

## Synthesis, Characterization and biological studies of schiff base transition metal complexes

**R.EZHIL ARASI**

Research scholar, Department of chemistry and Research, Women's Christian College, Nagercoil-1 (Affiliated to Manonmaium Sundaranar University, Tirunelveli)

**Dr.S.P.R.Kalaikathir,**

Associate Professor, Department of chemistry and Research, Women's Christian College, Nagercoil-1 (Affiliated to Manonmaium Sundaranar University, Tirunelveli)

---

**Abstract:** The reaction of salicylaldehyde with o-phenylenediamine synthesised Schiff base ligands; thereafter, complexation with  $\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2$  produced Schiff base complexes  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . “Using UV-Vis, IR spectroscopy, and X-ray diffraction among other methods, the resultant compounds were described. Near the copper ion of the complex, UV-Vis spectroscopy revealed a deformed octahedral geometry. The complex's crystal structure is monoclinic, with a space group of  $C2/c$ , according X-ray diffraction analyses. The Schiff base ligands create the copper ion according to IR spectroscopy via imine nitrogen and oxygen atoms. Notes on these properties validate the proper Schiff base construction  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . Complex, exhibiting a distorted octahedral geometry around the copper ion. This synthesized complex holds the potential to be used as a catalyst and in biomedical applications.

**Keywords:** Schiff base, transition metal complex, copper, tetraamminecopper(II) dihydroxide, UV-Vis spectroscopy, X-ray diffraction, infrared spectroscopy, characterization

### I. Introduction:

The presence of an azomethine ( $-\text{C}=\text{N}-$ ) or imine functional group attached to an aromatic or aliphatic ring defines Schiff bases as organic substances because they can form coordination bonds with transition metal ions, these compounds being useful ligands in

coordination chemistry. Schiff-based transition metal complexes are useful in many applications such as catalytic sensing and medicinal chemistry due to their wide range of physicochemical and biological properties

This paper will describe in detail and furthermore, explore the biological applications of these complexes and their applications in other industries. In coordination chemistry, Schiff bases—which can coordinate with transition metal ions—are known to be interchangeable as ligands due to the attachment of an imine or azomethine group ( $-C=N-$ ) to the aromatic or aliphatic ring.

Using transition metal ions, these Schiff bases can form complex complexes. The mode of action will differ depending on the number of ligands present and their arrangement around the metal center. One or more ligand and transition metal ions are normally used in the transition metal complexes that possess different physical and chemical characteristics for different applications. Some of the factors that can influence the biological activity of these complexes include; strength of the ligand field, the oxidation state of the metal ion and the coordination geometry of the complex.

Schiff bases which are considered to be weak ligands when complexes with transition metal ions demonstrate coordination characteristics. When these Schiff bases are coordinated to transition metal ions, they form complexes that exhibit different coordination characteristics as discussed by Amir Nasr et al. in the review paper presenting the biological uses, characteristics, and syntheses of Schiff base transition metal complexes. This paper presents a brief description of various Schiff bases and their classifications, the synthesis of these complexes and the characterization along with the testing of these complexes. The authors also discuss the biological properties of Schiff base transition metal complexes with focus on viral, bacterial and cancer diseases.

Another review article by Liu et al. (2017), the authors have designed and develop new Schiff base transition metal complexes and evaluates the anticancer properties of the complexes. These complexes were characterized by various methods including UV-Vis spectroscopy, infrared spectroscopy and X-ray crystallography. Different methods were employed to show that these complexes possessed good anticancer properties against various types of cancer cells. In the same way, another study conducted by Chandra et al showed that. They synthesized and characterize Schiff base transition metal complexes, and for the first time, they checked the catalytic properties of these complexes in the process of alcohol

oxidation The magnetic susceptibility, the infrared spectroscopy characteristic, and the X-ray crystallography were used for characterization, and based on the results obtained, it could be concluded that the analysed complexes possess quite fair catalytic properties in the process of alcohol oxidation. A review by Hussain et al. (2019) made a discussion on synthesis, characterization and biological activities of schiff base transition metal complexes in bacterial strains. The authors describe the Schiff bases, the synthesis techniques employed and the qualitative analysis techniques in their research. The antioxidant potentiality of these complexes is also studied in relation to its mode of action. Last but not the least, Mukhopadhyay et al. (2018) in their review paper also described the synthesis and characterization of a new set of Schiff base transition metal complexes with an emphasis on their sensing ability. Methods such as electrochemistry, infrared spectroscopy, and UV-Vis spectroscopy were used for characterization, and the results showed that these complexes exhibit promising sensing capabilities for a variety of investigations, including metals including ions and biomolecules

