Dhaka Univ. J. Sci. 74(1): 46-53, 2026 (January)
Prof. M. Muhibur Rahman Memorial Issue

ISSN 1022 - 2502, E-ISSN 2408- 8528
DOI: https://doi.org/10.3329/dujs.v74i1.83480

Synthesis, Characterization, and Properties of a Schiff Base and its Cu(II) Complex

Md. Ali Hasan Misbah Uddin, Johan Hossain Sakib, Md. Ershad Halim*, and M. Q. Ehsan*

Department of Chemistry, University of Dhaka, Dhaka -1000, Bangladesh

(Received : 4 August 2025; Accepted : 25 December 2025)

Abstract

The present study focuses on the preparation and characterization of a Schiff base, specifically salicylaldehyde-*o*-aminophenol, and its copper(II) complex. The ligand was synthesized through the condensation of *o*-aminophenol and salicylaldehyde using a mixed solvent system of water and ethanol. The resulting Schiff base and its copper complex were characterized using several techniques, including infrared (IR), UV-visible, proton nuclear magnetic resonance (^{1}H NMR) spectroscopy, thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), magnetic susceptibility measurements, and chemical analysis. Based on the results from thermogravimetric and elemental analyses, the proposed empirical formula for the complex is $[Cu(C_{13}H_9NO_2)(H_2O)]$. Geometry optimization studies confirmed that the structure is stable, and the moderate HOMO-LUMO gap suggests good stability and reactivity. Molecular docking studies indicated a strong binding affinity with biological targets, highlighting potential applications in medicinal chemistry.

Keywords: Schiff base, copper complex, UV-Visible, IR, and NMR spectroscopy, molecular docking

I. Introduction

The Schiff base, which contains the azomethine group (HC=N-), is formed through the condensation of primary amines with aldehydes or ketones. This compound was first identified by Hugo Schiff in 1864[1]. It functions as a flexi-dentate ligand, often coordinating through the oxygen atom of a deprotonated phenolic group and the nitrogen atom of the azomethine group[2]. Most Schiff bases are crystalline solids that exhibit weak basicity but can form insoluble salts when exposed to strong acids. The presence of nitrogen and other donor atoms, such as oxygen, plays a significant role in the coordination chemistry of Schiff base azomethanes. Consequently, there is interest in exploring how reduced Schiff bases interact with transition metals that are important in biological systems, as well as the coordination chemistry involved in these interactions[3].

A broad variety of Schiff base compounds and their behavior have been explored due to their flexible and diversified structure[4]. Schiff bases have many applications in various fields of chemistry, including catalysis [5,6], electrochemistry [7,8], organic synthesis [9,10] and, more importantly, medicinal values.

Acylation of Schiff bases by acid anhydrides, acid chlorides, and acyl cyanides has been proved beneficial in the synthesis of natural products [11]. Numerous investigations have shown that via condensation of salicylaldehyde with various heterocyclic compounds, a derivative with significant antibacterial and antifungal properties [12,13]. Schiff bases have been reported to possess antimicrobial [14,15], antiviral [16], anticancer [17,18], and anti-inflammatory activity [19].

Ligands are typically covalently bonded to metal ions through the donation of a lone pair of electrons into an empty metal orbital. Among the most critical metals in living organisms is iron, which is found in hemoglobin within red blood cells. In the lungs, iron binds with oxygen to form oxyhemoglobin[20], which circulates throughout the body and is later regenerated[21]. Copper can form a diverse array of coordination compounds with different ligands. Copper is a trace mineral essential for all living organisms and is primarily found in the liver, muscles, and bones of the human body[22]. Copper-containing proteins (blue copper proteins) play various roles in biological processes, including electron and oxygen transport, utilizing the simple interconversion between Cu^{+} and Cu^{2+}. The biological significance of copper emerged with the appearance of oxygen in the Earth's atmosphere[23]. These proteins employ electron transfer techniques to convey electrons[24]. Moreover, copper is present in many superoxide dismutases, which are proteins that catalyze the breakdown of superoxides into oxygen and hydrogen peroxide. Transition metal complexes generated from Schiff bases have also shown biological activity[25]. While copper is recognized for its vital nutritional and metabolic roles, an imbalance can lead to conditions such as microcytic normochromic anemia, Wilson's disease, and various other diseases in both humans and animals[26]. In this study, a reduced Schiff base ligand synthesized from salicylaldehyde and o-aminophenol was reacted with Cu(II) ion and investigated the properties of the complex.

II. Experimental

Materials and methods

Copper (II) nitrate trihydrate $[Cu(NO_3)_2 \cdot 3H_2O]$, Schiff base, and the solvents used in this study were of analytical grade and procured from Aldrich Chemical Company Ltd. Acids and disodium salt of ethylenediaminetetraacetic acid were obtained from BDH Chemicals Ltd. All chemicals, excluding the solvent, were used as received. Standard drying procedures were employed to dry the solvents. The melting and decomposition temperatures of the complex and ligands were determined using electrothermal melting point equipment. Infrared spectra of the compounds were

---

*Author for correspondence. e-mail: mqehsan@du.ac.bd, ershadhalim@du.ac.bd

obtained in the range of 400-4000 cm^{-1} with KBr pellets using an FTIR instrument Shimadzu Model-8900 spectrophotometer. Ultraviolet-visible spectrum analysis was performed using a double-beam Shimadzu UV-visible spectrophotometer, model UV-1650 PC. Throughout the research, rectangular quartz cells with a path length of 1 cm were utilized. The magnetic susceptibility of the compounds was measured using the SHERWOOD SCIENTIFIC Magnetic Susceptibility Balance from Cambridge, United Kingdom, and the Magway MSB Mk1 model. Thermal properties of the samples were analyzed using differential scanning calorimetry (DSC). The analysis was conducted with a platinum pan under a nitrogen atmosphere, at a flow rate of 20 mL/min. The temperature was increased from 30°C to 550°C at a rate of 10°C/min. Additionally, ^1H NMR spectra were recorded using a Bruker spectrometer in DMSO-d_6 as the solvent, with tetramethyl silane (TMS) serving as the internal standard.

