Chemical Data Collections

journal homepage: www.elsevier.com/locate/cdc

Synthesis, characterization, DNA interaction and anti-bacterial studies of Cu(ii), Co(ii) and Ni(ii) metal complexes containing azo-dye ligand

B.R. Kirthan^a, M.C. Prabhakara^{a,*}, H.S. Bhojya Naik^b, P.H. Amith Nayak^b, E. Indrajith Naik^b

^a Department of P.G. Studies and Research in Industrial Chemistry, Sir M.V. Government Science College, Bommanakatte, Bhadravathi 577 302, Karnataka, India

^b Department of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Shankaragatta 577451, Karnataka, India

ARTICLE INFO

Article history: Received 4 April 2020 Revised 22 June 2020 Accepted 4 August 2020 Available online 6 August 2020

Keywords: Azo-dye ligand DNA photocleavage Buffer Anti-bacterial Powder XRD

ABSTRACT

The derivatives of the pyrazole and its metal complexes are considered a pharmacologically important active frame that possesses that some types of pharmacological activities. From the above review highlights the synthesis of pyrazole based ligand through, the diazotization reaction of 5-methyl-2-phenyl-2,4-dihydro-3H-pyrazole-3-one with aniline forms a new azo-dye ligand having N and O donor atoms and their transition metal complexes having the general formula [M(L2).nH2O] where, [M= Co(II),Cu(II), and Ni(II); L = 3-methyl-1-phenyl-4-((E)-phenyldiazenyl]-4,5-dihydro-1H-pyrazole-5-ol]have been synthesized. The synthesized ligand and their metal complexes were characterized as by the melting point, solubility, elemental analyses, FT-IR, ¹H and ¹³C NMR, UV-Visible spectroscopy, and Powder XRD techniques. The DNA binding studies of the metal complexes with Calf-thymus DNA has been studied using absorption spectra, viscosity measurements, and thermal denaturation methods. Absorption spectral studies indicate that metal complexes containing ligand intercalated between the base pairs of the CT-DNA tightly with intrinsic binding constant (Kb) in Tris - HCI buffer containing 50 mM NaCI buffer was found to be 4.8 \times 10⁵M⁻¹, 3.89 \times 10⁵M⁻¹ and 3.26 \times 10⁵M⁻¹ for Co(II) Cu(II) and Ni(II) complexes respectively. Furthermore, the photocleavage studies were carried out by using pUC - 19 DNA monitored by gel electrophoresis. The antibacterial activity was carried by a well-diffusion method against pathogenic organism's gram-negative Klebsiella pneumonia, gram-positive Bacillus subtilis.

© 2020 Elsevier B.V. All rights reserved.

Corresponding author.
 E-mail address: mcpsmvgsc@gmail.com (M.C. Prabhakara).

https://doi.org/10.1016/j.cdc.2020.100506 2405-8300/© 2020 Elsevier B.V. All rights reserved.









Chemical Data Collections

journal homepage: www.elsevier.com/locate/cdc

Data Article

Effect of zirconium doping on the structural, optical, electrochemical and antibacterial properties of ZnO nanoparticles prepared by sol-gel method



caldata

E. Indrajith Naik^a, H.S. Bhojya Naik^{a,*}, R. Viswanath^a, B.R. Kirthan^b, M.C. Prabhakara^b

^a Department of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Shankaragatta, 577451, Kamataka, India
^b Department of P.G. Studies and Research in Industrial Chemistry, Sir M.V. Government Science College, Bommanakatte, Bhadravathi, 577

302, Karnataka, India

ARTICLE INFO

Article history: Received 15 April 2020 Revised 15 June 2020 Accepted 4 August 2020 Available online 6 August 2020

Keywords: Zr-doped ZnO X-ray diffraction Bandgap tunability Photoluminescence Cyclic voltammetry Antibacterial activities

ABSTRACT

The sol-gel approach has been used to synthesize $Zn_{1,x}Zr_xO(x = 0.00, 0.01, 0.03 \text{ and } 0.05)$ nanoparticles. Effect of Zr-doping on structural, optical, electrochemical, and antibacterial properties of ZnO nanoparticles is investigated. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Field emission scanning electron microscopy (FESEM), Transmission electron microscopy (TEM), UV-Visible spectroscopy (UV-Vis), and Photoluminescence (PL) analysis were used for the characterization of undoped and Zr-doped ZnO nanoparticles. Shifting of the absorption edge to lower wavelength and red-shift of the band gap are observed in UV-visible spectra of Zr-doped ZnO samples. Room temperature PL spectra exhibited band edge, violet, strong blue and green emission regardless of the concentration of doping, but intensity increased with levels of doping. Electrochemical performances towards uric acid individually and simultaneously were significantly affected by dopant and superior outcomes were acquired with the Zr-doped ZnO modified carbon paste electrode (MCPE). Antibacterial studies reveal that the Zr-doped ZnO nanoparticles possess improved antibacterial activity against both gram-positive (Bacillus subtilis) and the gram-negative (Klebsiella pneumonia) bacterial strains than the pure ZnO nanoparticles.