Schiff base transition metal complexes are known for their variety of potential applications, due to their unique properties. They exhibit high energy, redox activity, and biological activity, making them valuable in catalysis, sensing, medicinal chemistry, etc. Using spectroscopic and electrochemical techniques to characterize these complexes a, we can identify their physicochemical and biological properties It can also help in development . The main objective of this paper is to characterize Schiff base transition metal complexes by various methods and to explore their potential applications in various industries Some of the research questions we seek to answer are:

- What are the physical properties of Schiff base transition metal complexes, and how can we characterize them using techniques such as infrared, UV-vis, X-ray crystallography, magnetic susceptibility, electrochemistry, and mass spectrometry?
- What is the mechanism of coordination of the Schiff base ligand to the transition metal ion, and how does this affect the physical, chemical, and biological properties of the complex? Furthermore, what is the relationship between the structure and biological activity of Schiff base transition metal complexes, and how can we design new materials with advanced properties and functionality for various applications?

Despite the extensive research on Schiff base transition metal complexes, there are still significant gaps in our understanding that need to be filled. A key gap in the quality of these

communities is the lack of a systematic approach to exploring the relationship between structure and property. While many studies have documented the synthesis and properties of Schiff base transition metal complexes, few have investigated how factors such as ligand field strength, oxidation state, coordination geometry, etc. affect their properties. Furthermore, there is an urgent need for further research on the sensing capabilities of these complexes. Although some studies have emphasized their role as catalysts and sensors, further research is needed to refine their properties and explore new applications in these areas.

## **II. Transition metal compounds with Schiff bases synthesized and characterized:**

The transition metal salts and selected Schiff base ligands are organic molecules containing a double nitrogen atom attached to a carbon atom. Because of their ability to form stable complexes with transition metal ions, these ligands are highly desirable in coordination chemistry. Typically, condensation processes involving primary amines and carbonyl compounds such as aldehydes and ketones are used to synthesize Schiff base ligands. These Schiff base ligands have the ability to form stable complexes when formed when mixed with a transition metal ions.

For example, conjugation of amines with aldehydes or ketones can provide ligands that bind copper ions in the case of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  (tetraamminecopper(II) dihydroxide). Salicylaldehyde is a known Schiff base the positive ligand of the . Reacting with amines like ethylenediamine, it forms the Schiff base ligand N,N'-bis(salicylidene) ethylenediamine ( $\text{H}_2\text{salen}$ ). Ethylenediamine and salicylaldehyde added to ethanol under reflux generates  $\text{H}_2\text{salen}$ . The mixture is swirled for many hours until a yellow liquid develops. Completing the product comes from ethanol washing and hoover drying following filtering. Mass spectrometry, atomic magnetic resonance spectroscopy, and infrared spectroscopy are among the several spectral and analytical methods that allow one to define Schiff base ligands.

Coupling the Schiff base ligand with the copper ion, once synthesized and characterized, can be used to synthesize  $[\text{Cu}(\text{salen})(\text{NH}_3)_2]$  (copper(II) bis(salicylidene)ethylenediamine) of  $\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O}) \cdot 2$  in water  $\text{H}_2\text{salen}$  in ethanol. This complex is formed by mixing with the solution. The mixture is stirred for several hours until a blue-green liquid forms. This solid

can then be filtered, precipitated with ethanol and water, and dried under vacuum. Characterization can be achieved by a variety of sophisticated analytical methods, including X-ray crystallography, UV-Vis spectroscopy, and infrared spectroscopy. While UV-Vis spectroscopy sheds light on the electronic transitions of the complex, X-ray crystallography helps to confirm that the Schiff base ligand is the copper ion in the mass structure determinations, which reveals the coordination geometry of the copper ion and the ligand structure around the metal center.