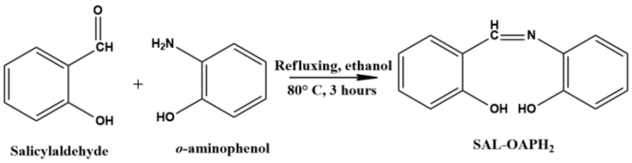
Computational methods

Density Functional Theory (DFT) calculations were performed using Gaussian 16 software to study the geometry, electronic structure, and stability of the copper (II) complex, using the B3LYP functional. The LANL2DZ basis set was applied for the copper ion, while the 6-31G(d) basis set was used for the lighter atoms. Geometry optimization was performed to determine the most stable arrangement of atoms in the complex[27-29]. The Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) were analyzed to calculate the HOMO-LUMO energy gap, a critical parameter that reflects the molecule's electronic stability and reactivity.

Molecular docking studies were conducted to explore the potential biological activity of the complex. Protein crystal structures were obtained from the Protein Data Bank (PDB)[30]. Docking was performed using PyRx, which evaluates the binding interactions between the ligand and target proteins. The docking principle involves calculating the binding affinity and predicting the most stable ligand-protein complexes based on non-covalent interactions such as hydrogen bonding, van der Waals forces, and π-π stacking. These computational techniques provided insights into the binding affinity and potential therapeutic applications of the synthesized complex. The docking results were saved in PDBQT file format for further analysis.

Synthesis of Schiff base Ligand

Salicylaldehyde-o-aminophenol, Sal-OAPH$_2$: Ethanolic solution of 2.5 mmol (0.2726 g) *o*-aminophenol was taken into a 50 mL conical flask. In another 50 mL conical flask ethanolic solution of 2.5 mmol (0.3046 g) salicylaldehyde was taken and both solutions were heated for about 10–15 minutes with continuous stirring. After that the ethanolic solution of salicylaldehyde was transferred into a refluxing flask and then the ethanolic solution of *o*-aminophenol was added gradually, and the mixture was refluxed at 80°C and continuously stirred for three hours. The orange-red precipitate appeared after the reaction mixture was kept overnight. The product was filtered and washed with water several times and dried at room temperature. The obtained crude product was subjected to recrystallization with a minimal amount of hot rectified spirit. The recrystallized product was dried and weighed.



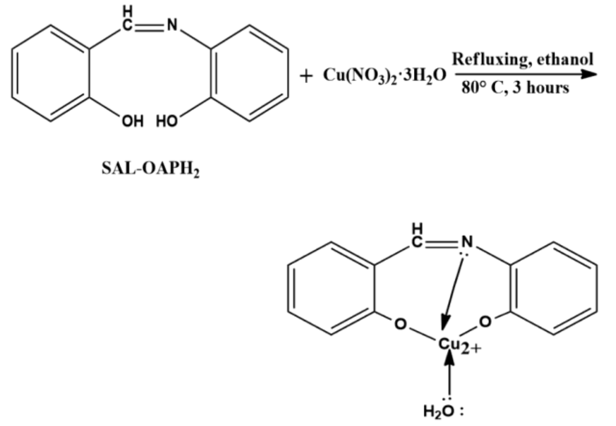
Scheme 1: Synthetic route towards SAL-OAPH$_2$ ligand from salicyladehyde and *o*-aminophenol

CHN analysis (Sal-OAPH$_2$): measured (calculated)- %N 6.58 (6.57), %C 72.67 (73.15), and %H 5.196 (5.16)

Yield: 76.83%, Color: Reddish brown, m.p.: 182-184℃,

FT-IR (cm^{-1}): 3427 (w, ν(O-H)), 3050 (m, ν_{as}(C–H)-aromatic), 2925 (m, ν_{sym}(C-H)-aromatic), 1630 (m, ν(C=N)), 1531 (m, ν(C=C)), 1275 (s, ν(C-N)), and 1223 (s, ν(C-O)).

Preparation of Cu (II) Complex with Sal-OAPH$_2$: Copper (II) nitrate trihydrate (0.5 mmol) was lightly warmed to dissolve in ethanol (30 mL). Another beaker was used to dissolve the synthesized Schiff base ligand (0.5 mmol) in the same solvent. Both solutions were gently heated for 10-15 minutes until the salt and the ligand were soluble in the solvent. Then the Cu (II) solution was added drop by drop to the ligand solution while stirring continuously. Upon mixing the components, instant precipitation occurred. To finish the reaction, the mixture was refluxed for about two to three hours with constant stirring using a magnetic stirrer. After allowing the mixture to stand, the precipitate produced was filtered out. Then it was washed with water, dried at room temperature and preserved in a desiccator.



Scheme 2: Synthetic route towards Cu(II)-SAL-OAPH$_2$ complex from SAL-OAPH$_2$ ligand and Cu(NO$_3$)$_2$.3H$_2$O

CHN analysis [Cu(II)(SAL-OAP)(H_2O)]: measured (calculated): % N 4.71 (4.79), % C 52.73 (53.38), and % H 3.319 (3.761) Metal Content, % 20.62 (21.71)

Yield: 72.23%, Color: Mint Green, m.p: >250,

^{1}H NMR (400 MHz, DMSO-d6, δ, ppm): 13.81 (s, 1H), 8.94 (s, 1H, CH=N), 6.45–7.60 (m, aromatic H).

