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Efficient Copper Ion Recognition Using A Naphthalene Derived Schiff Base Chemosensor

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ABSTRACT

A new naphthalene-based Schiff base chemosensor (L1) was synthesized using 2-hydroxy-1-naphthaldehyde and ethylenediamine and characterized using UV–Vis, FT–IR and ^1H NMR spectroscopic methods. The sensor showed a characteristic color change from yellow to colourless on the addition of Cu^{2+} ions, along with large spectral changes. Mechanistic studies showed that intramolecular proton transfer, keto–enol tautomerization and coordination with nitrogen and oxygen donor atoms are the mechanisms of Cu^{2+} recognition. In addition, paper-based sensing strips were also designed and used for rapid visual Cu^{2+} ion detection, which was successfully achieved. The results show that L1 can act as an efficient and convenient colorimetric chemosensor for copper ion detection.

Keywords: *Naphthalene, Colorimetric recognition, Selectivity, Copper, Schiff Base.*

I. INTRODUCTION

Copper, a trace metal essential to human health, is involved in a wide variety of biological reactions, including enzyme synthesis, cellular metabolism, and many more. Nonetheless, an overabundance of Cu2+ is detrimental to environmental and human health, especially due to the biological chain's amplifying effect; this chain can be enriched several times before entering the human body and inflicting central nervous system damage, such as in prion diseases, Alzheimer's, and Parkinson's. Environmental monitoring and healthcare concerns both rely on Cu2+ detection. The World Health Organization has stated that the maximum allowable concentration of Cu2+ in potable water is 31.5 M. Inductively coupled plasma spectroscopy, atomic absorption spectroscopy, and inductively coupled plasma mass spectrometry are some of the more traditional methods that have been developed for the purpose of identifying metal ions.

Recent articles on Cu2+ detection have also discussed impedimetric sensing and electrochemical monitoring, in addition to these methods. The high expense of equipment, the complexity of the processes, and the time of inspections are key practical limits of these methods, while they yield exact findings for metal ion detection. Detecting copper is crucial for a number of valid reasons. Additionally, it should be mentioned that copper is regarded as a "economically critical mineral" because of its significance in several consequential technologies. For this reason, it would be helpful to have portable, low-cost, sensitive, and selective copper characterisation sensors for use in prospecting and downstream process monitoring of copper production, particularly from unusual sources like industrial waste.

On the other hand, practical applications, such as the rapid on-site detection of metal ions, need the immediate development of reliable, affordable, and easy-to-understand measuring techniques. This includes electrochemical and optical sensing methods.

II. REVIEW OF LITERATURE

Kumar, Ram et al., (2025) L1 ((4-((E))-1-(((E))-2-hydroxybenzylidene)hydrazono)ethyl)benzene-1,3-diol) is a novel schiff base sensor that was achieved by the condensation reaction of 2-hydroxybenzaldehyde and (E)-4-(1-hydrazonoethyl)benzene-1,3-diol. Using ultraviolet-visible (UV-Vis) spectroscopy, we examined how the synthetic sensor L1 interacted with a range of metal ions. The stoichiometric ratio of the $Cu2^{+}$ ion and the sensor was 1:1, and the binding constant for the L1-$Cu2^{+}$ complex was determined to be $0.4 \times 10^{-}$ $M^{-}1$. Further evidence of its effectiveness throughout a wide pH range was provided by UV-Vis spectral fluctuations in L1 under different pH circumstances. With a limit of detection set at 32.2 nM, the sensor allowed for the detection of $Cu2^{+}$ ions in sub-second timeframes. In addition, the sensor's recyclability was evaluated by adding ethylenediaminetetraacetic acid (EDTA) to a solution that contained the L1-$Cu2^{+}$ complex. The stability and applicability of the L1-$Cu2^{+}$ complex for cupric ion detection were further supported by density functional theory (DFT) simulations, which confirmed the 1:1 binding stoichiometry. The developed Schiff base sensor L1 showed strong binding affinities to myoglobin, haemoglobin, bovine serum albumin (BSA), and human deoxyribonucleic acid (DNA) in molecular docking tests, indicating that it might be used in biological systems. The synthesised sensor's practical efficiency in detecting $Cu2^{+}$ in real water samples was also confirmed.