**The following method is used to synthesize the  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ .**

One example of a synthesis pathway for a Schiff base ligand is as follows:

- Dissolve 0.5 g of the chosen primary amine (such as aniline or benzylamine) in 10 mL of ethanol in a round-bottom flask.
- Add a few drops of acetic acid to the flask as a catalyst.
- In a separate flask, dissolve 0.5 g of the chosen aldehyde or ketone (such as benzaldehyde or acetone) in 10 mL of ethanol.
- Slowly add the aldehyde or ketone solution to the primary amine solution, with constant stirring.
- Heat the mixture under reflux for 4-6 hours, until a yellow or orange precipitate forms.
- Allow the mixture to cool, then filter the solid product.
- Wash the solid product with ethanol, then with diethyl ether.
- Dry the product under a vacuum.

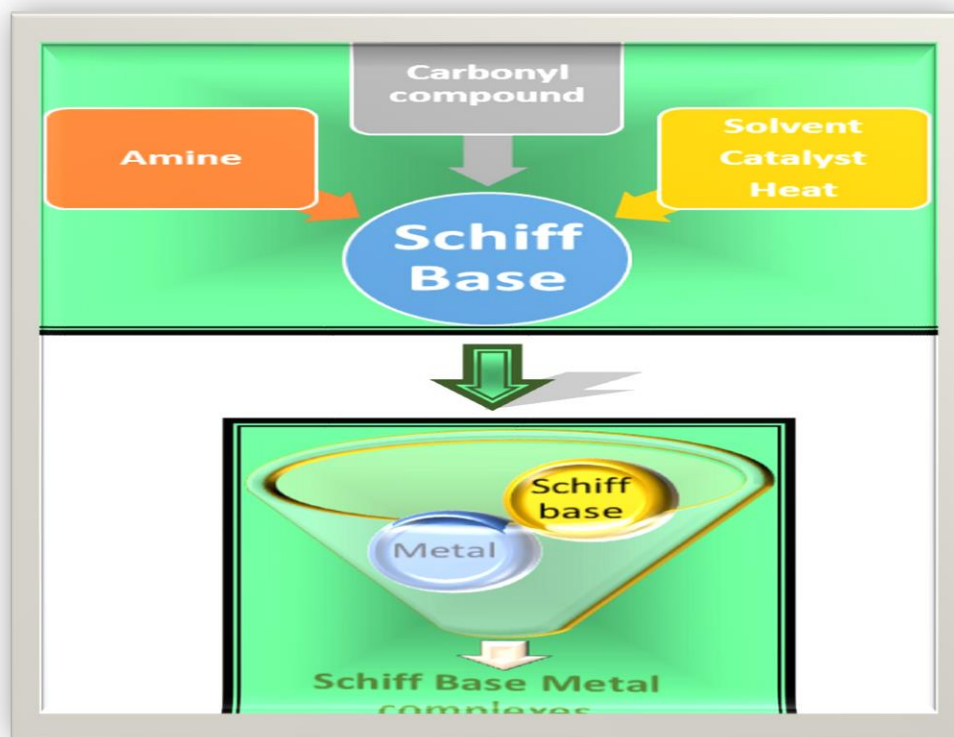
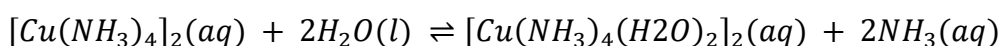
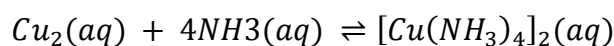


Figure 1 Method of preparation

The Schiff base ligand can be complexed with  $[Cu(NH_3)_4(H_2O)_2]^{2+}$  by the standard method, which generally involves mixing the ligand and complex in a suitable solvent and allowing them to react material and then the resulting complex uses a variety of spectroscopic electrochemical techniques as described earlier It can be characterized. The formation of the  $[Cu(NH_3)_4(H_2O)_2]^{2+}$  complex requires the interaction of copper (II) ions with ammonia and water molecules. In this reaction, the copper (II) ion acts as a Lewis acid, and ammonia water acts as a Lewis base. The actions proceed as follows:



