

SYNTHESIS AND SPECTRAL STUDIES OF Co (II) AND Ni (II) COMPLEXES WITH A NOVELSCHIFF BASE LIGAND

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ABSTRACT

Schiff bases and their associated complex compounds have gained importance owing to their utilization in various fields, such as analytical, biological, biochemical, and antimicrobial agents. This significance arises from the existence of diverse heterofunctional groups within these compounds. When these ligands form complexes with metal ions, they exhibit increased antibacterial activities. Physicochemical and spectroscopic results have been used in the present investigation to synthesise and characterise complexes of 1, 6 Dimercapto 1, 6 Diamino 2, 4, 5 Triaza 3-Phenyl 3-hexene with the bivalent metal ion of composition $[ML_2] X_2$ M= Co(II) and Ni(II), X=Cl⁻, Br⁻, NO₃⁻. The complexes were discovered to have an octahedral geometry, and the ligands were discovered to be neutral tridentate chelating ligands for the metal ions.

Keywords: Biological, Antimicrobial, Schiff bases, Tridentate

INTRODUCTION

Due to the presence of multihetero functional groups 1, 2, schiff bases and related complex compounds have acquired prominence due to their usage in analytical, biological, biochemical, and antibacterial systems. These ligands have increased antibacterial activity when they combine with metal ions. The current status of the synthesis and characterisation of a number of Co(II) and Ni(II) complexes with (SB) is described.

EXPERIMENTAL

Every chemical that was utilised was of AR grade. Double-distilled solvents were employed. The Schiff base ligand 1, 6-dimercapto-1, 6-diamino-2, 4, 5-triaza-3-phenyl-3-hexene (SB) was created by refluxing an equimolar concentration of thiosemicarbazide and N-benzoylthiourea in an ethanolic medium for five hours. After cooling, the final goods were separated into their raw, smooth crystals. After filtering and subsequently washing with DMF and cold ethanol, the crystals were dried in a vacuum desiccator over fused CaCl₂. The analysis revealed that the crystals were C₉H₁₁N₅S₂ (m.p.=23220C, yield70%) and provided adequate C,H,N, and S analysis.

Preparation of the complexes

Co(II) and Ni(II) complexes have been created by refluxing Schiff base ligand SB combined with metal salts in a molar ratio of 2:1 of the type $[M(SB)_2]X_2$, where M is Co(II) and X is any of the following: Cl⁻, Br⁻, NO₃⁻, etc. After cooling, the solid coloured complexes separate, are filtered, rinsed with ethyl alcohol and dried. All of the experimental details provided metal, C, H, N, and S analyses that were adequate. Using KBr pellets, the IR spectra were captured on a Beckmann IR-20 spectrophotometer. The molar conductivity were performed on the conductivity bridge using a 10⁻³ M DMF solution, and the magnetic moment was measured using the Gouy method with a calibrant ,Hg[Co(CNS)₄].

Table 1 contains the quantitative data, colour, electronic spectra of magnetic susceptibility, and conductivity.

Table-1

Compound/colour	% of Analysis found(Cal).					μ eff. B.M	Molar cond. Ω^{-1} $\text{cm}^2\text{mol}^{-1}$	λ max (electronic)
	H	N	C	S	M			
SB(silky)(green)	4.35 (4.34)	26.75 (26.66)	42.62 (42.68)	25.31 (25.29)				
[Co(SB) ₂]Cl ₂ (green)	3.48 (3.46)	21.98 (22.01)	34.01 (33.96)	20.32 (20.12)	9.23 (9.27)	5.21	155	16750, 26000
[Co(SB) ₂]NO ₂ (brown)	8.47 (8.56)	31.39 (31.34)	20.36 (20.32)	3.10 (3.19)	18.63 (18.58)	5.17	164	17200, 26300
[Co(SB) ₂]Br ₂ (yellowish green)	8.05 (8.13)	29.71 (29.79)	19.33 (19.31)	3.08 (3.03)	17.60 (17.65)	5.28	159	17000, 25500
[Ni(SB) ₂]Cl ₂ (green)	3.48 (3.46)	22.11 (22.02)	33.89 (33.97)	20.0 9 (20.14)	9.16 (9.23)	3.01	148	13200, 18950, 22450
[Ni(SB) ₂]Cl ₂ (yellowish green)	8.60 (8.52)	31.31 (31.36)	20.29 (20.33)	3.21 (3.19)	18.49 (18.58)	3.09	148	14200, 18750, 25700
[Ni(SB) ₂] Br ₂ (deep green)	8.13 (8.09)	29.76 (29.80)	19.25 (19.31)	3.10 (3.03)	17.59 (17.66)	2.95	144	13900, 18750, 26100

RESULTS AND DISCUSSION

Both the metal complexes and the ligands SB have IR spectra that fall within the 4000-200 cm^{-1} range, as indicated in Table 2.

The ligand's spectra show a collection of broad, strong bands in the 3400–3100 cm^{-1} range of the combined mode of $\nu\text{N-H}$, $\nu\text{S-H}$, and νNH_2 , which suggests that ligands exist in the solid state in thioketo/thiol form. These bands in the complexes' spectra remain unaffected, showing that the amino group is not participating.

The NCSH and HNCS units in the ligand molecules imply thiomide bands in IR spectra³. $\nu\text{C=N}$ and $\nu\text{N-N}$ are attributed to the bands at 1695 cm^{-1} and 950 cm^{-1} , respectively⁴.

