly alters the properties of the resulting complexes, enhancing their stability, solubility and biological activity [5]. Metal complexes of Schiff base, such as those derived from Co(II) and Ni(II), have been extensively studied for their antimicrobial and antifungal activities [6, 7].

Spectroscopic techniques such as ultraviolet-visible (UV-Vis), infrared (IR), nuclear magnetic resonance (NMR) and mass spectrometry were employed to characterize the Schiff base and their metal complexes [8]. The C=N stretching vibration in the IR spectrum is a distinguishing feature, while NMR provides valuable information about the electronic environment of the atoms in the complex [9]. These techniques, along with X-ray crystallography, were used to confirm the structure and coordination of the Schiff base complexes with Co(II) and Ni(II) ions [10].

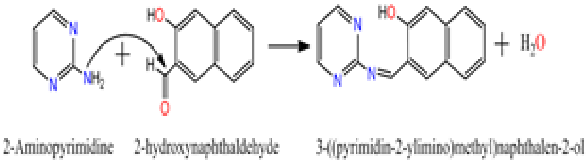
In conclusion, Schiff base and its metal complexes, particularly those derived from Co(II) and Ni(II) ions, show significant promise as therapeutic agent, especially due to its antimicrobial and antifungal activities. Its ability to form stable metal complexes and interact with biological macromolecules contributes to its potential in combating microbial infections, making it valuable candidate for further drug development [11, 12].

Experimental

All the chemicals used were of AR/GR grade. Pure sample of 2-aminopyrimidine, molecular formula $C_4H_5N_3$, molecular weight 95.10 g/mol, melting point~122-126°C was obtained from SRL Chemicals Ltd. Metal salts such as $CoCl_2$, $NiCl_2.6H_2O$ were of Merck. Solvents used were ethanol, acetone, DMF and dimethylsulfoxide (DMSO).

Synthesis Of Schiff Base

The compound was synthesized from 2-hydroxynaphthaldehyde and 2-aminopyrimidine by adding 2-hydroxynaphthaldehyde ethanolic solution (1.22g; 0.01mol) to same volume of ethanol solution of 2-aminopyrimidine (0.8144g; 0.01mol). The mixture was refluxed for 2 hrs and kept overnight at room temperature. The resulting solution was evaporated to 20% of its original solution and the product was collected by filtration, washed several times with ethanol, recrystallized from hot ethanol and then dried. The melting point of resulting yellow crystals was recorded.



Synthesis Of Complexes

The solid complexes were prepared by mixing ethanolic solutions of the ligand (HL) (0.18g and 0.01mol) with ethanolic solution of chlorides of Co(II) (0.059g and0.005mol), Ni(II) (0.049g and 0.005mol) separately. The resulting solutions were checked for pH and pH was adjusted by adding few drops of N/10 NaOH solution. The solutions were refluxed for 4 h and the refluxed solutions were kept for some days, solid crystalline complexes appeared in the solution which were filtered off, washed thoroughly with same solvent and finally with acetone, vacuum dried and weighed. Melting points of the complexes were recorded.

Analysis And Instrumentation

Elemental analysis was carried out on Vario MICRO V2.20 Elementar Analyse Systeme GmbH, from IIIM, Jammu. Metal contents were determined gravimetrically [13]. The infrared spectra were recorded on FT-IR Spectrophotometer Model RZX (Perkin Elmer) using KBr pellets from SAIF, Panjab University, Chandigarh. Molar conductance measurements were made in 10^{-3}M DMF solution on a Systronics Direct Reading Conductivity Meter (Model 303). The melting points of the ligand and the complexeswere recorded in open capillaries on a capillary melting point apparatus. Electronic spectra were recorded on a UV-VIS-NIR- Spectrophotometer Model Lambda 750 Perkin Elmer from SAIF, PU, Chandigarh. The magnetic susceptibility measurements were carried out on a Vibrating Sample Magnetometer from IIT, Roorkee.

RESULTS AND DISCUSSION

Through a condensation reaction, an amino group of aminopyrimidine in the pure compound was allowed to react with 2-hydroxynaphthaldehyde to form a Schiff base ligand (L) which was subsequently, reacted with metal ions to from Schiff base metal complexes. The ligand and the metal(II) complexes were isolated pure from EtOH in good yields.