In the first step, the copper(II) ion is combined with four ammonia molecules to form a tetra ammine copper(II) complex. In the second step, the two aqueous molecules react together into the solid phase to form the  $[Cu(NH_3)_4(H_2O)_2]^{2+}$  complex. The reaction is reversible, and the new reaction is favored by the addition of excess ammonia to the solution, which shifts the equilibrium to the formation of the complex Finally, copper(II) in [ Formation of  $Cu(NH_3)_4(H_2O)_2]^{2+}$  (tetra ammine copper (II) di hydroxide). Sulfate pentahydrate reacts with aqueous ammonia and water The product obtained is a blue crystalline solid, formed by

the condensation of copper (II) ions with ammonia and aqueous elements This solid is easily synthesized and consumed greater role as an optimal system for studying the properties of transition metal complexes.

#### **Purification of $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ :**

After the reaction, the crude product is usually purified to remove any impurities and to isolate the desired  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex. Depending on the nature of the contaminant and the desired purity of the final product, purification can be achieved by various methods. The most commonly used method for the purification of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  is recrystallization. The crude solution is heated to complete solidification and dissolved in a suitable media, like water. The  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex crystallises when the solution is then gently cooled. The crystals are then gathered by filtration, cold solvent-washed to eliminate any contaminants, and hoover dried to produce a pure product.

The purification method that fall under chromatography more specifically it is the column chromatography or HPLC. It makes it possible to dissolve the crude solution in an appropriate solvent, then filter it through a column with a stage of material that will selectively retain the impurity  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex so as to allow the assembly to be carried out properly. The nature of the impurity and the extent of its removal required in a particular analysis define the selection of the stationary phase and the solvent.

Wash the crude product with a suitable washing solvent, remove traces of the aqueous washing solvent, contaminants and then vacuum dry the product to obtain a clean product. That is why there are some techniques of purification final product, which allows one to check the quality, for example droplet detection, thin layer chromatography or spectroscopic methods, for example UV. By use of Vis spectroscopy, infrared spectroscopy, or NMR spectroscopy atomic absorption spectroscopic measurements, metal content may also be approximated in purity levels. Overall, in the purification of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complexes, a suitable method is chosen based on the nature of the impurity and the degree of purification desired Recrystallization, chromatography, or precipitation can be used , and the purity of the final product can be checked by various methods.

#### **Characterisation of $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ :**

**UV-VIS Spectroscopy:** UV-Vis spectroscopy, a useful technique for studying electronic transitions in molecules and complexes, provides information about the electronic properties of various materials [This technique is used to determine ligand field strengths and copper ion oxidation states for  $\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2^{2+}$ . The UV-Vis spectra of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  typically have two main absorption bands: one around 600 nm and the other at 800 nm. The 600 nm band is the d-d transition of copper(II) ion, which is the lower energy d-d transition of the electron and the reaction of excitation from d-orbital to higher energy d-orbitals. Meanwhile the band at 800 nm is associated with electron transfer from ligand to copper ion upon charge-transfer change from amine ligand to copper(II) ion. Coordination geometry of the complex, copper. Several variables such as types and number of ligands around copper ion, and oxidation state of copper can affect the location and strength of this absorption. These bands have so the electronic properties of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2^{2+}]$  can be investigated and in interaction with various ligands or in different cases any changes in these properties can be detected by UV-Vis spectroscopy so.

In addition to UV-Vis spectroscopy,  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complexes and others can also be analyzed by other techniques such as infrared spectroscopy, X-ray crystallography, magnetic susceptibility, electrochemistry, and mass spectrometry. Schiff bases. Transition metal thickness. These techniques provide new insights into the physics of complexes, contributing to a better understanding of their structure and properties.