FT-IR (cm^{-1}): 3428 (s, ν(OH)-H_2O), 3059 (sb, ν_{as}(NH)-aromatic), 3006 (m, ν_{sym}(C–H)-aromatic), 2928 (m, ν_{as}(C-H)-aromatic), 1612 (s, ν(C=N)-imine), 1529 (m, ν(C=C)), 1376 (s, ν(C-N)), 1293 (s, ν(C-O)), 744 (s, ν(Cu-N)), and 536 (s, ν(Cu-O)).

Complexometric technique[31,32] was used to determine the amount of Cu(II) in the complex. Hydrochloric acid was used to dissolve the metal complex at a temperature of about 100°C to make the stock solution. The copper (II) solution was titrated directly with standard EDTA solution in the presence of an ammonia-ammonium ion buffer and the Fast Sulphon Black F indicator.

III. Results and Discussion

The Schiff base ligand (SAL-$OAPH_2$) was synthesized via condensation of salicylaldehyde and *o*-aminophenol in ethanol. The reaction with $Cu(NO_3)_2 \cdot 3H_2O$ yielded a green copper(II) complex, [$Cu(C_{13}H_9NO_2)(H_2O)$], in good amount. The complex remained stable under ambient conditions and exhibited high thermal stability.

Characterization of Schiff base Ligand (Salicylaldehyde-o-aminophenol, Sal-OAPH$_2$)

FTIR Spectral Analysis: Important part of FTIR spectrum of SAL-OAP ligand is shown in **Fig 1.** The tentative assignments of the IR peaks have been done according to the standard references[33-35]

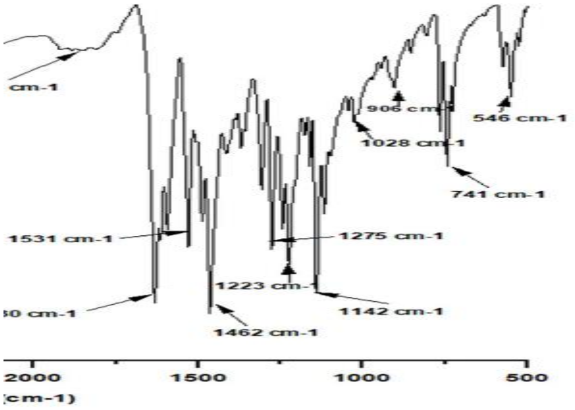


Fig. 1. Important portion of the FTIR spectrum of the ligand Salicylaldehyde-*o*-aminophenol

In the IR spectrum of (SAL-OAP) a weak board peak appears at 3427 cm^{-1} indicating O-H group in the aromatic ring. Asymmetric stretching and symmetric stretching of C-H were observed at 3050 cm^{-1} and 2925 cm^{-1}. The strong absorption peak near 1700-1660 cm^{-1} may be responsible for aldehyde and 1600- 1450 cm^{-1} for the aromatic ring. Peak at 1630 cm^{-1} was assigned as the medium band stretching for (C=N). This indicates the presence of a Schiff base through the characteristic C=N (imine) stretching vibration. C=C stretching at 1531 cm^{-1} was observed with a medium band. At 1275 cm^{-1}, a strong peak appears for aromatic amine (C-N), and at 1223 cm^{-1} a strong peak arrives for (C-O).

Ultraviolet-visible Spectral Analysis for SAL-OAP ligand: In Fig 2a, the UV-Vis absorption spectra of the ligand showed three bands at 267 nm, 349 nm, and 438 nm[36,37]. The band at 267 nm is due to the $\pi \rightarrow \pi^*$ transition within the aromatic ring of benzene and the second band appearing at 349 nm is assignable to $n \rightarrow \pi^*$ transition of non-bonding electrons presents on the nitrogen of the azomethine group (-HC=N-). The absorption peak above 400 nm has been previously assigned to the keto-imine structure of ortho-hydroxylsalicylaldimines in both polar and non-polar solvents. Tautomerism is believed to take place through an intramolecular hydrogen transfer to the imine nitrogen, or intermolecularly in protic solvent.

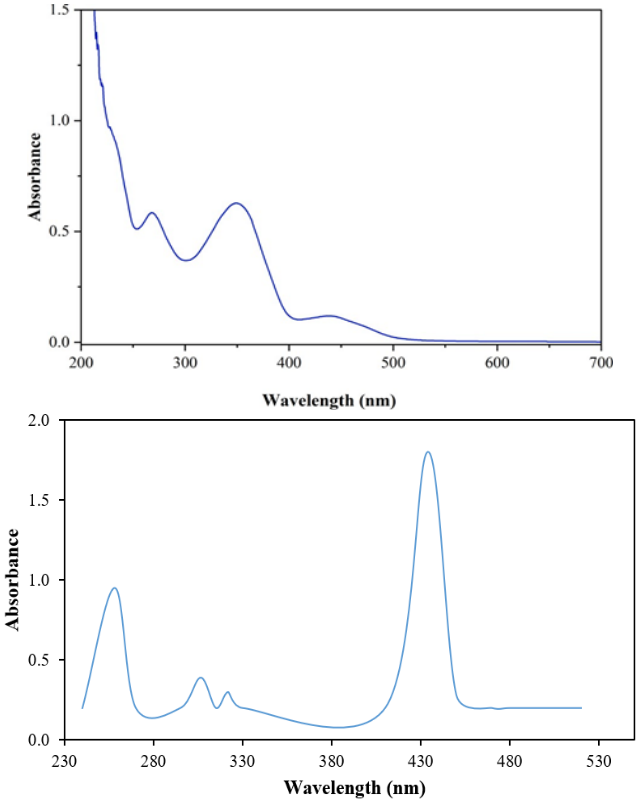


Fig. 2. UV spectra of (a) SAL-OAP ligand and (b) Cu complex of the ligand

Thermal Analysis of ligand (SAL-OAP): Fig 3a represents the TGA results of the SAL-OAP ligand [38, 39]. The curve shows that the ligand starts losing weight rapidly at 96.1ºC. The percentage of weight loss within the temperature range 96.1ºC–463.8ºC is 84.75%. This may be due to most of the weight loss of salicylaldehyde and *o*-

aminophenol. And above 463.8ºC the weight loss process is continuous and up to 642.3ºC the weight loss of the remaining 18.01% ligand occurred. Above 81.99% of the total weight loss is observed up to 800ºC.