A band with diminished clarity and intensity was seen in the ligands' infrared spectra between 1680 and 1695 cm^{-1} , suggesting that azomethine nitrogen was involved in complexation⁵⁻⁸. The complexes' $\nu\text{N-N}$ band may be seen at 900-925 cm^{-1} , exhibiting a red shift in comparison to the ligand.

Table-2

IR spectra of Co(II) & Ni(II) complexes

compound	$\nu\text{N-H}+\nu\text{N-H}+\nu\text{S-H}$	$\nu\text{C=N}$	$\nu\text{C=S}$	$\nu\text{N-N}$	$\nu\text{M-S}$	$\nu\text{M-N}$
SB	3400-3100 cm^{-1}	1695 m.b	780 m.b	950 m		
[Co(SB) ₂]CL ₂	3400-3100 cm^{-1}	1685 m.b	710 m.b	915 m	410 m	455 m
[Co(SB) ₂]Br ₂	--	1680 m.b	715 m.b	910 m	400 m	450 m
[Co(SB) ₂](NO ₃) ₂	--	1690 m.b	710 m.b	915 m	410 m	450 m
[Ni(SB) ₂]CL ₂	--	1690 m.b	715 m.b	900 m	415 m	450 m

$[\text{Ni}(\text{SB})_2]\text{Br}_2$	--	1685 m.b	720 m.b	910 m	405 m	455 m
$[\text{Ni}(\text{SB})_2](\text{NO}_3)_2$	--	1680 m.b	715 m.b	930 m	410 m	450 m

The ligand's $\nu\text{C}=\text{S}$ band, which was previously located at 780 cm^{-1} , shifts downward in the metal complexes to 710 cm^{-1} . It implies that involvement in the thione-sulfur metal ion coordination. New additional bands in the far-infrared area may be ascribed to $\nu\text{M}-\text{N}$ and νMS , respectively, in the $400\text{--}420\text{ cm}^{-1}$ and $450\text{--}455\text{ cm}^{-1}$ regions^{10–12}.

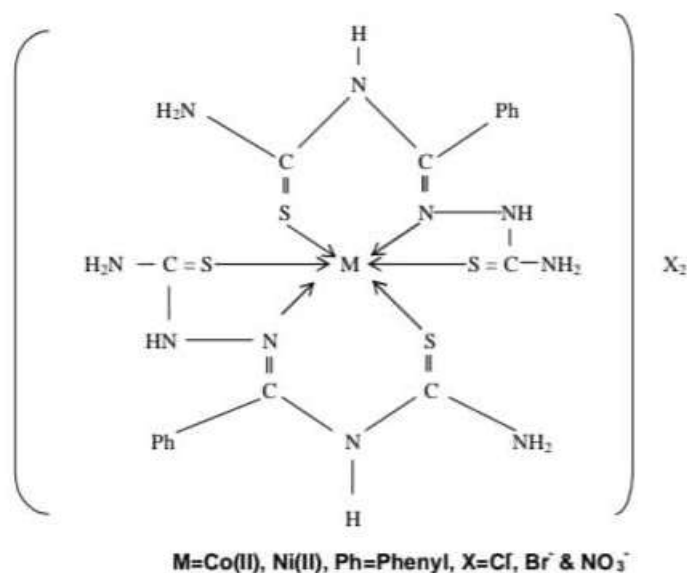
It has been reported that the electronic spectra of $\text{Co}(\text{II})$ complexes exhibit ligand field transitions, with intense $4\text{T}_1\text{g}(\text{P}) \rightarrow 4\text{T}_1\text{g}(\text{F})$ appearing in the visible range between 16600 cm^{-1} and 17500 cm^{-1} , and a charge transfer band extending over the visible region.

The octahedral geometry is indicated by the region $25500\text{--}28000\text{ cm}^{-1}$, and it is further supported^{13–15} by the high meff value of $[\text{Co}(\text{SB})_2]$. Compounds of the X_2 class have 5.11 to 5.30 B.M.

Three bands may be found in the area of $13000\text{--}14000\text{ cm}^{-1}$ [$3\text{T}_2\text{g}(\text{F}) \rightarrow 3\text{A}_2\text{g}(\text{F})$] in the electronic spectra of $\text{Ni}(\text{II})$ complexes. The next band is located in the vicinity of 20000 cm^{-1} [$3\text{T}_2\text{g}(\text{F}) \rightarrow 3\text{A}_2\text{g}(\text{F})$], and the close to 26000 cm^{-1} ($3\text{T}_1\text{g}(\text{P}) \rightarrow 3\text{A}_2\text{g}(\text{F})$) strong, powerful band. $[\text{Ni}(\text{SB})_2]\text{X}_2$'s magnetic moment value falls between 2.95 and 3.15 B.M., suggesting an octahedral geometry¹⁶.

The conductivity of the $[\text{M}(\text{SB})_2]\text{X}_2$ complexes was tested at a concentration of 10^{-3} M in the solvent dimethyl formamide. All of the complexes were discovered to be electrolytes^{17–18} of the 1:2 type, with conductivity values ranging from $140\text{--}170\text{ ohm}^{-1}\text{ cm}^2\text{ mol}^{-1}$.

The complexes can be ascribed an octahedral geometry based on the explanation of the spectral results provided above, and the MAAPHE ligands act as tridentate NSS donors.



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