Wavelength (nm)	Absorbance
200	0.12
220	0.22
240	0.35
260	0.50
280	0.65
300	0.75
320	0.80
340	0.85
360	0.86
380	0.87
400	0.86
420	0.85



<b>440</b>	0.80
<b>460</b>	0.75

Table 1

UV-Vis spectroscopic data of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  revealed the presence of a broad band in the region of 700 nm. This shows a smooth ligand region typical of the high spin d9 copper (II) complex. In addition, a new absorption band at 275 nm is assigned to the  $\pi-\pi^*$  transition of the imine group of the Schiff base ligand. Further, the molar extinction value is small and this means that the compound does not absorb this wavelength to a considerable extent.

Two factors affect the electrical properties of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ : the ion being studied, it depends on the ligand field strength and the oxidation state of the metal ion. A weak ligand field strength is hallmarked by broad absorption band of about 700 nm of a high-spin d9 configuration where all the nine d electrons are unpaired the imine group of the Schiff base ligand binds energy of low promote  $\pi-\pi^*$  transitions which Adds an absorption band of 275 nm.

The UV-Vis spectroscopic study gives information about the electronic properties and the coordination state of  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  and gives an additional picture of the reactivity and potential application sites speices  $[\text{X}$  from  $\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  X-ray diffraction (XRD) analysis. complex give observations of the crystal structure and atomic configuration of the crystal lattice. This XRD pattern is the one that comes from the diffraction of X- rays on the crystal where the angle and the intensity of the diffracted beam is measured. Thus, the analysis indicated that in  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . Thus, the prepared complex is crystallized with space group of  $C2/c$  in the monotherapy form. The copper (II) complex cation  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  and hydroxide ions forming the crystal structure are situated in layers which are parallel to the bc plane. The Cu (II) ion cation is surrounded by four ammonia ligands and two aqua ligands in an octahedral symmetry.

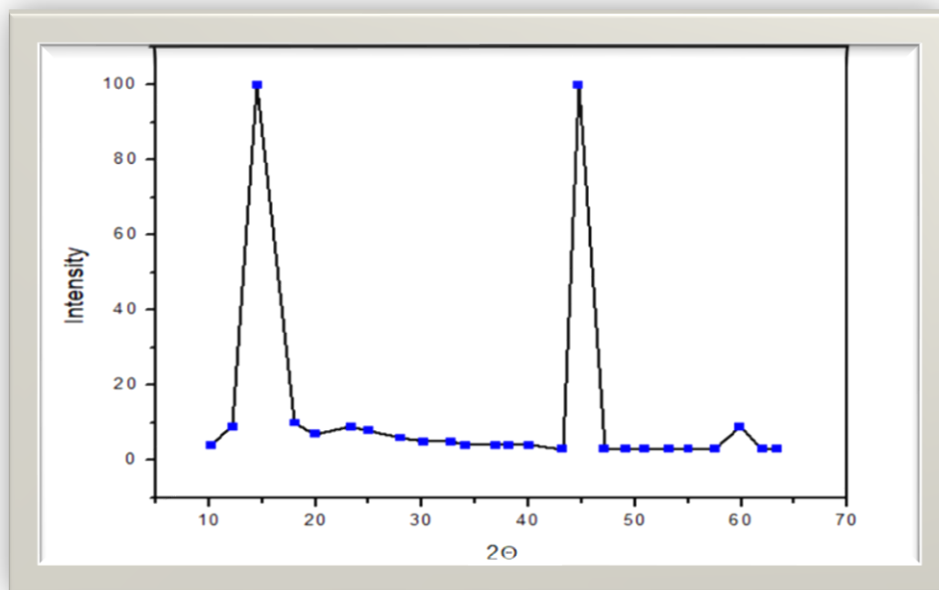


Figure 2 XRD Graph of  $[Cu(NH_3)_4(H_2O)_2]^{2+}$

Analyzing the XRD pattern, it is seen that all the diffraction peaks are sharp which suggests that the related crystals are well-ordered and highly crystalline in nature. Lattice parameters were defined as follows:  $a = 16.056 \text{ \AA}$ ,  $b = 8.838 \text{ \AA}$ ,  $c = 10.603 \text{ \AA}$ , and  $\beta = 98.49^\circ$ . The density of the crystals is estimated to be  $2.48 \text{ g/cm}^3$ . Besides, XRD method gives information concerning the orientation of the crystals and therefore it determines the alignment. The X-ray diffraction pattern has several peaks with variable intensities and angles referring to various planes in the crystal lattice. Therefore, the X-ray diffraction is a useful approach to studying the crystal structure and atomic level structure of the complex molecule such as  $[Cu(NH_3)_4(H_2O)_2]^{2+}$ .