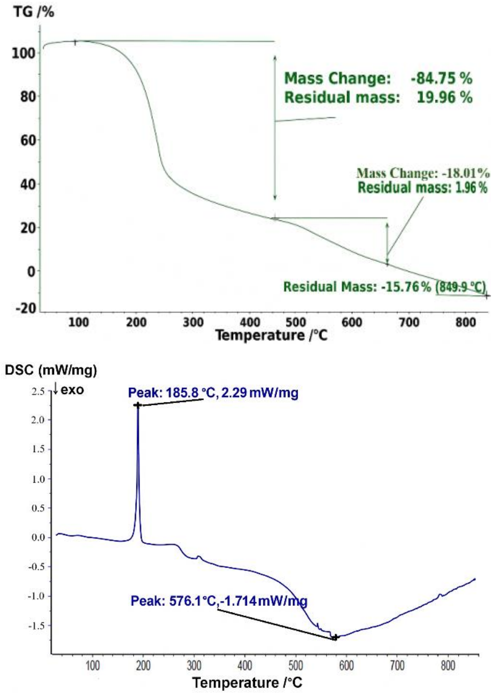


Fig 3: (a) TGA curve and (b) DSC curve of SAL-OAP ligand

Fig 3b shows the DSC curve of the SAL-OAP ligand, which indicates that the phase transition of the ligand occurs within 185ºC to 577ºC. Initially, the ligand releases 0.0645 mW/mg of heat, then relaxes and finally melts at 577 ºC temperature. The DSC curve shows an exothermic peak at around 185ºC and releases 2.29 mW/mg of heat indicating an exothermic reaction because of crystallization. The endothermic peak observed at around 577ºC refers to an endothermic reaction by melting.

^{1}H NMR spectrum analysis of Ligand [33, 34, 40]

Table 1. The ^{1}H NMR spectrum of the SAL-OAPH$_2$ ligand recorded in DMSO and showed signals (δ values).

(δ values) at: Chemical Shift δ (ppm)	Type of Proton	Coupling constant
8.963 s	H attached to C-7'	-
7.619 d	H attached to C-3'	7.2
7.540-7.499 t	H attached to C-5'	8.0
6.969-6.925 t	H attached to C-4'	8.8
6.897 d	H attached to C-6'	7.6
7.107 d	H attached to C-3	7.6
6.897-6.859 t	H attached to C4	7.6
7.402-7.366 t	H attached to C-5	7.2
6.634 d	H attached to C-6	7.6
9.737 s	H (Phenolic)attached to-C-1, 1'	

The ^{1}H NMR spectrum of the Schiff base ligand SAL-OAPH$_2$, recorded in DMSO-d$_6$, confirms the structure through distinct aromatic and phenolic proton signals. The spectrum displays multiple signals in the aromatic region (6.6–8.9 ppm), corresponding to protons on the substituted benzene rings, with splitting patterns (doublets, triplets) and coupling constants indicating typical ortho and meta couplings. A singlet at 9.737 ppm corresponds to the phenolic –OH proton, while the downfield singlet at 8.963 ppm is attributed to the imine proton, further confirming the formation of the Schiff base.

On the basis of the spectral data and chemical behavior the proposed structure of the ligand has been assigned as:

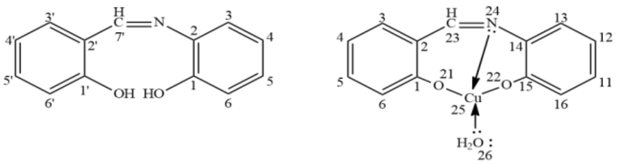


Fig. 4. Structural formula of (a) ligand (SAL-OP) and (b) the copper complex

Characterization of Cu (II) Complex: [Cu(II)(SAL-OAP)(H$_2$O)]

The solubility of a material in a given solvent indicates the substance's polarity. The Cu(SAL-OAP) complex is insoluble in water and methanol but shows slight solubility in methanol with heating. It is slightly soluble in ethanol and becomes fully soluble upon heating. The complex is completely soluble in DMF indicating nonpolar behavior of the synthesized complex.

FTIR Spectral Analysis: In the Cu complex the strong band appeared at 3428 cm^{-1} due to the -OH vibration of H$_2$O. The absorption peak found at the region 3059 cm^{-1} is due to (NH) of the NH$_2$ group. Symmetric stretching and asymmetric stretching of C-H were observed at 3006 cm^{-1} and 2928 cm^{-1}. The C=N group vibrates at 1612 cm^{-1} for the above compound and the C=C group shows the vibration at 1529 cm^{-1}. The strong peak of the C-N group shows the vibration at 1376 cm^{-1}. However, the (C-O) group vibrates at 1293 cm^{-1} for free SAL-OAP. Such a little shifting of (C-O) frequency for free SAL-OAP molecule may suggest the way of involvement of imine group in coordination with a metal ion. The compound shows a strong peak at 1377 cm^{-1} for the (C-N) region. The region at 1500-1300 cm^{-1} gives (N-H), sym & asym, and (C-C) aromatic peaks. A strong intensity absorption band at 744 cm^{-1} might be due to the metal-ligand bonds with the nitrogen of *o*-aminophenol. Then the compound shows a strong absorption peak of 536 cm^{-1} for a metal-ligand bond with the oxygen of salicylaldehyde.