Kumar, Ram et al., (2024) The compound 4-((E)-1-(((Z)-2,4dihydroxybenzylidene)hydrazono)ethyl)benzene-1,3-diol (L) was synthesised by condensing 2,4-dihydroxybenzaldehyde and a new Schiff base moiety, (E)-4-(1-hydrazonoethyl)benzene-1,3-diol (2). HRMS, ´H-NMR, ´³C NMR, and single-crystal XRD techniques were employed to characterise the resulting compound. To find out if the Schiff base could detect cupric ions better than the other transition metal ions, UV-vis absorbance tests were utilised. An additional peak at 462 nm emerged when Cu^{2+} ions were present. The expected binding stoichiometry for the L:Cu^{2+} partnership is found to be 1: according to the Job plot. 1. DFT calculations were used to validate structural correlations and absorption data. Additionally, docking tests for L showed a strong affinity for human haemoglobin, which provided important details on the ligand's optimal binding positions inside haemoglobin binding sites and its interactions with HHb. A binding coefficient of 3.02×10^{4} M^{-1} and a limit of detection of 42.09 nM were determined, respectively. The complex was shown to be reversible when EDTA was added to the L-Cu^{2+} solution, and when Cu^{2+} and EDTA were added to L, a colorimetric variation mimicking the "INHIBIT" molecular logic gate appeared. Moreover, the chemosensor's possible usage in detecting Cu^{2+} in its solid state using chemosensor L further validates its practical and versatile applicability in real-world applications.

Kumar, Gujuluva et al., (2024). In this investigation, a chemosensor that could detect Cu2+ ions in a THF:H2O combination (7:3, v/v) was utilised. The ligand used was a Schiff base (L = 6,6′-((1E,1′E)-(cyclohexane-1,2-diylbis(azanylylidene))bis(methanylylidene))bis(2,4-di-tert-butylphenol)). A 1:1 stoichiometric ratio between L and Cu2+ was validated by analysis using ESI-MS and Job's plot. L has an absorption band at 330 nm, which bathochromic shifts to 377 nm following contact with just Cu2+ ions, indicating a confined internal charge transfer mechanism of L. The capacity to detect Cu2+ ions at concentrations as low as 0.46 μM was proven by L. In addition, we probed L's use in creating molecular logic gates and its use in determining Cu2+ concentrations in water samples.

Kouser, Robina et al., (2022). A chemosensor probe 1 based on chromone was created and studied using FTIR, UV-vis, ´H NMR, ´³C NMR, and mass spectrometry. The first probe showed superior selectivity and sensitivity for Cu^{2+} ions compared to other metal ions studied by colorimetric, absorption, and fluorescence titrations, as well as Al^{3+}, Cr^{3+}, Co^{2+}, Cd^{2+}, Mn^{2+}, Fe^{3+}, Ni^{3+}, and Zn^{2+}. According to Job's plot

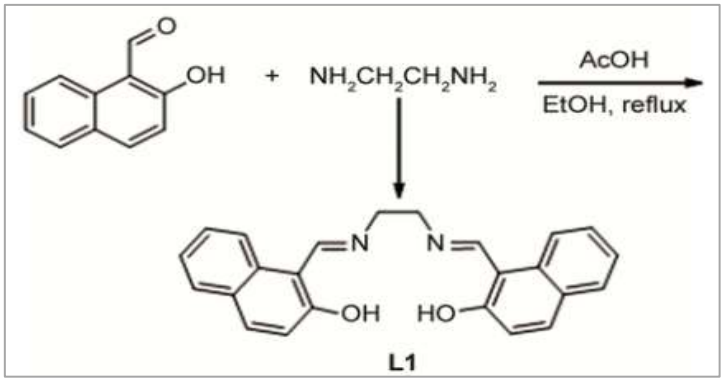
measurements, the binding mode of probe 1 with the Cu^{2+} ion was 2:1 stoichiometry. Using data from a non-linear least square fit, Probe 1 found an association constant of 8.48×10^{8} M^{-2}. The Cu^{2+} ion was determined to have a detection limit of 0.273×10^{-6} mol L^{-1} via probe 1. In addition, probe 1 was used to identify Cu^{2+} ions in various bovine liver tissues, including those affected by the liver fluke as well as those that were not. The sensing mechanism was supported by DFT studies. These tests show that probe 1 shows promise as a chemosensor for the rapid detection of Cu^{2+} ions in various biological samples using both fluorescence and the naked eye.

