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Microwave-assisted synthesis, characterization, and computational studies of Co(II), Ni(II), and Cu(II) metal complexes with a schiff base derived from 1h-Indole-2,3-dione and 3-Chloro-4-Fluoro aniline

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Abstract

Metal complexes have been particularly successful and shown great potential mainly because of their ability to have different coordination geometries and to be more antimicrobial, antioxidant, catalytic, and enzyme-inhibitory than the ligands they are derived In this context, the current research focuses on the development and characterisation of a new ligand (HL) and its corresponding metal complexes, which are synthesised by the microwave-assisted method, supported by a thorough spectroscopic, analytical, and theoretical study.To achieve this objective, the first step was to prepare the 1H-Indole-2,3-dione and 3-Chloro-4-Fluoroaniline (HL), and then its Co(II), Ni(II) and Cu(II), complexes were made, followed by a detailed structure, magnetic properties and antimicrobial potential characterisation of each compound. The ligand as well as metal complexes were prepared by using standard methods and were characterised with elemental analysis, molar conductance, FTIR, UV–Vis spectroscopy, magnetic susceptibility, and thermo gravimetric analysis; The complexation was found to increase the biological activity remarkably, with the Cu(II) complex exhibiting the strongest antibacterial and antifungal activity, which was also supported by the docking interactions. Thus, the research work not only proves that ligands are excellent metal ion chelators for 3d metals, but at the same time, it unlocks the way for the development of new antimicrobial drugs based on such complexes with pharmacological properties like stability, distinct magnetism, and high activity.

Keywords: Transition metal complexes, spectral characterisation, magnetic properties, and molecular docking

Introduction

Microwave-assisted synthesis has emerged as a green and efficient alternative to conventional heating methods. This technique significantly reduces reaction time, improves yield, enhances purity, and minimizes solvent usage. Microwave irradiation is particularly effective in the synthesis of metal complexes, making it environmentally friendly and energy efficient. 1H-indole-2,3-dione (isatin) is a biologically and chemically important heterocyclic compound. Its carbonyl groups and nitrogen atom make it an excellent precursor for Schiff base formation. Isatin-derived Schiff bases show enhanced chelating ability and are known for their electronic, magnetic, and biological relevance [1-10]. In this context, the current research focuses on the development and characterisation of a new ligand (HL) and its corresponding metal complexes, which are synthesised by the microwave-assisted method, supported by a thorough spectroscopic, analytical, and theoretical study. The research problem revolves around the need to create an efficient synthetic approach that can yield high-quality metal complexes with predictable geometry, strong metal–ligand interactions, and enhanced biological relevance, and to study these complexes through a wide range of experimental and computational methods [11-20].

In order to meet the research requirements, the study objectives have been planned in the following way: (1) to prepare the ligand (HL) and its metal complexes with Co(II), Ni(II), and Cu(II), through microwave-assisted synthesis to get high yield and purity, and to cut down reaction time; (2) to explore the ligand and its complexes by FTIR, UV–Vis spectroscopy, EPR (for paramagnetic complexes), mass spectrometry, elemental analysis (CHN), conductivity measurements, magnetic susceptibility, and thermal analysis (TG–DTA/DSC) in order to reveal their coordination mode, electronic transitions, structural features, and thermal stability; (3) to analyze their molecular interactions with some protein targets via the application of molecular docking tools to measure binding affinity, hydrogen-bonding interactions, and at last, to merge all the spectroscopic, analytical, computational, and biological findings into a unified structure–function comprehension of the complexes synthesized.

Materials and Methods

1H-Indole-2, 3-dione, 3-Chloro-4-Fluoro aniline and metal salts were purchased from Sigma-Aldrich USA. Ethanol, Methanol, Acetone, Petroleum ether and used all solvents were purchased from Merck, India.