© 2020 Elsevier B.V. All rights reserved.

Corresponding author.

E-mail address: hsb-naik@rediffmail.com (H.S.B. Naik).

https://doi.org/10.1016/j.cdc.2020.100505 2405-8300/© 2020 Elsevier B.V. All rights reserved. ORIGINAL RESEARCH ARTICLE



Synthesis, Characterization and Luminescent Properties of Mixed-Ligand Nickel Complexes for Opto-Electronic Application

P.H. AMITH NAYAK,¹ H.S. BHOJYA NAIK ⁽³⁾,^{1,3} H.B. TEJA,¹ B.R. KIRTHAN,² and R. VISWANATH¹

1.—Department of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Shankaraghatta 577451, India. 2.—Department of P.G. Studies and research in Industrial Chemistry, Sir MV Govt Science Collage, Bommanakatte, Bhadaravathi 577302, India. 3.—e-mail: hsb_naik@rediffmail.com

This paper reports the synthesis of a mixed ligand nickel complexes as an emissive layer in organic light emitting diode applications. Synthesized ligand and nickel complexes were characterized by Fourier transform infrared spectroscopy, ¹H nuclear magnetic resonance spectroscopy, mass spectroscopy, x-ray powder diffraction and scanning electron microscopy. This compound shows good thermal stability and film forming properties. Optical properties have been studied by UV-vis and photoluminescence (PL). Frontier molecular orbital theory energy levels of these compounds were demonstrated using density functional theory calculations. Photoluminescence (PL) emission peaks of complexes (1) and (2) show at 596 nm and 581 nm in solid state, respectively. The structure of the fabricated multi-layered device is: ITO/ αNPD(300 Å)/(1)(350 Å)/BCP(60 Å)/Alq₃(280 Å)/LiF(10 Å)Al(1500 Å) and ITO/ aNPD(300 A)/(2)(350 A)/BCP(60 A)/Alq₃(280 A)/LiF(10 A)Al(1500 A). Electroluminescence emission of devices (1) and (2) containing nickel complexes as the emissive layer emit at 568 nm and 561 nm, respectively. Commission Internationale de l'Eclairage chromaticity colour coordinates of devices (1) and (2) were found to be x = 0.426, y = 0.425 and x = 0.473, y = 0.447, respectively, which emits an orange colour. These results show that these nickel complexes can act as a promising emissive layer in opto-electronic applications as strong electroluminescent materials.

Key words: Nickel complexes, characterization, emissive layer, CIE, OLED

INTRODUCTION

Schiff base transition metal complexes are a group of organic transition metal compounds which possess many attractive applications in high-voltage quantum yield, energy efficient, opto-electronic devices such as light-emitting electrochemical cells (LEECs),¹ organic light-emitting diode (OLED) displays,^{2–4} conductors and semiconductors,^{5–8} with good luminescence intensity and stability, which shows their excellent photoluminescence (PL) and electroluminescence (EL) characteristics.^{9–11} The best use of these organic transition metal complexes is in the development of flat-panel OLED displays due to their strong luminescence at low drive voltage.^{12,13} Small molecule-based organic light-emitting diodes are thinner and lighter materials when compared to liquid crystals and they can work without the help of backlighting and filters.¹⁴ They are also referred to as solid-state lighting because, when an electric current pass through a formulated semiconductor diode, the material (semiconductor) produces visible light. Many pieces of research are

⁽Received September 19, 2020; accepted December 24, 2020; published online January 20, 2021)



Check for updates

Synthesis and opto-electronic properties of green light emitting metal Schiff base complexes

P. H. Amith Nayak^a, H. S. Bhojya Naik^a, H. B. Teja^a, B. R. Kirthan^b, and R. Viswanath^a

^aDepartment of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Shankaraghatta, India; ^bDepartment of Studies and Research in Industrial Chemistry, Sir M V Govt Science collage, Bommanakatte, Bhadaravathi, India

ABSTRACT

Schiff base copper complex for OLEDs application was synthesized and ligand was characterized by NMR, mass spectroscopy, FTIR, and powder XRD. Photo-physical properties were recorded on UV-visible and photoluminescence spectroscopy. Their phosphorescent emissive-layer in green light emitting multi-layered OLED device was investigated. It exhibits CIE chromaticity color coordinates at x = 0.377 and y = 0.583. The maximum brightness, current efficiency and power efficiency for the 3.0 weight% Cu(II) complex doped electroluminescent device are 6436 cd/m^2 , 15.4 cd/A and 6.7 Im/W, respectively. These results opens the route for the development of cost-effective metal complex for Opto-electronic applications as a part of strong electroluminescent materials.