Ultraviolet-visible Spectral Analysis for [Cu(II)(SAL-OAP)(H$_2$O)]: The UV-vis spectrum (Fig 2b) of the complex [Cu(II)(SAL-OAP)(H$_2$O)] showed bands at 321 and 434 nm which are assigned to $\pi\rightarrow\pi^*$ and $n\rightarrow\pi^*$, transition, respectively. These transitions involved here possibly arises due to the movement of an electron from a bonding π orbital to an antibonding π^* orbital or n to π^* orbital. No absorption peak was observed in the visible region of the complex though it is colored. Due to d-d transition, usually, weak absorption occurs (lower absorption co-efficient), in this type of complexes it may appear above 500 nm but in this case it does not appear.

Thermal Analysis of [Cu (II)(SAL-OAP) (H_2O)] complex: Fig 5a represents the TGA results of the [Cu (II)(SAL-OAP) (H_2O)] complex. The curve shows that the complex starts losing weight rapidly at 137.79ºC. The percentage of weight loss within the temperature range 137.79 ºC–223.79 ºC is 5.96 %. This may be due to the loss of one molecule of coordinated water present in the complex for which the calculated weight loss is 6.154%. Above 223.79ºC the weight loss process is continuous and up to 376.295ºC, the total weight loss is 36.397%. This may be due to the loss of one molecule of the *o*-aminophenol present in the complex for which the calculated weight loss is 37.31%. Above 376.295ºC the weight loss is continuous up to 523.795ºC. The percentage of weight loss within the temperature range 376.295ºC-523.795ºC is 41.97%. This may be due to the loss of one molecule of salicylaldehyde present in the complex for which the calculated weight loss is 41.75%. Above 84.33% of the total weight loss is observed up to 800ºC.

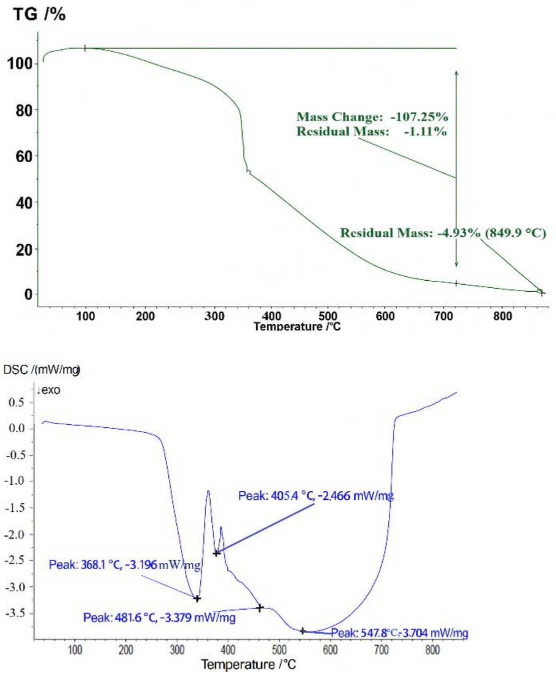


Fig. 5. (a)TGA curve and (b)DSC curve of [Cu(II)(SAL-OAP)(H_2O)] complex

Fig 5b shows the DSC curve of the [Cu(II)(SAL-OAP)(H_2O)] complex, which indicates the phase transition of the complex occurs within 368ºC to 548ºC. Initially, the complex releases 0.075 mW/mg of heat, then relaxes, and finally melts at 548ºC temperature. The DSC curve shows an endothermic peak observed at around 548ºC refers to an endothermic reaction by melting.

Magnetic Moment Measurement

The magnetic susceptibility of the complex was measured and the results are summarized in Table 2. The magnetic moment values furnish valuable information on the electronic configuration of the central ion in the complexes. The measured value given in the Table is in agreement with the divalent oxidation state of the copper ion. The complex is paramagnetic as suggested by the measured and standard magnetic moment values[41]. The color of the complex also supports this observation.

Table 2. Effective magnetic moments of Cu(II) complex in this study at 25ºC

Complex	C_{Bal}	l (cm)	m (g)	R	R_0	χ g (C.G.S unit)	μeff (BM)
[Cu(II)(SAL-OAP)(H_2O)]	0.989	2.1	0.0226	-5	-32	2.48×10^{-6}	1.34

^{1}H NMR spectrum analysis of Cu(II) complex: The observed ^{1}H-NMR spectral data of the Cu(II) complex were δ (d_6-DMSO): 13.81 (s, 1H), 8.94 (s, 1H), 6.45-7.60 (m) ppm. The Schiff base azomethine proton signal migrated upfield with 8.94 ppm was ascribed to the discharge of an electronic cloud in the direction of the metal ion, which signifies coordination with the metallic ion via the azomethine nitrogen. Chelation had no effect on the multi-signals in the 6.40–7.60 ppm range, which is attributed to the aromatic protons of both rings.

The main difference in the spectrum of Cu(II) complex is the absence of the -OH proton located at 9.737 ppm in the free ligand. This indicates deprotonation of this group during coordination with Cu(II) ion. A small peak at 13.81 may be due to presence of some impurities. Based on the results of the various studies described and discussed here, as well as an understanding of the essential criteria for complex formation that the associated ligands must meet, such as the coordination number and oxidation state of the metal ion, the most probable structure of the studied complex is provided in Fig 4b.

Optimized Structure of the metal complex

The structure of the prepared copper complex was optimized using Gaussian 16 software. The optimized structure is shown in Fig 6 and important bond distances and bond angles in coordination sphere are listed in Table 3. The structure obtained is distorted square planar, as shown in Table3 all Cu-O and Cu-N bonds are not equal and the O-Cu-O, O-Cu-N bond angles are more or less than 90 degree.

