

Heavy metal monitoring of beach sands through environmental magnetism technique: a case study from Vengurla and Aravali beaches of Sindhudurg district, Maharashtra, India

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Abstract Mineral magnetic, geochemical and statistical analyses were carried on surface sediments collected from Vengurla and Aravali beach, along west coast of India, premonsoon (PreM), monsoon(M) and postmonsoon (PM). Magnetic concentration parameters (χ_{lf} , ARM, SIRM and HIRM) are strongly correlated within them PreM during M and PM. Thermomagnetic analysis identifies titanomagnetite, magnetite, maghemite and hematite as the dominant magnetic mineralogy of the sediments. Strong correlation was deciphered between magnetic parameters and heavy metal (Cu, Cr, Zn and Ni) PreM and PM which obliterated in M. This shows influx of magnetic minerals and heavy metals is more in M than PreM and PM. The monsoonal influx is more haphazard and random in M because of enhanced weathering resulting in weak correlation between different mineralogical and geochemical entities. This finding outlines the efficacy of simple, rapid and non-destructive magnetic measurement which can be used as an indicator for heavy metal contamination. It can act as a proxy for measuring of heavy metal content in the coastal and beach environment.

Keywords Mineral magnetic · Heavy metal · Statistical · Geochemical · Beach · West coast

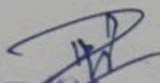
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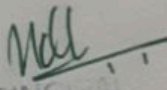
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Introduction

Investigating the compositional properties of rocks, sediments and soils using mineral magnetic measurements is nowadays a routine form of analysis (Thompson and Oldfield 1986; Walden et al. 1999; Maher and Thompson 1999; Oldfield 1999a, b). The technique has been applied to various depositional environments (e.g. Arkell et al. 1983; Oldfield et al. 1985, 1999; White et al. 1997; Walden et al. 1995, 1997; Schmidt et al. 1999; Wheeler et al. 1999). Many have also explored the relationship between mineral magnetic measurements and chemical/physical properties of sediments and soils (Oldfield et al. 1985; Oldfield and Yu 1994; Clifton et al. 1997, 1999; Chan et al. 1998; Petrovsky et al. 1998; Xie et al. 1999, 2000; Booth 2002). These investigations have revealed mineral magnetic measurements to be a suitable tool for determining sediment provenance (Oldfield and Yu 1994; Booth 2002; Gawali et al. 2010), sediment transport pathways (Lepland and Stevens 1996), which also serves as a proxy for geochemical, radioactivity, organic matter content and particle size data (Bonnett et al. 1988; Oldfield et al. 1993; Hutchinson and Prandle 1994; Clifton et al. 1997, 1999; Xie et al. 1999, 2000; Zhang et al. 2001). The environmental magnetic method has been successfully utilized for coastal investigations that include sediment sources and transport pathways, and determining contamination of heavy metals in estuaries and tidal flats (Oldfield et al. 1985; Lees and Pethick 1995; Zhang et al. 2001). Environmental magnetic methods (magnetic fingerprinting and magnetic inclusions) are extensively used to resolve various coastal research problems including investigating particulate pollution, to identify and characterize the sediment sources and to examine sediment dynamics in coastal


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Highly Stereoselective Direct Aldol Reaction of 4-Formylcoumarins with Acetone Catalyzed by L-Proline in Water-Acetone Mixtures

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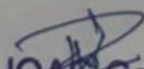


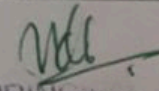
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Highly stereoselective direct aldol reaction of 4-formylcoumarins with acetone catalyzed by L-proline in water-acetone mixtures

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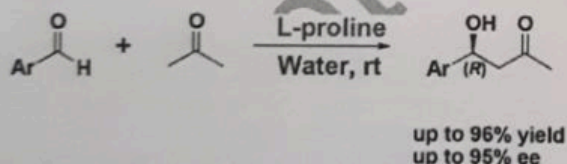
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Abstract

Organocatalyzed direct intermolecular aldol reactions has been developed for substituted 4-formylcoumarins with acetone in water using L-proline and phthalimido-prolinamide catalysts without use of additives. Stereoselective products obtained were in excellent yields (up to 97%) with high purity (up to 99%) and enantioselectivities (up to 95%). The isolated compounds were confirmed by IR, NMR, HPLC, MS and some of them by single X-ray crystallography study.