KEYWORDS

Copper complex; electroluminescent; OLEDs; Schiff base

1. Introduction

Recently, the design and development of metal-organic coordination complexes have got much more interest because of their molecular topologies and also their potential uses in opto-electronic applications such as luminescent devices, gas storage, magnetism, electrical conductivity, DND binding, and cleavages [1–3]. Several transitional metal complexes have an interesting attraction in developing low-cost, energy-efficient, and full-color flat panel display applications (OLED), which expose their dominant electroluminescent and photoluminescent (EL and PL) properties [4]. In the last decade, the development of green monochromatic material which can be used as dynamic emissive layers in organic light emitting layers is one of the key problems in modern material science. The application of such green emissive layers in the OLEDs and solid-state lightings are limited due to small lifetime and high roll-off efficiency in the electroluminescent devices [5, 6]. With the purpose of cost-effective thin devices while producing flexible and energy saving devices, the research on organic light emitting diodes has gradually increased until reaching the capability to replace the incandescent sources of light [7, 8]. Copper complexes are promising candidates for organic light emitting

Supplemental data for this article is available online at https://doi.org/10.1080/15421406.2020.1868053.
© 2021 Taylor & Francis Group, LLC



Materials Science for Energy Technologies



journal homepage: www.kesipublishing.com/en/journals/materials-science-for-energy-technologies

Structural, optical and photoluminescence enhancement of 2-mercaptoacetic acid capped Mn²⁺ doped CdS nanoparticles and their applications in efficient detection of latent fingerprints



E. Indrajith Naik^a, H.S. Bhojya Naik^{a,*}, R. Viswanath^a, I.K. Suresh Gowda^a, B.R. Kirthan^b

* Department of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Shankaraghatta, Karnataka 577451, India ^b Department of P.G. Studies and Research in Industrial Chemistry, Sir. M.V. Government Science College, Bommanakatte, Shimoga, Bhadravathi, Karnataka 577302, India

ARTICLE INFO

Article history: Received 13 August 2020 Revised 29 December 2020 Accepted 30 December 2020 Available online 5 January 2021

Keywords: Mn²⁺ doped CdS 2-Mercaptoacetic acid XRD Band gap tunability Photoluminescence Latent fingerprint

ABSTRACT

CdS:Mn2* nanoparticles (NPs) stabilized with 2- mercaptoacetic acid (MAA) as a capping agent at different concentrations were developed by co-precipitation method. The X-ray diffraction (XRD) measurement revealed the existence of the cubic phase for stabilized NPs. Scherer's method, Williamson-Hall (W-H) plot and size-strain plots (SSP) were helpful in the evaluation of the crystallite size and lattice strain of formed products. Ultraviolet-Visible absorption spectroscopy was adopted for energy gap determination, where Tauc's plots infer that the energy gap increased with the increase in MAA volume percentage. The existence of MAA capping on CdS:Mn²⁺ was confirmed by fourier transform infrared (FTIR) spectroscopy. The outcome of transmission electron microscopy (TEM) results indicated the presence of spherical shape particles with a typical size of 6-7 nm, which is an encouraging feature for numerous applications. Two emission peaks around 477 nm (blue) and 575 nm (yellow) were observed for MAA stabilized CdS:Mn2* NPs concerning photoluminescence (PL) spectroscopy. The disintegration and oxidation of the samples in the form of foremost weight loss and gain were studied by thermogravimetric analysis (TGA). Visualization of latent fingerprints (LFPs) under normal light on different porous and nonporous surfaces was conducted in the presence of MAA stabilized CdS:Mn2* NPs. The acquired emissive fingerprint powder gave superior images with high distinction and resolution connecting the ridges and space. Based on these results, MAA capped Mn2+ doped CdS NPs can be used for the recognition of LFPs in solving criminal cases.

© 2020 The Authors. Production and hosting by Elsevier B.V. on behalf of KeAi Communications Co., Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-ncnd/4.0/).

1. Introduction

A series of information can be collected by latent fingerprints (LFPs), which have been exploited as convincing physical proof only if they include the added donor information, specifically gender, incidence of human metabolites, and confirmation of getting in touch with explosives. LFPs suffer some shortcomings in certain cases, i.e. they are not purely visualized due to their unfortunate optical contrast when the human naked eye comes into consideration. This inconvenience created during the visualization makes

* Corresponding author.

E-mail address: hsb_naik@rediffmail.com (H.S. Bhojya Naik).

Peer review under responsibility of KeAi Communications Co., Ltd.



the researchers work for the development of superior procedures that facilitates their detection.

Powder dusting [1] ninhydrin spraying [2] cyanoacrylate fuming [3] and silver nitrates soaking have been categorized under traditional fingerprint methods. Among these, the simplest and commonly used one is the powder dusting method with high efficiency and effortlessness in use [1]. The materials used in this method in powder form are metal powders, magnetic powders, and fluorescent powders. These powders prove to be more effective in gaining the LFPs under numerous normal conditions. But still, the materials used in this method face some serious troubles in regards to low sensitivity, low contrast, high background interference, toxicity, and high auto-fluorescence interference.

A series of characteristic properties and applications of doped nano-sized semiconductors has achieved a great deal of attention in the modern-day researchers especially in their functionalized form [4]. These semiconductors in their nano form are different from their bulk materials for their chemical and physical proper-

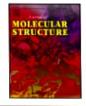
https://doi.org/10.1016/j.mset.2020.12.007

^{2589-2991/© 2020} The Authors. Production and hosting by Elsevier B.V. on behalf of KeAi Communications Co., Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).