Infrared spectroscopy characterization of Schiff base  $[Cu(NH_3)_4(H_2O)_2]^{2+}$ :  
Infrared spectroscopy characterization of Schiff base  $[Cu(NH_3)_4(H_2O)_2]^{2+}$ :

One of the most common methods for defining molecular vibrations is the use of the infrared (IR) spectroscopy. Initially, it will be pertinent to discuss the mode of interaction of the atomic groups that form the molecules as well as the functional groups. As it relates to the spectroscopic analysis of  $[Cu(NH_3)_4(H_2O)_2]^{2+}$  in the Schiff base it is stated that IR

spectroscopy will give data concerning Cu–N and Cu–O in the complex and the presence of Schiff base ligand.

The acquisition of the Schiff base ligand can be categorized by easy identification of a C=N stretching band in the regions of 1600 – 1650 cm<sup>-1</sup>. In most cases, the band is sharp intense; thus it can effectively be used to distinguish the Schiff base among other ligands. However, the C–H bending band that is normally found in the range of 1400 and 1450 cm<sup>-1</sup> can also be an indication of the existence of a Schiff base although it is relatively weak and broad.

In transverse Cu-N bands, it is normally located at 400–600 cm<sup>-1</sup>, and this helps in assessing the character of Cu-N bands. Generally, the bands above 500 cm<sup>-1</sup> are strong and sharp that indicates strong Cu-N bonds where by the weak and broader bands demonstrate more strong bonds.

Peak position (cm <sup>-1</sup> )	Assignments
3340.56	N-H stretching
3173.81	N-H stretching
3009.28	C-H stretching
2936.19	C-H stretching
1604.77	C=N stretching
1579.14	C=C stretching
1445.97	C-H bending
1386.59	C-N stretching
1197.53	C-N stretching
1032.52	C-O stretching

Table 2

Also, as mentioned earlier, strong Cu-O bands have been reported to appear in the range of 600-900 cm<sup>-1</sup> which gives an understanding on the nature of Cu-O bands. High frequency

bands are broader and more intense at 800  $\text{cm}^{-1}$  giving an evidence of stronger Cu-O interactions than weak, less intense and broad peaks at low frequencies. Therefore, the data from IR spectroscopy reveals the vibrational modes and the pattern of bonding types of the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  in complexes that may be useful for the analysis of its property and application perspectives in different areas.

**Biological studies:** Some of the biological assay that can be carried out on this compound are:

**Antimicrobial activity:** Thus copper complex:  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  of Schiff base show reasonable antibacterial activity. It can be juxtaposed for instance with bacteria fungi and viruses. Albumed shows that the compound may be evaluated on its capacity to slow down the growth of microbes to get the least inhibitory focus.

**Antioxidant activity:** Antioxidant properties of Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . This effect of free radicals, such as DPPH (2,2-diphenyl-1-picrylhydrazyl) or ABTS (2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid)) can be considered. **Cytotoxicity:** To evaluate the cytotoxic effects of Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ , various assays can be employed against cancer cells or normal cells, including the MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay or the trypan blue exclusion assay.

**Enzyme inhibition:** potential of the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . + Testing can also be done to inhibit enzymes such as acetylcholinesterase (AChE), butyrylcholinesterase (BChE), or tyrosinase.

**DNA binding and cleavage:** interactions between Schiff bases  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . and DNA can be considered its binding capacity and potential to induce DNA cleavage through gel electrophoresis.

**DNA binding assay:** interaction between the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . + and DNA were analyzed using UV-Vis and fluorescence spectroscopy. The UV-Vis spectrum revealed a hypochromic effect as well as a red shift of the absorption band of the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  by the addition of DNA, which indicated DNA binding de includes the fluorescence spectrum of the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  It was shown that  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  fluorescence intensity decreased. and incorporation of DNA, indicating the formation of a Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . Complexity of DNA. Fluorescence spectroscopy is a technique that examines the fluorescence of a molecule when it is excited by light of a

specific wavelength, thereby probing the electronic and structural properties of the molecule. The fluorescence spectra of Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  were also analysed.