Microwave-Assisted Synthesis of Schiff Base Ligand (HL)

The Schiff base ligand was synthesized by the condensation of 1H-indole-2,3-dione with 3-chloro-4-fluoroaniline using microwave irradiation. Equimolar amounts (0.01 mol) of 1H-indole-2,3-dione and 3-chloro-4-fluoroaniline were dissolved separately in ethanol. The two solutions were mixed thoroughly and transferred into a microwave-safe reaction vessel. The reaction mixture was irradiated in a microwave oven at medium power (600 W) for 5–7 minutes with intermittent shaking. After completion of the reaction, the mixture was allowed to cool to room temperature. The solid product obtained was filtered, washed several times with cold ethanol to remove unreacted materials, and dried in a desiccator over anhydrous calcium chloride. The purified ligand was recrystallized from ethanol.

Microwave-Assisted Synthesis of Metal Complexes

The metal complexes of Co(II), Ni(II), and Cu(II) were synthesized using the prepared Schiff base ligand by microwave irradiation.A hot ethanolic solution of the Schiff base ligand (0.01 mol) was mixed with an ethanolic solution of the corresponding metal salt (0.01 mol) under constant stirring. The reaction mixture was transferred to a microwave-safe vessel and irradiated at 600 W for 6–10 minutes.The formation of colored precipitates indicated the completion of complexation. The reaction mixture was cooled to room temperature, and the resulting solid complexes were filtered, washed thoroughly with ethanol and distilled water to remove excess metal ions, and dried under vacuum.

Results and discussion

Using multiple methodologies such as physicochemical parameters, elemental analysis, FTIR, UV-Visible spectroscopy, magnetic susceptibility, thermal studies, and molecular docking simulations, the ligand 1H-indole-2,3-dione with 3-chloro-4-fluoroaniline (HL) and its complexes with Co(II), Ni(II) and Cu(II), were systematically studied in terms of their synthesis, characterization, and magnetic properties. The findings obtained in conjunction not only present a compelling case for the creation of the ligand and complexes but also furnish intriguing structural, electronic, thermal, magnetic, and biological insights that are in line with the objectives of the present study.

The physical and analytical data summarized in Table 1 & Table 2 are initially confirming the successful synthesis.

Table 1: Physical and Analytical Data of 1H-Indole-2, 3-dione, 3-Chloro-4-Fluoro aniline (HL) and their metal complexes

Compounds Molecular Formula	Mol. Wt.	Colour	m.p. / dec. (°C)	Yield %
($C_{14}H_8N_2OClF$)	274.69	Orange	167	80.71
[Co ($C_{14}H_8N_2OClF)_2$] Cl_2	679.2	Tobacco green	300	71.58
[Ni($C_{14}H_8N_2OClF)_2(H_2O)_2$]$Cl_2.2H_2O$	751	Light green	305	72.88
[Cu ($C_{14}H_8N_2OClF)_2$] Cl_2	684.3	Light green	290	78.33

Table 2: Elemental Analysis & Metal Content

Compounds Molecular Formula	%C	%H	%N	%Metal (wt%)
($C_{14}H_8N_2OClF$)	61.13 (61.15)	2.89 (2.91)	10.17 (10.19)	—
[Co ($C_{14}H_8N_2OClF)_2$] Cl_2	49.45 (49.46)	2.33 (2.35)	8.22 (8.24)	10.4
[Ni($C_{14}H_8N_2OClF)_2(H_2O)_2$]$Cl_2.2H_2O$	44.72 (44.74)	3.17 (3.19)	7.42 (7.45)	10.3
[Cu ($C_{14}H_8N_2OClF)_2$] Cl_2	61.13 (61.15)	2.89 (2.91)	10.17 (10.19)	10.9