Journal of Molecular Structure





Optoelectronic, photocatalytic and biological studies of mixed ligand Cd(II) complex and its fabricated CdO nanoparticles



B.R. Kirthan^a, M.C. Prabhakara^{a,*}, H.S. Bhojya naik^b, R. Viswanath^b, P.H. Amith Nayak^b

^a Department of P.G. Studies and Research in Industrial Chemistry, Sir M.V. Government, Science College, Bommanakatte, Bhadravathi, 577302, Karnataka, India

^b Department of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Jnana Sahyadri, Shankaraghatta, 577451, Karnataka, India

ARTICLE INFO

Article history: Received 19 April 2021 Revised 7 June 2021 Accepted 8 June 2021 Available online 18 June 2021

Keywords: Mixed ligand Cd(II) complex CdO Cyclic voltammetry Photoluminescence Photodegradation Photocleavage

ABSTRACT

This existing examination focuses on the synthesis of the novel Azo-imine ligand obtained from the simple condensation of 2-hydroxy-3-methoxy benzaldehyde with 4-amino-azobenzene and its Mixed ligand Cd(II) Complex was synthesized using Azo-imine ligand as primary ligand and 8-hydroxy Quinoline as a secondary ligand in the equimolar ratio. Further, the obtained complex was fabricated as CdO through the thermal decomposition method. The obtained compounds were illuminated by the different spectroscopic techniques and the formation of the nanoparticles was confirmed by Powder-XRD and TEM Analysis. The CV and PL properties of the synthesized compounds have been investigated in different conditions. Photoemission wavelength at 481 nm and 498 nm specified that both Cd(II) complex and CdO enhance strong Blue luminescence on photoemission. From the electrochemical studies, the reduction of Cd(II) was found to be Quise-reversible in a 0.1 M KOH and give evidence for the formation of a mixed ligand Cd(II) complex in the molar ratio 1:1:1. For Acid red dye under Visible light, CdO shows effective photodegradation than the mixed ligand Cd(II) complex. The DNA Binding study of mixed ligand Cd(II) complex with CT-DNA was investigated by the absorption spectroscopy method and the results gave the evidence for the classical intercalation. The DNA Cleavage results are the indication that the metal complex has good costs in the cleavage of pUC -18 DNA. Further, the antibacterial study of the compounds shows satisfactory results against Gram-positive (Staphylococcus Aureus) and Gram-negative (Proteus) bacterial strains.

© 2021 Elsevier B.V. All rights reserved.

1. Introduction

Metal complexes comprise the azo-Schiff base ligands and their derivatives archives a very good application in physical, analytical, optical, and as well as in the biological field due to their immense behavior of the azo-Schiff base moiety [1-2]. The azomethine and azo-Schiff based ligands and their metal complexes are the most suitable session of composites for particular pharmacological effects such as antibacterial, antifungal, ant amoebic, antileishmanial, antimalarial, antitumor, immunosuppressive, analgesic, vasorelaxant, and plasmodial, anticonvulsant, and antihypertensive activities [3-6]. In the homogeneous and heterogeneous reactions like oxidation, hydroxylation, aldol condensation and epoxidation, transition metal complexes of the Schiff base ligands play important role as a catalyst [7]. Cadmium has their own noticeable

Corresponding author.

E-mail address: mcpsmvgsc@gmail.com (M.C. Prabhakara).

features compare to the other transition metal ions usually, it has a low melting point, the spherical d¹⁰ configuration of this element simplifies miscellaneous coordination geometries and Cd(II) related coordination compounds are proved to be less toxic compare to the Cd(II) ions [8-9].

More than that, the metal complexes have another important nature; they will act as the processor in the fabrication of metal oxides (CuO, CoO, NiO, CdO, etc.,) by combustion method [10]. From the literature, both metal complexes and metal oxide nanoparticles enhance good photocatalytic, electrochemical, and optical behavior due to their flexible and redox nature of the compounds [11]. Synthetic organic dyes the colorants that are enormously used in the textile industries cause environmental pollutions likely in the aquatic region owing to their nonbiodegradability, toxicity, and low photocatalytic activity. To decrease the pollution caused by the dyes developed a large number of nanomaterials as photocatalysts [12] and these nanoparticles are used as the catalyst for the decontamination of wastewater under UV irradiation [13]. Compare to the other nanoparticles CdO



SEVIER

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs



Green light emitting fluorescent [Zn(II)(Schiff base)] complexes as electroluminescent material in organic light emitting diodes



P.H. Amith Nayak , H.S. Bhojya Naik , R. Viswanath , B.R. Kirthan

^a Department of Studies and Research in Industrial Chemistry, School of Operated Sciences, Resemps University, Shanhuraghana, 577451, India ^b Department of Studies and Research in Industrial Chemistry, Sir M V Cost Science College, Bertmanakana, Bhuduravashi,577302, India