Graphical Abstract



KEYWORDS: Aldol reaction; recyclable organocatalyst L-proline; phthalimido-prolinamide; 4-formylcoumarin; Acetone

INTRODUCTION



Secondary electrochemical doping level effects on polaron and bipolaron bands evolution and interband transition energy from absorbance spectra of PEDOT: PSS thin films

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ABSTRACT

Doping induced effect on interband transition energy levels of PEDOT: PSS films deposited by spin coating have been studied experimentally by following changes in vibrational, optical and electrochemical properties. Absorbance spectra of films have been used as a tool to study formation of polaron/bipolaron bands, their energy shift and binding energies with change in doping concentration. Energy level structure evolving from optical spectra has been sketched and corresponding energies required for transition at different doping levels have been indicated. Electrochemical studies show redox peaks in agreement with spectroscopic results demonstrating storage of charge in sub-band states in the form of polarons/bipolarons. Increased absorption due to $\pi-\pi^*$ transitions on secondary doping reveal non linear characteristic in the plot of hue vs. chroma traversing from faint blue to deep blue region in the chromaticity diagram.

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1. Introduction

Conducting Polymers (CP) like polyaniline, polypyrrole, polythiophene have been attracting widespread attention for a number of novel applications because of their innate properties [1,2]. Polyaniline and polypyrrole are conducting polymers with high conductivity but lack properties of solubility and processibility [3,4]. However, by controlling the pendant chain chemistry, Polythiophene, can be used to prepare new polymers with tunable properties. Polythiophene and its derivatives have been found to be stable both in their doped and undoped states. They also exhibit high stability of the optical spectrum and high conductivity retention at elevated temperatures for long intervals [5]. Poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT:PSS), a polythiophene derivative is one such CP with exceptional optical, conductive and solubility properties. It forms a dispersion of oxidatively doped cationic derivative PEDOT electrostatically bound to a polyanion PSS in water [6]. PSS also acts as a charge compensating counter-ion and stabilizes the p-doped PEDOT. The solution-processability of this aqueous colloidal dispersion can be used to achieve a thin, virtually transparent film

for use as a flexible electrode numerous electronics applications, as well as in anti-static coatings, supercapacitor materials, sensors, OLED applications, transparent electrodes, solar cells, organic transistors [7–13] etc. Doped PEDOT:PSS has been used widely for depositing thin, transparent films for use as an electrode in electronics applications [14]. Thin films of PEDOT:PSS show high conductivity of the order of several hundred S/cm. It is also a promising candidate for electrochromic device (ECD) like windows/displays due to its fast response time, small electronic bandgap, low redox potentials and facile fabrication [15,16]. PEDOT: PSS thin films can be easily deposited using different techniques like template synthesis, CVD, spin coating, inkjet printing, electro-polymerization and spraying [17,18].

PEDOT:PSS is a low bandgap p-type semiconducting material with its energy gap lying in the VIS-NIR range (1.6 eV for $\pi-\pi^*$ transition) and shows an absorption maximum in the middle of the visible spectrum at 600 nm. Doped PEDOT:PSS is almost transparent in the visible region (with a light blue tint) and while neutral polymer possesses a blue-black color. In its pristine state, a film of PEDOT:PSS consists of a mixture of undoped and doped PEDOT units in the ratio 1:4, corresponding to an intermediate state between the fully doped (oxidized) and undoped (reduced) state. Electrochemical doping of PEDOT:PSS results in addition of mid-gap energy levels, producing absorptive transitions in the visible region that invoke an observable color change. This high-contrast