The analytical data of the complexes correspond with 1:2 (metal: ligand) stoichiometry. Thus, the general formula $[M(L_2)]$ where [M(II) = Co, Ni], has been assigned to the metal complexes, respectively. They are very air stable solids at room temperature without decomposition for a long time. The complexes are non-hygroscopic, insoluble in water and other common organic solvents but soluble in DMF and DMSO. The molar conductance value of the complexes (measured in 10^{-3}M DMF) reveals the non-electrolytic nature of the complexes [14]. The magnetic moment data indicated all the complexes to be paramagnetic in nature. The physico-chemical characterization and analytical data and molar conductance values are given in Table 1 and Table 2.

Table: 1 Physico-Chemical Characteristics of Ligand APN And Its Complexes

S. No	Ligand/ Complexes	Colour	% Yield	M.P °C	Molar Conductance Ω^{-1} cm^2 mol^{-1}
1	APN	Light yellow	75	170	-
2	$[Co(APN)_2]$	Light Purple	70	195	13.7
3	$[Ni(APN)_2]$	Greenish Brown	73	230	12.5

Table 2: Analytical And Physicochemical Data Of Ligand APN And Its Complexes

S. No.	Molecular Formula (Molecular Weight)	Elemental Analysis (%) Found (Calculated)				Magnetic Moment B.M.
		C	H	N	Metal	
1	$C_{15}H_{11}N_3O$ (249.27)	72.19 (70.09)	4.40 (4.18)	16.08 (15.99)	-	-
2	$C_{30}H_{22}N_6O_2Co$ (557.47)	64.44 (63.07)	3.93 (2.47)	15.03 (14.55)	19.95 (18.60)	5.38
3	$C_{30}H_{22}N_6O_2Ni$ (621.23)	66.44 (64.05)	3.93 (3.89)	15.04 (14.09)	12.06 (11.90)	3.18

Magnetic Measurements

The magnetic moment data are presented in Table 2. The Co(II) complex showed a value of 5.38 B.M., which is slightly lower than the spin only value of 5.92 B.M. for high spin octahedral Co(II) complexes [15]. Ni(II) complex showed magnetic moment values of 3.18 B.M., slightly higher than the spin only (2.83B.M.) value, indicating an octahedral environment around Ni(II) ion [16,17].

Electronic Spectra

The electronic spectra of the complexes were recorded in the solution state. The energies of the observed spin allowed bands in all the complexes agreed with the octahedral geometry. The electronic spectrum of Co(II) complex shows bands at 10000cm^{-1}, 19810cm^{-1} and 20746 cm^{-1},which can be assigned to $^4T_1g(F) \rightarrow {}^4T_2g(F)$, $^4T_1g(F) \rightarrow {}^4A_2g(F)$ and $^4T_1g(F) \rightarrow {}^4T_1g(P)$ respectively, for Co(II) ion in an octahedral field [18].

The electronic spectrum of the Ni(II) complex displayed three bands at 12500 cm^{-1}, 18900 cm^{-1} and 26400 cm^{-1}, assigned to $^3A_2g(F) \rightarrow {}^3T_2g(F)$, $^3A_2g(F) \rightarrow {}^3T_1g(F)$ and $^3A_2g(F) \rightarrow {}^3T_1g(P)$ transitions, respectively, which indicate octahedral geometry of the Ni(II) complex [19,20].

Infrared Spectra

IR spectra of complexes indicates that the Schiff base (ligand) acts as a tridentate ligand, using phenolic oxygen andazomethine nitrogen and nitrogen of pyrimidine ring as donor atoms. The IR spectrum of the Schiff base shows a strong band at 1609 cm^{-1} attributed to $\upsilon_{(-HC=N)}$ stretching vibrations of the azomethine group, which gets shifted to higher frequency region 1628 cm^{-1} in the complex representing involvement of the nitrogen atom of azomethine group [21,22]. The band at 1569 cm^{-1} is due to the $\upsilon_{(C=N)}$ stretch and this frequency shifted to a lower value of 1535 cm^{-1} in the complexes confirming the involvement of the (C=N) in the coordination with the metal ions [23]. The stretching vibrational band C-O of the ligand lies at 1373 cm^{-1} frequency [24, 25]. This band shifts to the 1420 cm^{-1} higher frequency side in the complex. Further, the bonding is supported by the appearance of new bands in the 501 cm^{-1}, 520 cm^{-1}, 614 cm^{-1} and 593 cm^{-1} regions which are assigned to $\upsilon_{(M-N)}$ and $\upsilon_{(M-O)}$ vibrations respectively.