Kim, Min et al., (2017). For the detection of Cu2+, Co2+, and S2-, a novel colorimetric chemosensor 1 based on Schiff was created. A simple colour change from colourless to yellow would allow Sensor 1 to monitor Cu2+ and Co2+. A 2:1 complexation stoichiometry was established for the binding modes of 1 to Cu2+ and Co2+ by use of Job plot and ESI-mass spectrometry analysis. The World Health Organization (WHO) suggested a value of 31.5 μM for Cu2+ and the Environmental Protection Agency (EPA) a value of 1.7 μM for Co2+, although the detection limits for Cu2+ and Co2+, respectively, were lower at 0.02 μM and 0.63 μM. That one could identify and measure Cu2+ in actual water samples is crucial. Additionally, Cu2+-2·1 combination has the potential to be employed as a very selective colorimetric sensor for S2-, even when other anions are present, without causing any interference. Additionally, theoretical computations clarified the Cu2+ and Co2+ sensing processes by 1.

III. EXPERIMENTAL SETUP

Analytical reagent (AR) grade chemicals and solvents were purchased from conventional commercial providers in India for the current experiment. There was no further purification of the reagents before use. In all of the experiments, freshly made double-distilled water was used. The absorption spectra of ultraviolet light were captured using a UV-Visible spectrophotometer within the 200-800 nm wavelength range. Infrared spectra were acquired by means of the KBr pellet method. Tetramethylsilane (TMS) was used as an internal reference standard for proton Nuclear Magnetic Resonance (~1H NMR) spectra recorded in DMSO-d6 solvent. The digital melting point equipment was used to determine the melting points, and the results are presented without correction.

Condensation of 2-hydroxy-1-naphthaldehyde and ethylenediamine produced the Schiff base chemosensor L1. Ethanol was used as a solvent for the continuous stirring of 2-hydroxy-1-naphthaldehyde (2.2 mmol) and ethylenediamine (2.0 mmol). In order to speed up the condensation process, a little quantity of acetic acid was added. Eight hours were spent refluxing the reaction mixture at 80°C. Collecting the brilliant yellow precipitate when the reaction was complete, we rinsed it with ethanol several times to eliminate any remaining unreacted substances, and then dried it under vacuum. We used FT-IR, ^1H NMR, elemental analysis, and ESI-mass spectrometry to characterise the synthesised chemical, which we got in 85% yield. See Scheme 1 for a simplified plan of the chemosensor L1's assembly.



Scheme 1: Synthesis and Structure of L1

A solution of dimethyl sulfoxide (DMSO) was used for the metal ion sensing experiments. Metal ion stock solutions and the synthesised sensor were made independently. By introducing different quantities of Cu^{3+} ions to the sensor solution and documenting the spectrum changes, UV-Vis absorption measurements were performed. The interaction mechanism between the sensor and Cu^{2+} ions was investigated by FT-IR and ^1H NMR titration studies. In addition, for real-world detection trials, we impregnated filter paper with the sensor solution and made paper-based sensing strips.

IV. RESULTS AND DISCUSSION

Observing the shifts in the complexation reaction's absorption spectra allowed us to probe Cu2+'s recognition capability. The chemical L1 in DMSO has a yellow hue and a robust absorption peak at 402 nm and 426 nm, as seen in Figure 1. The sensor displayed a remarkable transition from yellow to colourless and a blue shift in the absorption peak to 375 nm and 400 nm upon addition of Cu2+ (10 equivalents) to the L1 solution.

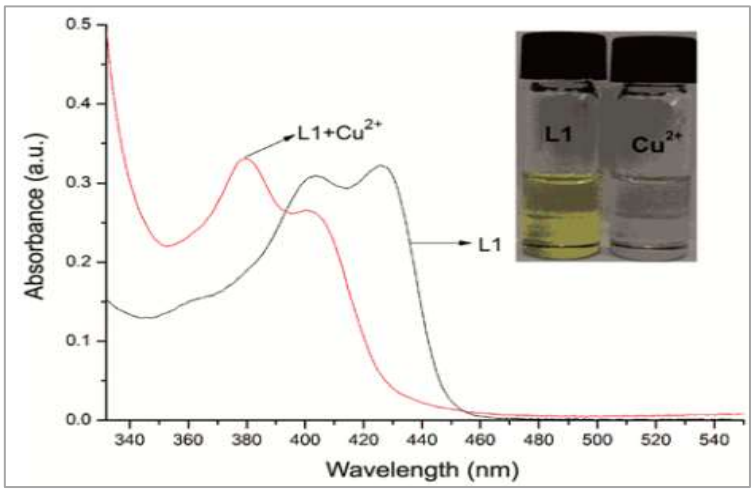


Figure 1: Absorption Spectra of L1 in DMSO before and after Complexation with Cu^{2+}

The FT-IR analysis revealed the chemical process that led to the complexation of L1 with Cu2+. Fig. 2. Compound L1's FT-IR spectra showed distinct peaks at 1613 cm-1 and 1547 cm-1, which were determined to represent the stretching vibrations of C=N and C=C, respectively. Nevertheless, with incorporation of Cu2+, the absorption peaks associated with C=N vanished, while two further peaks emerged at 1643 cm-1 and 3218 cm-1, correspondingly, caused by the stretching vibration of C=O/N-H. At the same time, there was a red shift to 1574 cm-1 in the stretching vibration absorption peaks of C=C, which means that Cu2+ had complexed with compound L1.