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Research Paper

Studies on electrochemical activity of CNT/PANI composite thin film coating on ITO coated glass surfaces: Effect of concentration on fractal dimension

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ABSTRACT

Thin films of CNT/PANI composites have been deposited potentiostatically by electrochemical polymerization from a solution of CNT dispersed in aniline monomer and H₂SO₄ on ITO coated glass substrates. H₂SO₄ concentration in aniline monomer solution has been varied and its effect on electrochemical properties of films has been studied. To elucidate information about the degree of surface disorder, surface growth mechanism and the kinetics of electrochemical reactions at the surfaces, fractal dimensions has been evaluated using two electrochemical techniques: cyclic voltammetry and electrochemical impedance spectroscopy. It is observed that as acid concentration in the deposition solution increases, fractal dimension of the deposited film varies from $D_f = 1$ corresponding to a series of isolated islands, increasing to 2 for a planar 2D configuration for smooth surfaces and finally reaching a value of $2 < D_f < 3$ for rough and porous surface of the electrodes. Results obtained from both the techniques are found to be in good agreement with the fractal dimension values lying between those for smooth and porous/rough surface.

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1. Introduction

Since the advent of conducting polymers (CP) by Shirakawa, et al. [1] in the year 1977, interest in these exotic materials has risen exponentially. The enormous amount of work done and research papers published in this field bear a testimony to the fact that properties of CP, belonging to the new group of advanced materials can be tuned according to the user's needs. These materials reportedly have excellent properties like conductivity, ease of deposition and so on and so forth. Further work is still going on to produce CP with improved properties like tractability, transparency, increase in conductivity, bandgap tuning etc. for applications like electrocatalysis, anticorrosion coating, electrochromic devices, camouflage devices, antistatic agents and transparent electronic devices [2] in general. The ability of these CPs to be drawn into wires, deposited as films or coatings over any shape make them popular materials for diverse purposes. After the successful synthesis of polyacetylene, many new CP like PANI, PEDOT, PPy,

PPrDOT etc. have been synthesized and characterized for use in various applications. Among these PANI appears to be the natural choice of materials because of its ease of deposition, exceptional conductivity and various other properties [3,4]. Over the last few decades, much research has been carried out to improve the stability, adherence, optical properties and conductivity of Polyaniline (PANI) by using different fillers and studying their properties. Using non conductive fillers like PAA, CSA, PVA [5–7] etc. as binder, surfactant etc. to deposit a film ends up reducing conductivity of PANI, defeating the choice of a CP for a specific application. To overcome this problem, choice of filler must be such that it does not interfere with the conductivity of PANI, but aids it along with providing the necessary stability and strength to the film. A number of schemes have been proposed to increase the conductivity of PANI. One of the most frequently investigated methods is incorporation of highly conductive carbon species like graphene or Carbon nanotubes (CNTs) in such polymers [8]. CNTs possess unique structures and exhibit extraordinary electrical, optical, chemical, and mechanical properties, which are somewhat complementary to those of CPs [9]. So the combination of CNT/PANI is expected to create new materials with advanced properties and greater potential applications in mechanical, thermal, electrical,

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Sediment Texture and Geochemistry of Beaches between Redi-Vengurla, Sindhudurg, West Coast of India

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ABSTRACT

Hanamgond, P.T.; Gawali, P.B.; Lakshmi, B.V.; Mahesh Babu, J.L.V.; and Deendayalan, K., 0000. Sediment texture and geochemistry of beaches between Redi-Vengurla, Sindhudurg, west coast of India. *Journal of Coastal Research*, 00(0), 000-030. Coconut Creek (Florida), ISSN 0749-0208.