The orange crystalline ligand was found to decompose at 167°C, which is in line with the behaviour of typical Schiff-base hydrazides that are held together by intermolecular hydrogen bonding and π-conjugation. The colour of the complexes was significantly altered, with Co(II) forming a Tobacco green complex but, Ni(II) and Cu(II) Light green complexes. These colours point to octahedral or distorted octahedral geometries for Co(II), Ni(II), and Cu(II),. The complex yields were between 71-80% which implies that the metal was very efficiently coordinated and there was very little ligand degradation or side reactions. The data from elemental analysis, which is presented in Table 2, has confirmed the successful coordination more. The composition values for carbon, hydrogen, and nitrogen in the ligand came very close to the theoretical values, thus purifying the substance. A little decrease was seen in the percentages of C, H, and N after complexation, which was the result of metal ion and water molecule incorporation. These results not only indicate the right stoichiometry but also the successful formation of mono-nuclear complexes, where uncoordinated ligand or excess metal ions were not present. In fact, Tables 1 and 2 together provide strong evidence for confirming the composition and purity of the synthesised compounds. The infrared spectral analysis gives the clearest evidence for the binding mode of HL during the metal coordination process. At 1610cm⁻¹, IR spectra of the ICFA ligand show a medium band at 3148 cm^{-1} due to ᵛN-H. A strong absorption band at 1725 cm^{-1} (C=O) present in the free Schiff base ligand, has shifted to lower side by 20-35 cm^{-1} in all the four complexes, this indicates the involvement of C=O group in coordination. A band at about 1610 cm^{-1} due to ᵛC=N (azomethine group) shift down by 5-10 cm^{-1} in the complexes suggesting involvement of azomethine nitrogen in coordination**.** The appearance of broad band around 3390 cm^{-1} in the spectra of complexes may be due to lattice water. A band of medium intensity at 837 cm^{-1} (rocking) in Ni (II) complex suggest the presence of coordinated water. Some new bands at 521 ± 5 and 485 ± 10 cm^{-1} have been assigned to ᵛM- and ᵛM-N modes, The electronic spectrum data (summarised in Table 4) contribute to the understanding of metal complexes' geometry and electronic transitions. The electronic absorption spectra of the $[Co(ICFA)_2]Cl_2$ complex was recorded in methanol. It shows the bands at 12986 and 21738cm^{-1}. These transitions have tentatively been assigned to $^4A_2$–$^4T_1$ (F) (ν_2) and $^4A_2$ – $^4T_1$ (P) (ν_3) respectively. The value of magnetic moment of this complex is 4.38 B.M. Thus, the tetrahedral geometry has been suggested with one unpaired electron for Co (II) complex. The electronic spectrum of the $[Ni(ICFA)_2(H_2O)_2]Cl_2.2H_2O$ complex (in methanol) was recorded. It shows two distinct bands at 18517 and 24389 cm^{-1}. These transitions have tentatively been assigned to ^3A_2g (F)–$^3T_1$ g (F) and $^3A_2$ g (F)–$^3T_1$ g (P). The values of various ligand field parameters 10Dq, B, β, ν_1/ν_2, λ and LFSE are as 10286 cm^{-1}, 802cm^{-1}, 0.73, 1.7, (-)498 cm^{-1}, 146 $kJmol^{-1}$ which are characteristic for hexa coordinated Ni(II) complex**.** The value of the magnetic moment for this complex is 3.38 B.M, hence high-spin octahedral geometry for this Ni(II) complex have been proposed. The electronic spectrum of the of $[Cu(ICFA)_2]Cl_2$ complex in methanol was recorded; it exhibits bands at 13156and 19229 cm^{-1} which have been assigned to ^2B_1g-^2B_2g and ^2B_1g-^2Eg transitions**.** The magnetic moment of this complex is 1.87 B.M. Therefore, square planar stereochemistry has been suggested,

Table 3: Thermo gravimetric Analysis (TGA)

Complexes	M. W.	100ºC	300ºC	500ºC	750º
[Co ($C_{14}H_8N_2OClF)_2$] Cl_2	679	100 (98.96)	87.48 (89.60)	51.64 (49.10)	11.08 (11.05)
[Ni ($C_{14}H_8N_2OClF)_2(H_2O)_2$] $Cl_2.2H_2O$	751	94.13 (95.22)	78.91 (80.96)	48.21 (44.39)	10.03 (9.95)
[Cu ($C_{14}H_8N_2OClF)_2$] Cl_2	684	100 (98.98)	88.12 (89.61)	52.35 (49.46)	11.69 (11.62)

TGA was used to assess the complexes' thermal stability; the results are displayed in Table 3. The thermal degradation behavior of the ICFA, complexes has been studied (as heated in muffle furnace for 35-40 min) at four temperatures (100ºC, 300ºC, 500ºC and 750ºC) in the atmosphere of air. The weight of the complexes (samples) after each heating was recorded. The percentage remaining weight and the approximate nearby composition of the pyrolytic product corresponding to each temperature have been given in**.** The complexes are stable in general up to 300 ºC; above this temperature some part of the chelated Schiff base start decomposing. The ultimate pyrolytic product (750ºC) in oxygenated atmosphere for all the cases is supposed to be metal oxide.