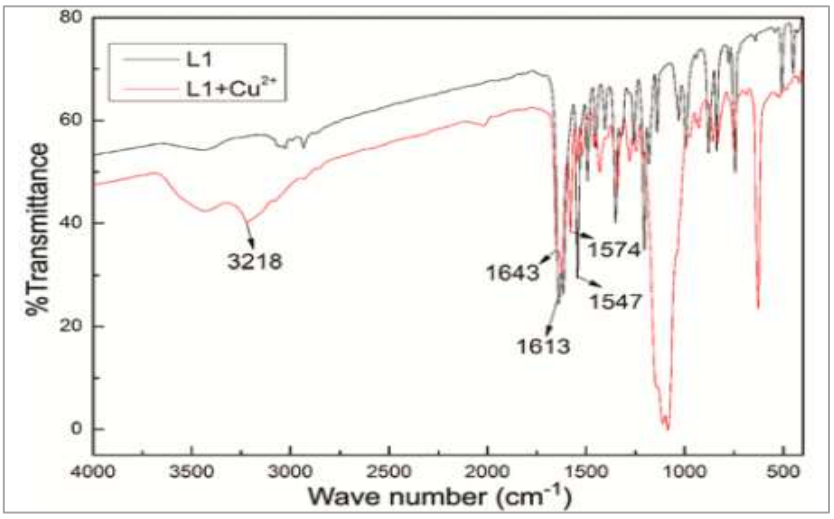


Figure 2: Comparative FT–IR Spectra of L1 and Its Cu^{2+} Adduct

The 1H NMR titration showed the same thing. Figure 3 shows that in a DMSO solution, chemical L1 exhibited two distinct peaks at 14.23 and 9.15 ppm, associated with the protons of OH and CH=N, respectively. A new peak progressively emerged at 10.65 ppm and the proton of the phenolic OH at 14.23 ppm vanished after Cu2+ was added to the L1 solution. A new peak of N-CH= emerged at 8.4 ppm in the high field, suggesting that the molecule L1 has been coordinated with Cu2+ by intramolecular proton transfer, whereas the protons of CH=N at 9.15 ppm progressively faded away as the amount of Cu2+ increased.

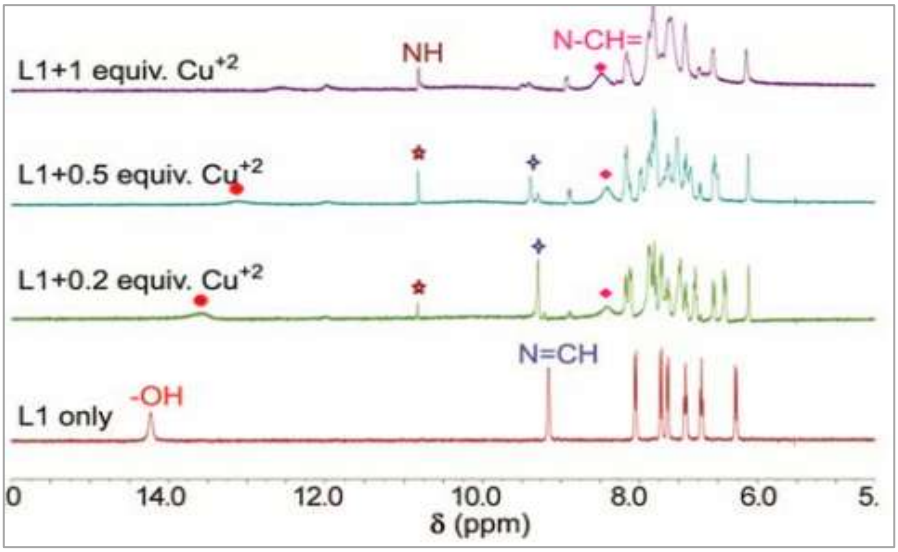
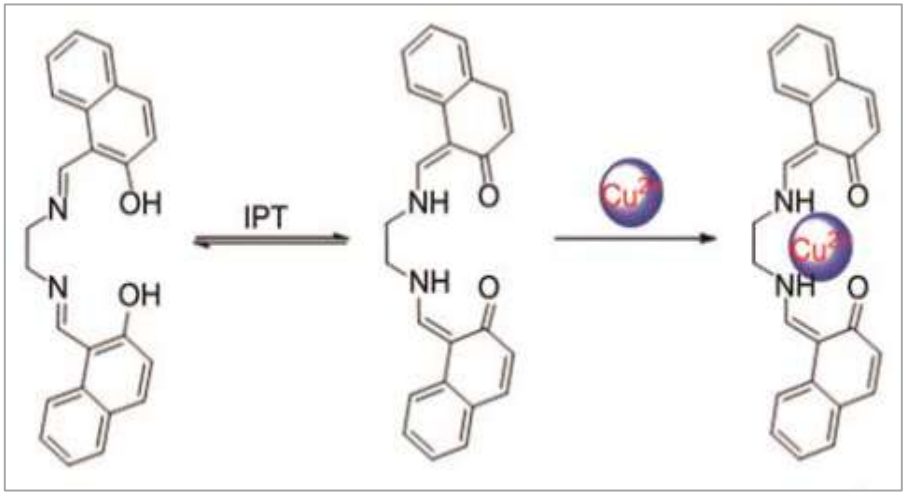