Table: 3 IR Spectra Band Values (cm^{-1}) Of Ligand And Its Complexes

Ligand/ Complex	$\upsilon_{HC=N}$	υ_{C-O}	$\upsilon_{C=N}$	υ_{O-H}	υ_{M-N}	υ_{M-O}	Chelate ring
APN	1609s	1373s	1569s	3425s	-	-	1425s
APN-Co	1628s	1420s	1535s	-	501_b	614_b	1408s
APN-Ni	1645s	1246s	1543s	-	520_b	593_b	1445s

Mass Spectra

The mass spectrum of $[Ni(C_{30}H_{22}N_6O_2)]$ shows a molecular ion peak at 557.23 (I) due to $[Ni(L_2)]^+$ Which is in accordance with the proposed formula of the complex [26-27]. The other peaks observed are due to fragmentation of ligand from its complex by formation of radical cations at m/z values 307.96, 281.94, 222.22, 112.11 and 72.06. The intense peaks observed at m/z 307.96 (II) is due to loss of $[(C_{15}H_{11}N_3O)]^+$ from (I) and at m/z 281.94 (III) due to loss of –CN group from (II). The other peaks at m/z 249.27 (IV) is due to loss of $[C_{15}H_{11}N_3O_3O(Ni)]^+$ from (I), at m/z 222.22 (V) due to loss of $(C_2H)^+$ from (IV), at m/z 196.02 (VI) due to loss of $(CN)^+$ group from (V) $(L)^+$, at m/z 112.11 (VII) is due to loss of $(C_4H_6NO)^+$ from (VII) and at m/z 72.06 (VIII) due to loss of $(C_2H_6N)^+$ from the ligand $(L)^+$, indication the aminopyrimidine loss. The mass spectrum of $[Co(C_{30}H_{22}N_6O_2)]$ shows molecular ion peaks at /zvalues of 557.47 due to $[Co(L)_2]$, which are in accordance with the proposed formula of the complexes. The other peaks at / values of 308.02, 282.18, 249.27, 226.1, 223.25, 196.2 and 112.11 may be due to the radical ions $(C_2H_3)^+$, $(CN)^+$, $(C_4H_6NO)^+$ and $(C_2H_2N)^+$ of the complexes. The base peaks at / 223.25 may be due to the metal Co linked to the donor atoms of the ligand.

Antibacterial Activities

Antibacterial activity of Schiff base and its metal complexes was tested in vitro against representative Gram- positive bacterial species such as S.aureus and Lactobacillus and Gram-negative bacteria species such as E. coli and P. aeruginosa by agar well diffusion method. Compounds inhibiting growth of one or both microorganisms were further tested for their minimum inhibitory concentration (MIC) of the compound. Schiff base ligand is more active against almost all microbes. Furthermore, all the complexes showed very good activity against all organisms (MIC = 25µg/mL). However, the synthesized compounds showed relatively higher or lower activity than the standard drug, Streptomycin. It may be due to the nature of the metal ion, the nature of the ligand and orientation of the ligand around the metal ion [28-30]. The results are summarized in Table 4.

Table 4: Antibacterial Activity Of Ligand And Its Metal Complexes, MIC Showing Inhibition Zone In Mg/ml

Ligand/ Complexes	Gram-positive		Gram-negative	
	S. aureus µg/mL	Lactobacillus µg/mL	P. aeruginosa µg/mL	E. coli µg/mL
$C_{15}H_{11}N_3O$	22	20	19	22
$Co(C_{30}H_{22}N_6O_2)$	17	13	13	19
$Ni(C_{30}H_{22}N_6O_2)$	19	15	19	13
Streptomycin	27	26	24	23

MIC: Minimum inhibitory concentration

CONCLUSIONS

Based on stoichiometry and analytical data, it is concluded that the ligand is neutral, tridentate coordinating through the "N," "N," and "O" of the azomethine group, pyrimidine ring, and phenolic group, respectively. All the complexes possesses 2:1 (L: M) stoichiometry based on analytical and spectral data and octahedral structures have been proposed for the complexes. The ligand and the complexes showed very good activity against all bacteria.

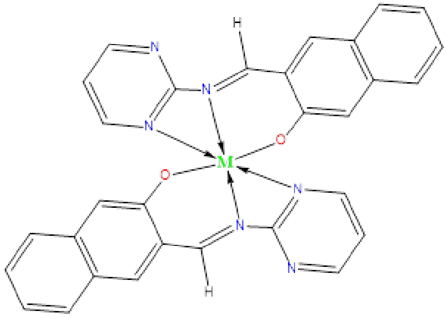


Fig: 1 Structure of Schiff Base metal Complex
Where M= Co(II) and Ni(II)

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