Textural and geochemical determinations were carried out on three beaches (Vengurla, Aravali, and Redi) of the Sindhudurg district, Maharashtra, west coast of India. Seasonal sediments from the beach were collected during 2003-04 to understand the sediment dynamics (texture, dispersal pattern, depositional environment, etc.) and geochemical characteristics. In general, a seaward grain size fining is seen along Vengurla beach (swash-backwash phenomenon), with a coarsening seaward trend along Aravali and Redi beaches (high-energy conditions). The CM pattern studies reveal traction currents as the transport mechanism. Thus, the sediments of the study area are deposited under moderate to high-energy conditions. The geochemical study shows that the percentages of V, Cr, and Zr are greater in premonsoon; Si, Al, K, Sr, Mn, Ti, and P are greater in monsoon; and Mg, Ca, K, Mn, Na, S, Cl, and P are greater in postmonsoon at Vengurla beach. At Aravali beach, the percentages of Si and Al are more than those observed at Vengurla or Redi beaches. The percentages of Mn, Na, S, and Cl are greater premonsoon; Si, Al, Fe, K, Ti, Cr, and Zr are greater in monsoon compared with the other two seasons; and Mg, Ca, Sr, Mn, P, and V are greater in postmonsoon. At Redi, Cr and Ca are greater than at the two other beaches. Percentage of Fe is greater in all the seasons at Redi. Mn and Ti are quantitatively greater in premonsoon; Si, Al, Fe, and K are greater in monsoon; and Fe, Mg, Ca, Sr, Na, S, Cl, P, V, Cr, and Zr are greater in postmonsoon. These seasonal changes can be attributed to changing wind, wave, and current regimes prevalent in this coastal tract, which seem to be dissimilar even though the three beaches are adjacent (but separated by headlands or a creek).

ADDITIONAL INDEX WORDS: Dynamics; Maharashtra.

INTRODUCTION

Beaches are nonstatic and ever-changing landscapes formed by complex interactions involving sediment source, wave and wind energy, river discharge, precipitation intensity, and ambient geomorphology. The beaches are sensitive to changing climatic and environmental conditions involving variation in atmospheric pressures and subsequently generated winds (Simm, 1996). These changes also influence the effect that waves, tides, and currents have on the morphology of beaches, not least the sea level, which is one of the most important components of shoreline position change (Leatherman 2001).

Mineralogical and geochemical characteristics of beach sands are closely related to geology and hydrodynamics. Analysis of such sediments for their compositional makeup can provide valuable insight into the local and regional hydrodynamics, patterns of sediment dispersal/transport, distribution, and source. Beaches are sensitive to erosive and accretionary processes, and these changes can be easily quantified by morphological changes it undergoes within a span of weeks, months, or years. Since many recreational facilities line this coastal transect all over the world, any

deleterious change effected on a beach has economic and societal effects that need to be addressed and prioritized. Beaches and their adjacent nearshore zones act as buffers to wave energy. Consequently, they are sensitive to change over timescales ranging from a few seconds to several years. The study of beach changes assists in forecasting coastal erosion and deposition, among other things. Wind, waves, and long-shore currents are the driving force behind coastal erosion, wherein valuable property frequently is lost to the dynamic beach-ocean system, posing many problems to coastal communities. However, understanding of the coastal processes is rudimentary.

Relationships between different textural and sedimentological, geochemical, and compositional parameters in varied depositional settings of beach sediments have been used extensively to understand pathways, detrital types, and grain size characteristics to determine sediment provenance or source characteristics (Basu, 1976; Dickinson and Suczek, 1979; Di Giulio *et al.*, 2003; Gawali, Basavaiah, and Hanamgond, 2010; Hanamgond and Chavadi, 1992, 1993; Ibbeken and Schleyer, 1991; Ingersoll, 1990; Kasper-Zubillaga and Dickinson, 2001; Le Pera and Critelli, 1997). However, this is not always so straightforward, because some coastal sands do not necessarily reflect the composition of the source rock (Kasper-Zubillaga and Carranza-Edwards, 2005).