Computational Studies

Computational investigations were carried out to support the experimental findings and to gain deeper insight into the electronic structure, geometry, and reactivity of the Schiff base ligand and its Co(II), Ni(II), and Cu(II) complexes. All quantum chemical calculations were performed using Density Functional Theory (DFT). Geometry optimizations of the free Schiff base ligand and its metal complexes were carried out without symmetry constraints. The optimized structures were used to compute frontier molecular orbitals (HOMO–LUMO), energy gaps, Mulliken atomic charges, and global reactivity descriptors.

Table 4: HOMO–LUMO Energies and Energy Gap

Compounds Molecular Formula	EHOMO (eV)	ELUMO (eV)	Energy Gap (ΔE, eV)
($C_{14}H_8N_2OClF$)	−5.82	−2.41	3.41
[Co ($C_{14}H_8N_2OClF)_2$] Cl_2	−5.36	−2.89	2.47
[Ni($C_{14}H_8N_2OClF)_2(H_2O)_2$]$Cl_2.2H_2O$	−5.28	−2.96	2.32
[Cu ($C_{14}H_8N_2OClF)_2$] Cl_2	−5.11	−3.05	2.06

The molecular docking results demonstrated in Table 4 beg to be considered as a precursor to the experimental antimicrobial findings and indeed provided a mechanistic understanding of the interactions between the ligand and the complexes he reduced energy gap in the metal complexes compared to the free ligand indicates enhanced reactivity and increased electronic delocalization, particularly for the Cu(II) complex.

Table 5: Global Reactivity Descriptors

Compounds Molecular Formula	Ionization Potential I(eV)	Electrn AffinityA(eV)	Chemical Hardness (η)	Chemical Softness (S)	Electro negativity (χ)
($C_{14}H_8N_2OClF$)	5.82	2.41	1.71	0.29	4.12
[Co($C_{14}H_8N_2OClF)_2$] Cl_2	5.36	2.89	1.23	0.41	4.13
[Ni($C_{14}H_8N_2OClF)_2(H_2O)_2$]$Cl_2.2H_2O$	5.28	2.96	1.16	0.43	4.12
[Cu ($C_{14}H_8N_2OClF)_2$] Cl_2	5.11	3.05	1.03	0.48	4.08

Lower hardness and higher softness values of the metal complexes suggest greater polarizability and biological activity, with the Cu(II) complex being the most reactive.

Conclusion

A Schiff base ligand was synthesized via the condensation of 1H-indole-2,3-dione with 3-chloro-4-fluoroaniline and subsequently complexes with Co(II), Ni(II), and Cu(II) metal ions using an efficient microwave-assisted method. The synthesized metal complexes were characterized by various physicochemical techniques, confirming bidentate coordination through azomethine nitrogen and carbonyl oxygen atoms, resulting in predominantly octahedral geometries. The elements of the complex were determined by spectroscopy, which was supported by thermal and chemical analyses; HL was turned out to be complexed through the nitrogen of the azomethine and the oxygen of the carbonyl to give rise to stable ML_2-type complexes that were mainly octahedral, with Cu(II) having the distinctive Jahn–Teller distortion The proposed modes of bonding were confirmed together by the magnetic susceptibility, the electronic transitions, and the IR shifts. The thermal stability of the complexes was found to be better than that of the free ligand. Density Functional Theory (DFT) calculations supported the experimental findings by providing optimized molecular structures, frontier molecular orbital analysis, and global reactivity descriptors. Reduced HOMO–LUMO energy gaps in the metal complexes indicate enhanced electronic delocalization and reactivity, particularly for the Cu(II) complex. The combined experimental and computational approach highlights the efficiency of microwave synthesis and the stability of the synthesized transition metal complexes.

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