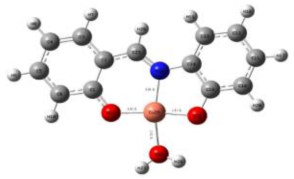


Fig. 6. Optimized structure of [Cu($C_{13}H_9NO_2$)(H_2O)]

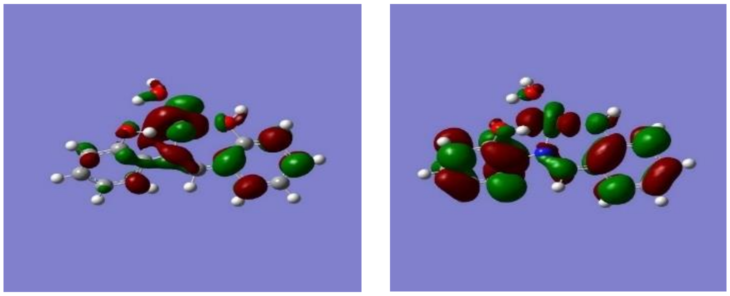
Table 3. Important bond lengths and bond angles of the coordination sphere

Bonds	Distance (Å)	Bond angles	Angles
Cu(25) – O(21)	1.8492	O(21)–Cu–O(22)	~89.6
Cu(25) – O(22)	1.8459	O(22)–Cu–N(24)	~93.7
Cu(25) – N(24)	1.9292	N(24)–Cu–O(26)	~91.2
Cu(25) – O(26)	2.0127	O(26)–Cu–O(21)	~87.4
C(1)–C(2)	1.4405		
C(2)–C(3)	1.4188	**Dihedral angles**	**Angles**
C(3)–C(4)	1.3791	O(21)–Cu–N(24)–C(14)	2.04
C(4)–C(5)	1.4087	N(24)–Cu–O(26)–H(27)	-2.71
C(5)–C(6)	1.3818	O(21)–Cu–O(26)–H(28)	~2.37
C(6)–C(1)	1.4189		
C(1)–O(21)	1.3111		
C(14)–N(24)	1.4102		
C(23) – N(24)	1.285		
C(15)–O(22)	1.3270		

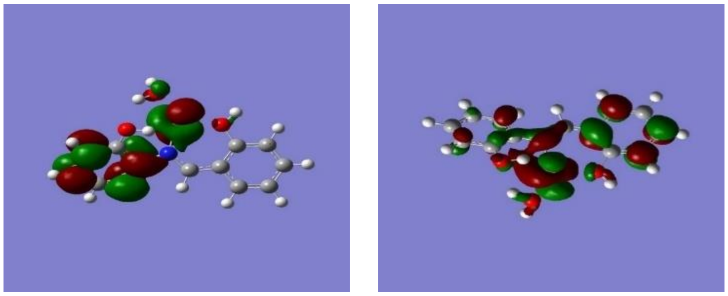
HOMO-LUMO band energy gap calculation of the metal complex

The energies of the frontier molecular orbitals of the copper complex were calculated; metal coordination significantly alters the frontier orbital energies and overall electronic behavior. This approach allowed us to gain insights into the electronic stabilization and potential applications of the metal-bound species.

The HOMO was found at -5.09 eV and the LUMO at -1.70 eV. The resulting energy gap of 3.39 eV suggests that the complex possesses moderate electronic stability along with a favorable degree of reactivity. The HOMO was mainly distributed over the aromatic moieties and donor atoms, while the LUMO was localized around the copper center and coordinated oxygen atoms. This indicates a possible ligand-to-metal charge transfer (LMCT) upon excitation. The nature of the HOMO–LUMO distribution supports effective conjugation within the complex and provides insight into its electronic behavior, which may relate to its potential catalytic or biological applications. The visual representations of the frontier orbitals are shown in Fig. 7. Here, ‘UP’ and ‘DOWN’ denote α-spin and β-spin orbitals, respectively, based on spin-unrestricted DFT calculations. This distinction arises due to the presence of unpaired electrons in the Cu(II) complex.



HOMO(UP) LUMO(UP)



HOMO (DOWN) LUMO (DOWN)

Fig. 7. Selected frontier molecular orbitals (HOMOs and LUMOs) of [Cu(II)(SAL-OAP)(H2O)]

Molecular Docking of different proteins against the Schiff base ligand

Binding affinity is a measure of how strongly a molecule can fit into a receptor and interact with it through non-covalent bonding. To find out the binding affinity as well as protein interaction, we performed docking of our synthesized compound 2-Salicylideneaminophenol with (a) CYCLOOXYGENASE-2 complexed with a selective inhibitor, SC-558(PDB ID:1CX2), (b) MMP9 (gelatinase B) (PDB ID:1L6J), and (c) IIa ATPase/AMP-PNP (PDB ID: 1ZXM). As a result, the compound showed binding affinity with the proteins having energy -7.6 to -8.1 kcal/mol and hence showed good non-covalent interactions. These proteins are an inducible enzyme that plays a key role in the inflammatory response, converting arachidonic acid into prostaglandins, in tissue remodeling, inflammation, and cancer metastasis. Human DNA Topoisomerase IIα is bound to DNA and an inhibitor, etc. The ligand may inhibit the activities of these proteins substantially.