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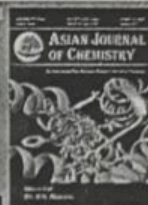
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Effect of Resin Structure and Resin Fixed Ion on Selectivity of Perchlorate and Nitrate in Aqueous and Mixed Media†

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The anion exchange of perchlorate and nitrate against chloride was investigated at different temperatures on weak base anion exchangers in aqueous and mixed media. The selectivity sequence observed for the resin Tulsion A-10X (MP) having acrylic matrix with polyamine group is $\text{NO}_3^- > \text{ClO}_4^- > \text{Cl}^-$ and for polystyrene based Amberlyst A-21 (MP) and Tulsion A-23 (Gel) having tertiary and quaternary ammonium groups respectively is $\text{ClO}_4^- > \text{NO}_3^- > \text{Cl}^-$. The study reveals that nitrate is more preferred than perchlorate on the resin having polyamine group. However the resins having tertiary and quaternary ammonium groups prefer perchlorate over nitrate. It is also observed that there is effect of temperature and solvent on selectivity of perchlorate and nitrate.

Keywords: Selectivity, Anion exchange, Resin matrix, Resin fixed ion.

INTRODUCTION

In separation of anions from the water and wastewater, selectivity plays important role as it reflects the preference of resin for particular ion in presence of other ions. Important factors governing anion selectivity in systems with monovalent and divalent ions include the spacing of the active sites, type of resin matrix, hydrophobic or hydrophilic nature of the resin matrix [1-3] and percentage of divinyl benzene [4]. The anion exchange selectivity data available for resins with polyacrylic matrix is inadequate, whereas anion exchangers with polystyrene matrix having cross linkages of divinyl benzene are used for exchange study of perchlorate and nitrate against chloride in aqueous and mixed media by various researchers [5,6]. Perchlorate and nitrate ions are hazardous to human health if their concentration in water is more than the permissible limit [7]. Hence, the present research deals with anion exchange selectivity of perchlorate and nitrate against chloride on weak base anion exchangers of different resin

matrix at various temperatures in aqueous and mixed media. Anion exchangers used for the study are weak base Tulsion A-10X (MP), Amberlyst A-21 (MP) and strong base Tulsion A-23 (Gel).

EXPERIMENTAL

Anion exchange resins Amberlyst A-21 (MP) from Himedia Laboratories Pvt. Ltd., Mumbai, India and Tulsion

A-10X (MP) and Tulsion A-23 (Gel) resin samples received from Thermax Pvt., Ltd., Pune, India were used for the present work. Table-1 summarizes resin type, matrix structure and capacities of the resins used. All the reagents used were of analytical grade. The 0.05 M solutions of HCl, HClO_4 , KNO_3 and KCl were prepared in water and water organic solvent mixed media.

Selectivity studies were carried out by taking 250 mg of air dried resin into 100 cm^3 stoppered volumetric flasks. 0.05 M electrolyte solutions of exchanging counter ions were added to the flask in different proportions to give a total volume of 30 cm^3 and total ionic strength of 0.05 M. The flasks were tightly closed and kept to attain equilibrium in reciprocate type Toshiba make mechanical shaker. After equilibration a known aliquot (10 cm^3) from external solution phase was pipetted out and estimated for Cl^- ions by Mohr's method using standard 0.05 M silver nitrate solution and potassium chromate as an indicator.

The selectivity coefficients $K_{\text{Cl}^-}^{\text{ClO}_4^-}$ and $K_{\text{Cl}^-}^{\text{NO}_3^-}$ were evaluated using the following equation.



where $\text{B}^- = \text{ClO}_4^-, \text{NO}_3^-$

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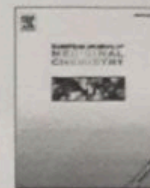
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Research paper

Synthesis, characterization and molecular docking studies of substituted 4-coumarinylpyrano[2,3-c]pyrazole derivatives as potent antibacterial and anti-inflammatory agents