ARTICLEINFO	ABSTRACT
Keynanti: Schiff baue	Developing an electroluminescent material, doped with a host organic layer which used as an emitting layer that has high efficiency and brightness for organic light-emitting diodes, leading to strong commercial interest. The
Zinc completes Thermal stability CIE OLED	efficiency and color saturation in light-emitting devices can be altered by introducing an emissive layer fabri- cated with photoluminescent material. In this context, we have developed the Schiff base zinc metal complexes, which can be suitable for efficient light-emissive materials for Optoelectronic applications such as organic light- emitting diades. The synthesized compounds were characterized by various spectroscopic studies. Photo-
	luminescence spectra showed that emission peaks of zinc complexes lie in the range 500-600 nm. Electrolu- minescence emission of the device containing zinc complex 2nL1 and 2nL2 as emissive layer emits at 546 nm and 552 nm respectively. Commission internationale de l'éclairage chromaticity color coordinates were found to be
	x = 0.41, $y = 0.57$ for ZnL1 and $x = 0.49$, $y = 0.46$ for ZnL2 which emits green and yellowish-orange color

respectively. These results are the identification that these zinc complexes can act as a promising emissive layer in opto-electronic applications as a part of strong electroluminescent materials.

1. Introduction

In the last decades, the combination of organic-inorganic systems has dragged much more attraction in the field of flat panel display applications such as organic light emitting diodes. The lnorganic layers in the solid-state lighting give semiconducting properties, high charge-carrier mobility, and thermal stability. The organic layers on the conducting side of an indium tin oxide glass enhance their brightness due to efficient light-matter coupling. The mechanical arrangement of the simplest optoelectronic devices involves three molecular layers, a hole transport layer [1], an electron transport layer, and an emissive layer (usually organic) [2], inserted between two conductors, an anode, and a cathode usually made up of appropriate alloy [3].

Hybrid device structures contain active layers composed of polymer mediums which are surrounded by some nanoparticles, inorganic donor/organic acceptor structures, inorganic-organic p-n junctions, hybrid multilayer device structures, microstructures etc. [4-11].

Monolayer organic emitters such as Tris(8-hydroxyquinolinato) aluminium coated on Aluminium oxide deposited silica wafers reported to exhibit high luminescence properties, they are also a promising candidate for highly sensitive fluorescent chemical sensors [12]. According to spin-statistics, not more than 25% quantum yield obtained from electroluminescent of small molecular fluorophores, but in phosphorescent compounds, their electroluminescence can theoretically achieve quantum yields nearly 100% since both singlet and triplet excitations can be stored for the emission [13]. Lifetimes and applications of organic light emitting diodes depend on their physical and chemical properties like polarization, morphology, chemical reactivity, and diffusion [14]. Due to their unique properties like low power consumption, full color, high-efficiency, and ease of fabrication for a full area flat panel display application, these organic light-emitting diodes can replace the broadly used plasma display and liquid crystal displays [15]. Luminescence quenching can be controlled by proper doping of phosphorescent layers on a host matrix in a narrow and balanced concentration leads to the most efficient phosphorescent OLEDs [16].

Color tuning is very important for the preparation of full color displays. The desired tuning can be made by property chosen substituent that help to Schiff the emission wavelength, i.e., color of emitted light. Many fluorescent dyes and charge transport materials have been developed to this purpose [17–19], yet efforts are still going on in terms of color tuning. The use of metal complexes as efficient electroluminescent materials has received great attention as the emission properties

Corresponding author.
 E-mail address: hub naik@vediffmail.com (H.S.B. Naik).

https://doi.org/10.1016/j.jpcs.2021.110288

Received 30 March 2021; Received in revised form 11 June 2021; Accepted 23 July 2021 Available online 28 July 2021 0022-3697/© 2021 Elsevier Ltd. All rights reserved.



Check for updates

Fabrication, depiction, DNA interaction, antibacterial, DFT and molecular docking studies of Co(II) and Cu(II) complexes of 3-methyl-1-phenyl-4-[(E)-(pyridin-2-yl)diazenyl]-1H-pyrazol-5-ol ligand

Kirthan Bhadravathi Ramashetty^a, Prabhakara Mustur Channabasappa^a, Bhojyanaik Halehatti Seetyanaik^b, Ereshanaik^a, Viswanath Ranganaik^b, Amith Nayak Peerya Nayak Hemla Nayak^b, Ravikumar Shivakumar^c and Kotresh Kyathanahally Rajashekarappa^d

⁴Department of P.G. Studies and Research in Industrial Chemistry, Sir M.V. Government Science College, Bhadravathi, Karnataka, India; ^bDepartment of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Shankaragatta, Karnataka, India; ^cDepartment of PG Studies and Research in Biotechnology, School of Biosciences, Kuvempu University, Shankaraghatta, Karnataka, India; ^dDepartment of PG Studies and Research in Biochemistry, School of Chemical Sciences, Kuvempu University, Shankaraghatta, Karnataka, India