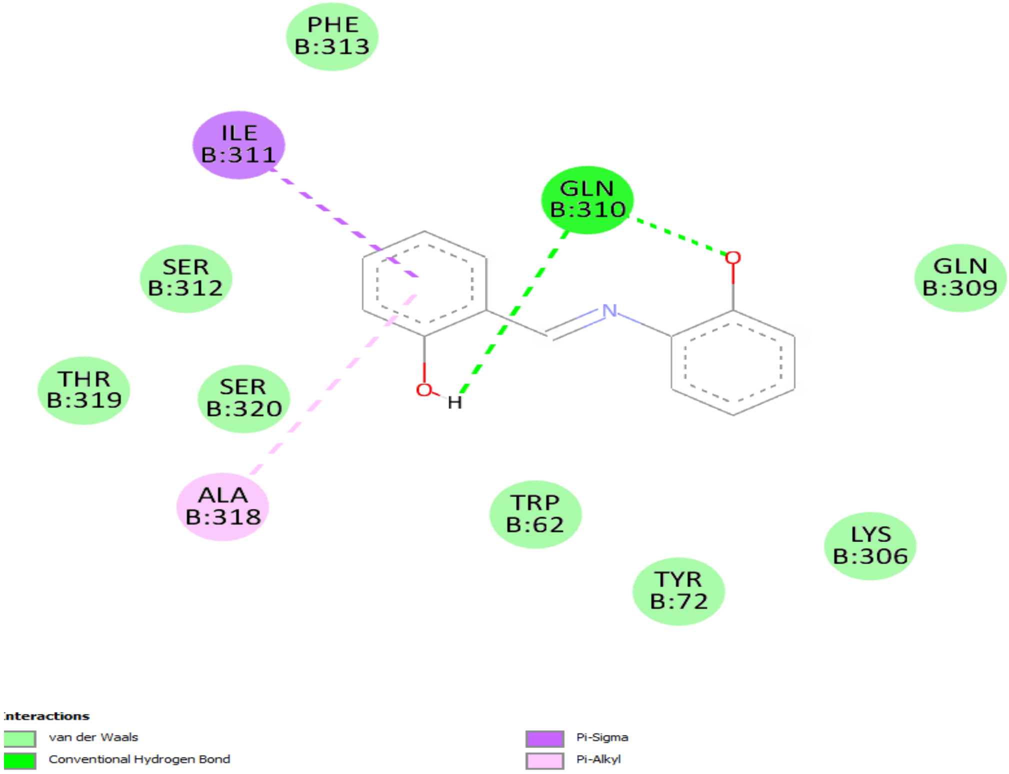


Fig. 8. 2D interaction of the Schiff base with Human Topoisomerase II protein

IV. Conclusion

The Schiff base and its metal complex were synthesized successfully and characterized by elemental analysis, IR, UV-visible, and ^{1}H NMR spectroscopy, thermal analyses, such as TGA and DSC. The thermal analysis confirmed that one molecule of water forms a coordination bond to Cu(II) ion. Magnetic susceptibility value of the complex indicates that the Cu(II) complex is paramagnetic due to the presence of one unpaired electron in its 3d orbital of the copper ion.

From computational methods using Density Functional Theory (DFT), geometry optimization revealed the most stable square planar structure of the complex, providing details about the bond lengths, bond angles, and coordination environment around the copper center. The calculated HOMO-LUMO energy gap offered insights into the molecule's electronic properties, suggesting good stability and potential reactivity due to the moderate band gap. Study of the interaction potential of the ligand through molecular docking studies showed a strong binding affinity to specific target proteins, highlighting its potential applications as an anti-inflammatory agent and anticancer agent, and suggesting its possible applications in fields such as medicinal chemistry and catalysis.

References

1. Worku, D., M., Negussie, V.J.T., Raju, S., Theodros, J.A., Jonsson, 2002. Synthesis and characterization of Schiff base complexes. *Bull. Chem. Soc. Ethiop.* 29, 1-6.
2. Worku, D., M., Negussie, V.J.T., Raju, R., Negussie, 2002. Synthesis of Schiff base complexes. *Bull. Chem. Soc. Ethiop.* 17, 30-35.
3. Gamet, P., J., Reedsk, 2006. Schiff bases in inorganic chemistry. *Eur. J. Inorg. Chem.* 29, 147-155.
4. Paquette, L.A., W.A., Benjamin, 1968. Principles of Modern Heterocyclic Chemistry. *J. Chem. Soc. Eth.* 318, 218-225.
5. Sharma, V.B., S.L., Jain, B., Sain, 2004. Catalysis by Schiff base complexes. *J. Mol. Catal. A: Chem.* 219(1), 61-64.
6. Bhunora, S., J., Mugo, A., Bhaw-Luximon, S., Mapolie, Van J., Wyk, J., Darkwa, E., Nordlander, 2011. Organometallic chemistry of Schiff base derivatives. *Appl. Organometal. Chem.* 25, 133-145.
7. Ershad, S., L., Sagathforoush, G., Karim-Nezhad, S., Kangari, 2009. Schiff base ligands in electrochemistry. *Int. J. Electrochem. Sci.* 4(6), 846-854.