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Anti-inflammatory

Molecular docking

ABSTRACT

A green, eco-friendly and efficient protocol has been developed and synthesized a series of coumarin based pyrano[2,3-c]pyrazole derivatives (**3**) by multi-component reaction (MCR). Unexpected 3-coumarinyl-3-pyrazolylpropanoic acids (**4**) have been isolated by the reaction of compound (**3**) in acidic conditions. Further, intramolecular cyclization of compounds (**4**) leads to C₄-C₄ chromons (**9**) and these compounds were screened for their biological activities using array of techniques. Most of the compounds exhibited promising antibacterial activity, in particular Gram-positive bacteria. The anti-inflammatory assay was evaluated against protein denaturation as well as HRBC membrane stabilization methods and compounds exhibit excellent anti-inflammatory activity in both methods. Molecular docking study has been performed for all the synthesized compounds with *S. aureus* dihydropteroate synthetase (DHPS) and results obtained are quite promising.

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1. Introduction

Coumarin analogues are a group of bioactive molecules, found substantially in nature with a wide range of structural modifications [1]. Coumarins are a privileged oxygen heterocycles widely distributed in various species of plants as well as animals and microbial metabolite, playing an important role in the agricultural and pharmaceutical industries [2]. They exhibit antiviral [3], anti-cancer [4], anti-fungal [5], anti-inflammatory [6], anti-HIV [7] properties. They have been known to be particularly effective against Gram-positive bacterial species [8]. Incorporation of bio-compatible fragments like vanillin and paracetamol onto coumarin nucleus

has resulted 4-aryloxymethyl coumarins which are exhibiting anti-inflammatory activity [9]. Coumarin based anti-biotics viz. novobiocin and clorobiocin affect the functioning of DNA gyrase, which is the basis for their broad spectrum of antibacterial activity [10]. The naturally occurring bromotyrosine derivatives have exhibited anti-microbial effect on the methicillin resistant *S. aureus* (MRSA) [11].

Pyrazolones fused pyran rings compose a very important class of compounds in the heterocyclic area [12], and are extensively used as important precursors in the field of medicinal chemistry due to their potential biological and pharmacological properties such as antimicrobial [13], anti-inflammatory [14], anticancer [15] insecticidal [16], and inhibitors of human Chk1 kinase [17]. Medicinally important pyrano[2,3-c]pyrazole derivatives have been synthesized via two component [18], three component [19], and more

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Synthesis of Naked-eye Detectable Fluorescent 2H-chromen-2-One 2, 6-Dicyanoanilines: Effect of Substituents and pH on Its Luminous Behavior

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Abstract A variety of new coumarin derivatives containing C-4 bridged 2,6-dicyanoanilines (**4a-4d**) were synthesized via multicomponent one pot approach. These novel sensors were characterized by spectral analysis and a series of pH sensing fluorescence studies were performed, the results indicating that the sensors are highly selective and more effective at various pH. The fluorescence colour changes at different pH could be directly detected by naked eyes.

Keywords Coumarins · 2,6-dicyanoanilines · Fluorescence pH sensors · Acceptor-donor-acceptor system

Introduction

In recent years, the design of fluorescent molecular sensors have been flourishing interest in the research and development of pH sensors for monitoring acidity especially in biological [1, 2], material [3, 4], environmental science [5, 6] and other fields, in which the fluorescent pH chemical sensors play a convincing role. The pH values can provide important information about objects and characteristic nature. Numerous

chemical and biochemical analytes (e.g. cations, anions, neutral molecules and gases, etc) can be detected by fluorescence [7]. The success of fluorescent sensors can be explained by the distinct advantages offered by its detection in terms of sensitivity, selectivity, local observation (e.g. by fluorescence imaging spectroscopy) and response time etc. [8]. Several fluorescence pH sensors have been reported in the literature [9] in which the most widely used techniques are the measurements of fluorescence intensity.