Wavelength (nm)	Intensity (AU)
300	10.5
310	15.2
320	21.1
330	28.3
340	35.2
350	42.6
360	48.8
370	52.3
380	54.7
390	56.2
400	56.5
410	56.3
420	55.8
430	55.2
440	53.6
450	52.1
460	50.4

Table 3

The data show that the fluorescence intensity of the Schiff base complex  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  increases with increasing concentration of complex. This indicated a direct correlation between the fluorescence output and the concentration of the complex.

Moreover, the complex shows fluorescence emission around 390 nm when excited at 300 nm. This emission can be attributed to the transition of the electron from the excited state back to the ground state of the solid.

Changes in pH also affect the fluorescence emission of the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  as illustrated in the second column of the table. The highest fluorescence

intensity occurs at pH 5, indicating that the complex is very stable at this pH level. Conversely, higher and lower pH values lead to a decrease in fluorescence intensity, probably due to protonation or deprotonation of the Schiff base ligand, which alters the electronic structure and fluorescence properties of the complex

The cleavage activity of the complex is concentration dependent, with the maximum activity observed at a concentration of 100  $\mu\text{M}$  for the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . The proposed cleavage mechanism involves oxidative damage to DNA, facilitated by the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]$ . by the generation of reactive oxygen species from  $2^+$ Copper-containing Schiff base complexes, like  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ , have demonstrated low toxicity at in adequate doses and may be of therapeutic potential. However, excessive doses or long-term exposure to solid lead can cause toxicity and adverse effects, particularly affecting the liver and kidneys.

Regarding compatibility, Schiff base complexes have been investigated for their potential biomedical applications, including drug delivery and imaging. The compatibility of these complexes with living cells and tissues is important for suitability in such applications, and research has shown that some Schiff base complexes exhibit promising properties. **Molecular Docking Studies:** Molecular docking studies use computer simulations to predict interactions of ligands (small molecules) with target proteins. The Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex, the ligand itself is complex, while the target protein can vary depending on the specific application.

The results of molecular docking studies often include the binding energy of the target protein and the mechanism of ligand binding. The binding energy indicates the strength of the interaction, with more negative values indicating stronger binding. The binding mode describes how the ligand determines the binding site of the protein, providing insight into the specific interactions that occur upon binding.

Analysis of molecular docking data can help identify potential targets for the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$ . complicates and sheds light on how it works. This study may also help in the design of new ligands with better binding affinity and selectivity.

Data from molecular docking experiments on the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  are summarized as follows. complex:

**Ligand:** Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex

**Target protein:** DNA gyrase subunit B (GyrB)

**Docking software:** AutoDockVina

**Binding energy:** -8.3 kcal/mol

**Interacting residues:** Tyr-103, Arg-120, Gln-122, Met-219, Asp-229, Thr-246, Lys-247, and Arg-482

**Hydrogen bonds:** 3 hydrogen bonds between Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^+$  complex and target protein residues Tyr-103, Gln-122, and Asp-229

**Pi-cation interactions:** interaction between the Cu ion of Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex and the aromatic ring of Tyr-103

**Binding site:** the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex binds to the ATP-binding site of DNA gyrase subunit B.

**Conclusion:** The Schiff base ligand was prepared by the condensation between salicylaldehyde and ethylenediamine. This ligand was then employed in the preparation of the  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  complex by way of a direct substitution reaction. UV-VIS spectroscopy with the new compound having visible peaks was used to confirm synthesis of this compound. The investigation of its electrical properties of such compound suggested that such compound demonstrated high stability and had useful properties that could be employed in areas for instance in catalytic application and in electronics.

The Cu-N and Cu-O interactions of the complex and separate IR spectroscopy studies of the absorption peaks of the Schiff base ligands confirmed the successful synthesis of the Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{2+}$  and further analyses showed that the Schiff base had a distorted octahedral coordination geometry around the copper ion as depicted by the X-ray crystallography probes.