8. Martínez, P.E., B.N., Martínez, C.R., de Barbarín, 2006. Schiff base complexes in material science. *Adv. Technol. Mater. Process. J.* **8(1),** 41-48.
9. Tanaka, H., H., Dhimane, H., Fujita, Y., Ikemoto, S., Torii, 1988. The role of Schiff bases in organic synthesis. *Tetrahedron Lett.* **29(31),** 3811-3814.
10. Mathews, I.I., H., Manohar, 1991. Polyhedron derivatives of Schiff base complexes. *Polyhedron* 10(23-24), 2851-28513.
11. Desai, K.R., R.B., Patel, P.S., Desai, K.H., Chikhali, 2003. Schiff base acylation reactions. *J. Indian Chem. Soc.* **80,** 138-142.
12. Okabe, M., R.C., Sun, G.B., Zenchoff, 1991. Schiff base derivatives in organic synthesis. *J. Org. Chem.* 56, 4393-4397. Jolly, V.S., Arora, G.D., Talwar, Preeti, 1990. Synthesis of Schiff bases. *J. Indian Chem. Soc.* 67, 1001-1005.
13. Chohar, Z.H., P.A., Humayun, K.M., Khan, 2004. Schiff base derivatives with biological activity. *J. Enzyme Inhibition Med. Chem.* 19, 161-165.
14. Valent, A., M., Melnik, D., Hudecova, B., Dudova, R., Kivekas, M.R., Sundberg, 2002. Schiff bases in medicinal chemistry. *Inorg. Chim. Acta* 340, 15-20.
15. Singh, U.I., R.K.B., Singh, W.R., Devi, C.B., Singh, 2012. Schiff base complexes in pharmaceutical chemistry. *J. Chem. Pharm. Res.* **4(2)**, 1130-1135.
16. Singh, S.P., S.K., Shukla, L.P., Awasthi, 1983. Antimicrobial Schiff bases. *Current Science* **52(16)**, 766-769.
17. Sathisha, M.P., V.K., Revankar, K.S.R., Pai, 2008. Metal-based drugs in medicinal chemistry. *Metal-Based Drugs* 2008, 11 pages.
18. Kandeel, M. M., S.M., Ali, E.K.A., Abed ElALL, M.A., Abdelgawad, P.F., Lamie, 2012. Schiff base complexes in drug development. *J. Chem. Pharm. Res.* 4(9), 4097-4106.
19. Bawa, S., S., Kumar, 2009. Schiff base complexes in medicinal chemistry. *Indian J. Chem. Sect. B: Org. Chem. Incl. Med. Chem.* 48B(1), 142-145.
20. Garrett, A.B., E.T., Loppincatt, F.H., Verhock, 1968. *Chemistry: A Study of Matter*. Baisdel Publishing Co., Massachusetts, p. 545.
21. Lyster, A.A., 1969. *A First Course in Hygiene*. University Tutorial Press Ltd., London, 11th ed., p. 27.
22. Johnson, M.D., E., Larry, 2008. Copper. *Merck Manual Home Health Handbook*, Merck Sharp & Dohme Corp., a subsidiary of Merck & Co., 7 April 2013.
23. Decker, H., N., Terwilliger, 2000. COPs and robbers: Putative evolution of copper oxygen-binding proteins. *J. Exp. Biol.* 203(Pt 12), 1777-1782.
24. Lippard, S.J., J.M., Berg, 1994. *Principles of Bioinorganic Chemistry*. University Science Books, Mill Valley, CA.
25. Aliyu, H.N., I., Ado, 2010. Studies of Mn(II) and Ni(II) complexes with Schiff base derived from 2-aminobenzoic acid and salicylaldehyde. *Bayero J. Pure Appl. Sci.* 3(1), 245-249.
26. White, A., P., Harder, E.L., Smith, 1964. *Principles of Biochemistry*. International Student Ed., 3rd ed., p. 189.
27. Frisch, M. J. TGW. Tracks and mony othars, *Gaussian 16*, Revision C.01, Gaussian, Inc., Wallingford CT, USA, 2016.
28. Becke, A. D., “Density-functional thermochemistry. III. The role of exact exchange,” *J. Chem. Phys.*, 1993, 98, 5648–5652.
29. Hay, P. J. and W. R., Wadt, “Ab initio effective core potentials for molecular calculations. Potentials for the transition metal atoms Sc to Hg,” *J. Chem. Phys.*, 1985, 82, 270–283.
30. Foresman. J.B., A. Frisch *Exploring Chemistry with Electronic Structure Methods*, (1996). 2nd ed, Gaussian Ink, Pittsburgh, USA
31. Schwarzenbach, G. and H., Flaschka, *Complexometric Titrations*, Methuen & Co. Ltd., London, 1969.
32. “*Vogel’s Textbook of Quantitative Chemical Analysis*”, 5th ed. ELBS series, (1991), 324
33. Pavia, D. L., G. M., Lampman, G. S. Kriz, and J. R., Vyvyan, *Introduction to Spectroscopy*, 4th ed., Cengage Learning, USA, 2014.
34. Silverstein, M. R., C. G Bassler, and C. T. Morril, (1981) "*Spectroscopic Identification of Organic Compounds*" 4th ed, 135
35. Nakamoto K.,"*IR and Raman Spectra of Inorganic and Coordination Compounds*", (1978), 3rd ed, John Wiley and Sons, N.Y, 211
36. Roberts J. D., and M.C Caserio, “*Basic Principles of Organic Chemistry*”, 1977, W.A. Benjamin, 2nd Edn, 1105
37. Lever B. P, “*Inorganic Electronic Spectroscopy*”, 1984, Elsevier Pablishing Company, New York, 1st. Edn., 52
38. Yakuphanoglu F., 2015, Thermal analysis methods used in solid state physics and chemistry to obtain kinetics and thermodynamics parameters of solid materials by TGA, DTA and DSC analyses, *Journal of Materials and Electronic Devices*, 17-23
39. Ghanshyam Kumar1 and R. P. S. Chauhan1, 2021 Thermogravimetric Analysis and Kinetic Parameters, Determination of Co (II) Complexes, *IOSR Journal of Applied Chemistr*y, **14**, **(9),** PP 63-67
40. Janet Blumel, Peter Hofmann and Frank H. Kohlert, 1993 NMR Spectroscopy of Paramagnetic Complexes Part 39*-Natural Abundance *H NMR of Paramagnetic Sandwich Compounds MAGNETIC RESONANCE IN CHEMlSTRY, **31**, 2-6
41. Figgis, B. N. and J. Lewis, 1960., *Modern Coordination Chemistry*, Interscience Publishers, New York,