In search of a suitable indicator dye for pH sensing, our attention has focused on 2,6-dicyanoaniline derivatives [10]. The luminescence investigation of 2,6-dicyanoanilines continues to be an area of inquisition in view of their Acceptor-Donor-Acceptor (A-D-A) system incorporating one electron donor and two electron acceptors [11]. These are excellent fluorophores with relatively high fluorescent quantum yields, Stokes shifts, flexible and tunable physicochemical properties [12]. The promising relevance of these molecules are artificial photosynthesis [13], materials presenting semiconducting or nonlinear optical properties [14] and molecular electronic devices [15].

Coumarin itself is not fluorescent, but it exhibits intense fluorescence by various functional groups substitution at 6 and 7 positions [16, 17]. Properly substituted derivatives yield intense fluorescence which are widely used in different branches of chemistry, biology, medicine and physics. These derivatives are an important part of fluorescence probes, sensors and switches [18, 19]. The fluorescence of coumarins is widely used as a research tool in polymer science as photoinitiators, fluorescent solar collectors and as reporters of radical reactions [20–22]. Recently, these have been utilized for enantioselective sensing [23]. The fluorescence of coumarin is strongly influenced by substituting the electron-donating or withdrawing groups at some positions or by lengthened π -conjugation [24]. In general, electron-donating substituents

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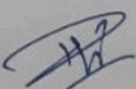
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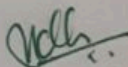
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An efficient and catalyst free methylthiolation of 4-(bromomethyl)-2H-chromen-2-ones with DMSO

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ABSTRACT

The first simple, metal free, and efficient protocol has been established for the methylthiolation of structurally diverse 4-bromomethyl-2H-chromen-2-ones using dimethyl sulfoxide (DMSO) as methylthiolation source at higher temperature. The experimental method is highly economical and provides excellent yields of highly pure products which do not require further purification. All novel 4-[(methylthio)methyl]-2H-chromen-2-ones were characterized by ¹H, ¹³C NMR, and single-crystal X-ray analysis.

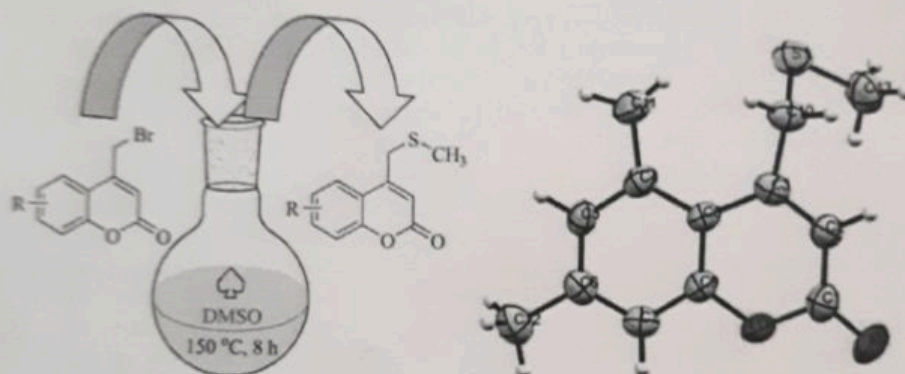
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4-Bromomethyl-2H-chromen-2-one; 4-[(methylthio)methyl]-2H-chromen-2-one; DMSO; methylthiolation

GRAPHICAL ABSTRACT



Introduction

Thioethers are very useful as synthetic intermediates with numerous features in organic and medicinal chemistry mainly involving synthesis of heterocycles which exhibit diverse biological activities.^{1,2} Generally, the synthesis of thioethers involves the condensation of a thiol (disulfide) with a halide in the presence of a base.³ On the other hand, thiols are malodorous, and handling requires more safety precautions. Therefore, the synthesis of thioethers from thiols sometimes is disadvantageous. Thiols are commonly synthesized by the reaction of halides with a source of sulfur, typically sodium hydrosulfide or thiourea derivatives.⁴ Symmetrical benzyl thioethers were achieved using sodium hydrosulfide and benzyl bromide with less satisfactory results.⁵ Moreover, gaining good quality of products with excellent yield is challenging. In the recent development, various methodologies have been used for carbon-sulfur bond formation. For instance, the cross-coupling reaction of thiols

and aryl halides with metal catalyst has been achieved with significant increase in the yield and purity of the compound.⁶