ABSTRACT

Cobalt(II) and copper(II) complexes of the (3-methyl-1-phenyl-4-[E-(1iazinyl-2-yl)1iazinyl]-1H-pyrazole-5-ol) ligand were obtained by the diazotization reaction of 5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one with 2-amino pyridine. The synthesized compounds were confirmed by analytical, and spectroscopic analyses (like, UV-Visible, FT-IR, NMR, and mass spectroscopy). Calf thymus DNA interaction with metal complexes is inspected by UV-Visible spectra, viscosity measurements, and thermal denaturation techniques. The intrinsic binding constant (K) was found to be 1.17×10^6 M⁻¹, and 0.98 x 10⁶ M⁻¹ for Co(II) and Cu(II) complexes respectively. The Cleavage of pUC-19 DNA was monitored by gel electrophoresis. The computerized in silico molecular dockage studies of the composites with the target receptor Glu-6p and results showed that the compounds are potent drugs for the target enzyme. Further, the optimized structure of the azo dye ligand was obtained by the density functional theory (DFT) by Gaussian09 program by the RB3LYP at 6-311G (++, g, d, p) basis set. Furthermore, screened for the bacterial action in contradiction of pathogenic organism's gram-negative Klebsiella pneumonia, gram-positive Bacillus subtills by a diffusion method.

ARTICLE HISTORY

Received 6 April 2021 Accepted 6 October 2021

KEYWORDS

Azo-dye complexes; photocleavage; anti-bacterial; molecular docking; DFT; Powder XRD

Introduction

Heterocyclic compounds containing nitrogen and oxygen atoms have been expansively considered owed to their stimulating biological properties and



INDIAN CHEMICAL SOCIETY

Journal of the Indian Chemical Society

journal homepage: www.editorialmanager.com/JINCS/default.aspx

DNA interaction studies of Cu(II), Co(II), and Ni(II) chelates derived from schiff base ligand



Ereshanaik^a, M.C. Prabhakara^{a,*}, H.S. Bhojya Naik^b, B.R. Kirthan^a, H.M. Kumaraswamy^c, R. Sandeep Kumar Jain^c

* Department of PG Studies and Research in Industrial Chemistry, Sir. M.V. Govt. Science College, Bemmanakatte, Bhadravathi, 577 302, Karnataka, India

^b Department of PG Studies and Research in Industrial Chemistry, Jnana Sahyadri, Kuwempu University, Shankaragatta, 577 451, Karnataka, India

^e Department of PG Studies and Research in Biotechnology, Jnana Sahyadri, Kuvempu University, Shankaragatta, 577 451, Karnataka, India

ARTICLE INFO

Keywords: Absorption spectra Viscosity DNA-Cleavage Gel-electrophoresis

ABSTRACT

Chelates of the type $M(L)_2$ (where, M = Co(II), Ni(II) and Cu(II), and $L = 3-\{(E)\cdot\{(2-hydroxy-3-methaxyphenyl) methylidene]amino}pyridin-4(1H)-one)\}$ were synthesized by using the Schiff base ligand in the stochiometric ratio 2:1 (L:M) and Schiff base ligand (L) was synthesized by simple condensation between 2-hydroxy-3-methoxybenzaldehyde with 3-aminopyridin-4-ol. The structure and formation of synthesized compounds were established by different analytical and spectroscopic methods like, elemental analysis, UV- spectroscopy, FT-IR, Proton and Carbon NMR, mass spectrometry and Powder XRD. Further, the synthesized chelates screened for the DNA binding studies of Calf Thymus (CT)-DNA by exploiting electronic absorption spectra, relative viscosity measurements and thermal denaturation methods. The proposed DNA binding mode supports the enhancement in the binding activity of the complexes in presence of newly synthesized ligand. The cleavage activities of the PUC-18 DNA in the presence and the absence of the complexes were recorded with the help of gel-electrophoresis. The cleavage experiment results reveals that all the synthesized chelates can cleave pUC-18 DNA effectively.

1. Introduction

Ever since, Hugo Schiff introduced the term Schiff bases also known as imines or azomethines have attracted the phenomenal popularity because of its preparation, stability, relatively cheap precursors such as carbonyl compounds and primary amines and their chelating ability. When the functional groups such as -SH, -NH2 and -OH near the site of condensation, those with potentially coordinating to the metal centre act as very good chelating agents [1]. Their capacity to chelate with metal centre is commonly increased by imparting the donor atoms at appropriate positions in the molecule, allowing a huge number of transitions chelates with interesting structures [2-4]. The chemistry of the Schiff base compounds, which contains (-N=CH-) groups, takes the fore front position in the development of the co-ordination chemistry of the symmetrical transition chelates [5,6]. Several transitions chelate having Schiff base ligand play a prominent role in pharmaceutical and biological activities like anti-bacterial, anti-microbial, anti-cancer, anti-fungal, antiviral, anti-malarial, anti-inflammatory and antioxidant as well as catalytic activities [7,8]. This enhanced biological activity of these

compounds is due to their synthetic flexibility and structural stability. Schiff base chelates of transition metals have been of continuing interest because of their roles as biological models, as catalysts for organic reactions and components in the formation of new materials [9]. Complexes of transition metal ions have received a growing attention in recent years. It has been an interesting area for chemists, physicists and biologists, since these complexes form the basis for several research fields such as bio-inorganic chemistry, magneto chemistry, material science, catalysis, super conductivity, multi electron redox chemistry etc. [10–12].