Figure 3: 1H NMR Titration Study of L1 with Varying Concentrations of Cu^{2+}

In two stages, it is possible to show that the reaction between L1 and Cu2+ has begun: Compound L1 undergoes intramolecular proton transfer upon Cu2+ addition, as shown in Scheme 2, resulting in keto-enol tautomerization. The blue shift and colour fading are caused by the Cu2+ forming a short conjugated length with the N and O atoms on the keto form of chemical L1.



Scheme 2: Proposed complexation mechanism of the sensor L1 towards Cu^{2+}

To demonstrate its usefulness, test strips were made by soaking filter papers in a weak hydrochloric acid solution, rinsing with distilled water to neutralise the acid, and finally drying them in a vacuum. After being soaked in the sensor L1 solution (0.01 mol L-1), the filter sheets were dried in a vacuum and then used to detect Cu2+. The test strips containing L1 appeared yellow in Figure 4, but when Cu2+ was added, the colouration became colourless. The results demonstrate that the test strips are capable of detecting Cu2+ in real-time.

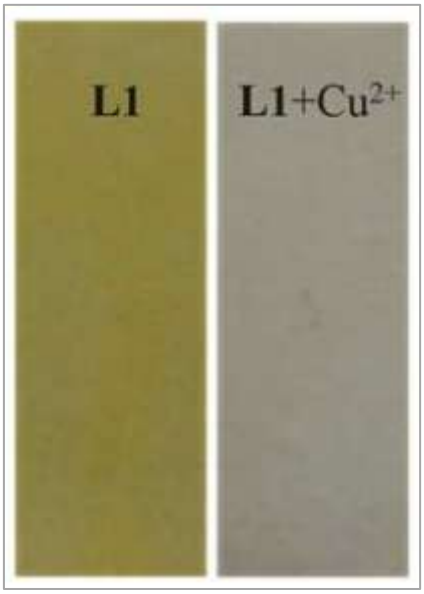


Figure 4: Test strips of L1 and L1+Cu2+

V. CONCLUSION

The sensor showed very good sensing ability with Cu^{2+} ions and produced a clear colorimetric response which enabled it to be easily detected visually. The UV-Visible absorption studies showed that there are significant changes in the spectra as well as a blue shift when the ions of Cu^{2+} are introduced, confirming good complex formation. The sensing mechanism was further investigated by FT–IR and ^1H NMR showing that the recognition of copper ion is associated with intramolecular proton transfer, keto–enol tautomerization and coordination of the N and O donor sites of the recognition molecule. The optical responses and color fading were attributed to these structural changes. The developed chemosensor was further demonstrated to be practically applicable by fabricating paper-based sensing strips that constitute a fast and convenient platform for on-site detection of Cu^{2+} ions. The attractive colour change of the test strips makes them ideal for field analysis and environmental monitoring. The Schiff base sensor L1 is a promising selective copper ion sensor due to its simplicity of synthesis, high sensitivity, distinct colorimetric behavior and practical applications.

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