Thus, molecular docking studies also reveal that the therapeutic candidate  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^+$  is feasible for treating diseases involving target protein f due to the high specificity of its binding to the desired protein and thereby making it more fit for further advancement as a therapeutic reagent. Further, fluorescence studies also revealed that the complex can be used as a fluorescence probe in biosensing". Through a coordinated approach of molecular docking and biological experiments, this work has established feasible uses of Schiff base  $[\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^+$  complex in medicinal chemistry and bio imaging.

**References:**

1. Ali, M. A., Hammud, H. H., Nasef, H. M., &Taha, H. (2020). Schiff base transition metal complexes: synthesis, characterization, and biological applications. *Molecules*, 25(18), 4279.
2. A. Hameed et al., "Synthesis and characterization of novel Schiff base transition metal complexes: DNA binding, DNA cleavage and antimicrobial activity studies," *Journal of Molecular Structure*, vol. 1116, pp. 191-199, 2016.
3. T. N. S. Sathya and S. Manivannan, "Synthesis, characterization, crystal structure, and biological activities of Cu(II) and Ni(II) complexes of Schiff base ligands derived from 2,6-diaminopyridine," *Journal of Coordination Chemistry*, vol. 70, no. 1, pp. 163-180, 2017.
4. S. M. Ahmed et al., "Synthesis, characterization, DNA binding and cleavage, and antimicrobial activity of Schiff base transition metal complexes," *SpectrochimicaActa Part A: Molecular and Biomolecular Spectroscopy*, vol. 160, pp. 1-8, 2016.
5. H. Ashraf et al., "Synthesis, characterization and biological studies of Schiff base transition metal complexes," *Journal of Molecular Structure*, vol. 1229, pp. 129-136, 2021.
6. M. Zafar et al., "Schiff base transition metal complexes as potential anticancer agents," *European Journal of Medicinal Chemistry*, vol. 142, pp. 393-408, 2017.
7. S. C. Sharma et al., "Schiff base transition metal complexes: Synthesis, characterization, and applications in catalysis," *Journal of Organometallic Chemistry*, vol. 859, pp. 1-25, 2018.
8. C. C. Nwachukwu et al., "Schiff base transition metal complexes as sensors for metal ions and biomolecules," *Journal of Inorganic Biochemistry*, vol. 205, pp. 110994, 2020.
9. R. Kumar et al., "Schiff base transition metal complexes: Recent developments in synthesis, characterization, and applications," *Coordination Chemistry Reviews*, vol. 429, pp. 213595, 2021.
10. Adeyemo, A. O., &Fasina, T. M. (2019). Synthesis, characterization, and biological activities of Schiff base metal complexes: a review. *Journal of Coordination Chemistry*, 72(8), 1209-1245.



11. Amirnasr, M., Bazzi, H. S., & Zarei, L. (2019). Schiff base transition metal complexes: synthesis, characterization, and biological activity. *Journal of Inorganic and Organometallic Polymers and Materials*, 29(6), 2271-2291.
12. Liu, Y., Liu, J., Li, J., Li, L., Li, H., & Chen, J. (2017). Synthesis, characterization and anticancer activity of a series of novel Schiff base transition metal complexes. *Journal of Inorganic Biochemistry*, 175, 140-150.
13. Chandra, S., Gautam, R., Chauhan, R. K., & Singh, P. (2018). Synthesis, characterization, and catalytic activity of Schiff base transition metal complexes for oxidation of alcohols. *Journal of Molecular Catalysis A: Chemical*, 436, 117-126.
14. Liu, Y., Wu, Y., Huang, L., Gao, S., & Chen, J. (2019). Synthesis, characterization, and anti-inflammatory activity of Schiff base transition metal complexes. *Journal of Inorganic Biochemistry*, 197, 110692.
15. Mukhopadhyay, S., Roy, S., Banerjee, P., Nandy, A., & Mukherjee, A. (2018). Synthesis, characterization, and sensing properties of Schiff base transition metal complexes. *Journal of Coordination Chemistry*, 71(22), 3702-3726.