DNA binding with numerous small molecules will take place via noncovalent modes like groove, electrostatic and intercalation. Out of these, intercalation type of binding mode is one of the authoritative binding modes and is associated to the anti-tumour activity of metal compounds [13]. For the last few decades, the DNA interaction of transition chelates is of great interest in bio-inorganic chemistry owing to their possible application for designing new anticancer therapeutic agents and their photochemical activity, that will take them to potential probes of DNA structure and conformation [14,15]. Thus, the transition chelates are

* Corresponding author. E-mail address: mcpsmvgsc@gmail.com (M.C. Prabhakara).

https://doi.org/10.1016/j.jics.2021.100288

Received 16 September 2021; Received in revised form 6 November 2021; Accepted 27 November 2021 0019-4522/© 2021 Indian Chemical Society. Published by Elsevier B.V. All rights reserved.



Inorganic Chemistry Communications

journal homepage: www.elsevier.com/locate/inoche



Short communication

Optoelectronic, Photocatalytic, and DNA interaction studies of synthesised Cu(II), Co(II), and Ni(II) complexes containing schiff base ligand



B.R. Kirthan^a, M.C. Prabhakara^{a,*}, H.S. Bhojyanaik^b, P.H. Amith Nayak^b, R. Viswanath^b, H. B. Teja^b, Ereshanaik^a

^a Department of PG Studies and Research in Industrial Chemistry, Sir M.V. Government, Science College, Bommanakatte, Bhadravathi, Karnataka 577 302, India ^b Department of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Jnana Sahyadri, Shankaragatta, Karnataka 577451, India

ARTICLE INFO

Keywords: Schiff base DFT Cyclic voltammetry Photoluminescence Malachite green CT-DNA

ABSTRACT

An innovative, active Cu(II), Co(II), and Ni(II) complexes of Azomethine ligand [5-(*diethylamina*)-2-hydroxyphenyl]methylidene)benzo hydroxide] were synthesized. The afresh made ligand and its metal complexes were premeditated by elemental analysis, FT-IR, UV–Visible, ¹H & ¹³C NMR, LC-MS spectroscopy, and X-ray powder diffraction. The Optimized structure of the compounds was done by Density Functional Theory (DFT) in Gaussian09 program at the basis set RB3LYP at 6-311G (++, g, d, p). The PL emission of the metal complexes was tuned in the Ultraviolet region, which concluded that it is shown that the metal layer leads to an enhanced photoluminescence efficiency of metal complexes. The redox behavior of the metal complexes was investigated by the cyclic voltammetry technique. Photocatalytic results related degradation of Malachite green indicated that the metal complexes dramatically enhance the catalytic activity. This means that metal complexes showed virtuous photocatalytic activity under UV light irradiation. Further, the metal complexes have also shown significant DNA binding with CT-DNA and pUC-19 DNA cleavage activities.

1. Introduction

Schiff base transition metal complexes like copper, cobalt, nickel, iron, manganese zinc, cadmium etc., having the ONS hetero atoms play a vital role in the bio-inorganic, electrochemical, optical, and medicinal research due to their stability, special molecular structure, stretchability, unique coordinative behaviour and biological properties [1-4]. Largely, Schiff base ligands were attained by the condensation reaction between the aldehyde or ketones with amines [5]. Schiff bases have been investigated in relation to a wide range of contexts, including antimicrobial, antiviral and anticancer activity. They have also been considered for the inhibition of amyloid-ß aggregation. Schiff bases are common enzymatic intermediates where an amine, such as the terminal group of a lysine residue, reversibly reacts with an aldehyde or ketone of a cofactor or substrate. Schiff base ligands and its 3d-metal complexes also hold a unique position in drug discovery and lead a prominent role in biological activities like anti-bacterial, anti-microbial, anti-cancer, antioxidant, and analgesia [6]. The majority of the ligands and its metal complexes have special characteristics such as extractability. colours suitable for photometric analysis, and intense biological activity [7]. Copper, cobalt, nickel, and zinc are the essential metal for the human beings. in these bio-essential elements copper play a prominent role in may physiological process [8]. Transition metals like cobalt, copper, ruthenium may potential to the antitumor drug due to their bioactivities [9–11].

Moreover, dyes are the leading environmental pollutants in the aquatic region, the decolouration slow biological degradation, and the high COD nature of the dyes, which becomes toxic and hazardous to many organisms. The decontamination of wastewater was extremely done by photocatalysts and their heterostructures under light irradiation [12,13]. From the last several years, a series number of studies were adopted for the removal of hazardous dyes in the pollutants are Reverse osmosis, Ultrafiltration, Activated carbon, Chlorination, Biodegradation, COD, and Photodegradation. Nowadays, photocatalysis is the emerging technique to overawed the environment and water pollution [14]. CuO, TiO₂, ZnO, Fe₂O₃, and some other metal oxides were extremely used for photocatalytic applications. Largely, Imine (C = N) based ligands and their metal complexes consist of electron-donating

* Corresponding author. E-mail address: mcpsmvgsc@gmail.com (M.C. Prabhakara).

https://doi.org/10.1016/j.inoche.2021.109109

Received 30 September 2021; Received in revised form 18 November 2021; Accepted 30 November 2021 Available online 4 December 2021

1387-7003/@ 2021 Elsevier B.V. All rights reserved.

NJC



PAPER

Check for updates

Cite this: New J. Chem., 2022, 46, 1943

Received 29th October 2021, Accepted 14th December 2021 DOI: 10.1039/d1nj05156c

rsc.li/njc

1. Introduction

Nanoparticle research is currently an area of intense scientific interest due to their wide variety of potential applications in biodegradation,¹ pollution control,² biomedicine,³ and the optical and electronic fields.⁴ Different phenomena of lightmatter interactions can be studied using metal-substituted nanoparticles, which serve as a versatile platform, and their conductivity can be redesigned by intercalating impurities into their crystal lattice. When metal materials are prepared in the nanometre size range, the density of their electronic states changes in a systematic manner, which impacts the properties of the synthesized nanomaterial. Ferrites are a useful tool in photocatalytic applications. Ferrites are assorted metal oxides having iron oxides as their main components, possessing

^b Department of P.G. Studies and Research in Industrial Chemistry, Sir M. V. Government, Science College, Bommanakatte, Bhadravathi, 577302, Karnataka, India

Combustion-assisted green-synthesized magnesium-doped cadmium ferrite nanoparticles for multifunctional applications

Vishnu G., 😳 ^a H. S. Bhojya Naik, 😳 *^a R. Viswanath, ^a B. R. Kirthan, ^b P. H. Amith Nayak 😳 ^a and Mohammed Abdullah Bajiri 😳 ^a

Magnesium-doped cadmium ferrite nanoparticles, $Mg_XCd_{1-X}Fe_2O_4$ (where, X = 0, 0.2, 0.4, 0.6, 0.8, 1) were synthesized by a combustion method using curd as fuel. The synthesized nanoparticles were characterized using XRD, FTIR, SEM, HRTEM, XPS, PL and UV-VIS spectroscopy. XRD studies reveal that the synthesized nanoparticles exhibit a cubic spinel structure, and the average crystalline size and lattice parameters decrease with the increase in magnesium doping. The vibrational stretching modes of the octahedral and tetrahedral sites were confirmed by FTIR, and the applomerated and nanoflake-like structure was confirmed by SEM and HRTEM. The elemental composition and oxidation and transition states of the synthesized nanoparticles were revealed by X-ray photoelectron spectroscopy. Luminescence spectroscopy reveals that the luminescence intensity decreases with the increase in magnesium doping. From the UV-VIS spectroscopy, the band gap of the synthesized nanoparticles is determined, which decreases as the magnesium doping increases. The photodegradation capabilities of the synthesized nanoparticles were assessed for the degradation of malachite green dye, under visible light irradiation. Electrochemical studies reveal that the synthesized nanoparticles show appreciable electrochemical performance. Pure CdFe₂O₄ and Mg-doped CdFe₂O₄ were inspected against the Gram-positive bacteria S. aureus and Gram-negative bacteria Shigella, and it was found that the antibacterial activity improved with magnesium doping compared to the pure CdFe₂O₄ nanoparticles.

> optical, magnetic, and electrical properties, and are suitable for a broad range of applications, such as the photodegradation of industrial wastes or dyes,5 piezoelectric catalytic performance or the piezoelectric catalytic degradation of organic pollutants,6,7 electrode components for batteries," window materials for solar cells,9 as well as in biological systems, such as bio-imaging, magnetic resonance imaging,10 nano-materials with both luminescent¹¹ and magnetic properties,¹² either paramagnetic or ferromagnetic. Another new green technology is piezocatalysis, where the surfaces of the piezocatalyst particles exhibit heatexcited free electrons and holes under the influence of mechanical vibration, generating active free radicals with a strong oxidation ability to decompose organic pollutants.13,14 Photocatalysts are capable of degrading various organic pollutants or dyes. They harness light energy to excite photo-induced electrons. The photogenerated electrons from the valence band (VB) are transferred to the conduction band (CB), which results in the recombination of the charge carriers and helps degrade particular pollutants or dyes.15,16 Synthetic dyes are utilized in a broad range of commodities, such as clothes, accessories made of leather and furniture, but a side effect of their widespread use is that up to 12% of these dyes are wasted in the course of the colouring

^a Department of Studies and Research in Industrial Chemistry, School of Chemical Sciences, Kuvempu University, Shankaraghatta-577 451, India. E-mail: hsb_naik@rediffmail.com