Simple methods for the synthesis of aryl methyl thioethers involve reduction of sulfoxide,⁷ or reaction of aryl halides with dimethyl disulfide.⁸ DMSO has been used as oxidizing agent to convert alkyl/aryl halides to aldehydes.⁹ Recently, DMSO has been used for *ortho*-methylthiolation of 2-arylpyridine and C-H thiolation of heteroarenes.¹⁰ However, the utility is confined to heteroarene substrates. An important progress in this field using CuI as a catalyst and ZnF₂ as a promoter has been reported by Cheng et al.¹¹ The methylthiolation of heteroaryl alkyl halides reported so far involve the use of various metals as catalysts. Hence, here we report a new, simple and efficient methodology for the heteroaryl alkyl methylthiolation of 4-(bromomethyl)-2H-chromen-2-ones (1) to 4-[(methylthio)methyl]-2H-chromen-2-ones (2) using DMSO as the thiomethylation agent.

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A Review of Ochratoxin Contamination Effects and Its Control

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Ramesh Ch. and Santoshkumar Jayagoudar. (2017). A review of ochratoxin contamination effects and its control. International Journal of Agricultural Technology 13(4): 457-468.

Mycotoxins are secondary metabolites produced by spectrum of fungi. Mycotoxin contamination of agricultural commodities is one of the major problem in agricultural trade and food industry, fungal contamination causes a considerable damage to quality and taste of the agricultural commodities. Fungal contamination occurs from field to fork level. In recent years, mycoflora and mycotoxin contamination of agricultural commodities had drawn the attention of the people; by their damage and harmful effects on humans and animals by the consumption of such contaminated food and food materials.

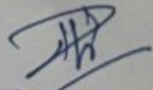
Among mycotoxins, aflatoxin and ochratoxins are the common most mycotoxins; aflatoxins produced by *Aspergillus flavus* and *Aspergillus parasiticus*, Ochratoxins are produced by mainly *Aspergillus ochraceus* and other related *Penicillium* species. Ochratoxins are classified into Ochratoxin-A, B, C among these Ochratoxins, Ochratoxin-A is the most common. OTA is classified as class-2B toxin, Ochratoxin-A contamination was recorded in various agricultural commodities, there are various influencing factors which contribute to the growth and development of the fungi, among those temperature and relative humidity plays very important role, Ochratoxins are having the several health effects on humans and animals. There are several efforts have been made to reduce Ochratoxin contamination in agricultural commodities and food materials. viz. good agricultural and hygienic practices, preservation, storage, transportation etc. leads to reduction in the level of Ochratoxin contamination along with these efforts, several International agencies trying their level are best to reduce OTA contamination in food and agricultural industry.

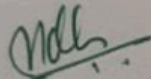
Keywords: Agricultural commodities, Mycoflora, Mycotoxins, Ochratoxins, OTA

Introduction

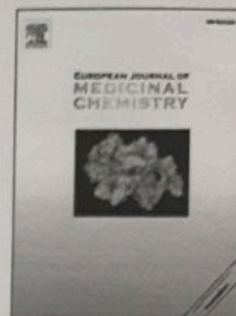
Mycotoxin contamination is common problem in agriculture and food industry. Fungal contamination of food agricultural commodities takes place at various level viz. during harvesting, processing and transportation, levels. When the fungi get suitable atmosphere for the growth and development, they grow and colonize. There are many fungal species which were isolated from various agricultural commodities. A spectrum of mycotoxins were screened by various analytical methods. (Garrido *et al.*, 2013 and Makun *et al.*, 2013). There are reports even OTA screened

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Accepted Manuscript



Green, unexpected synthesis of bis-coumarin derivatives as potent anti-bacterial and anti-inflammatory agents

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Green, unexpected synthesis of bis-coumarin derivatives as potent anti-bacterial and anti-inflammatory agents

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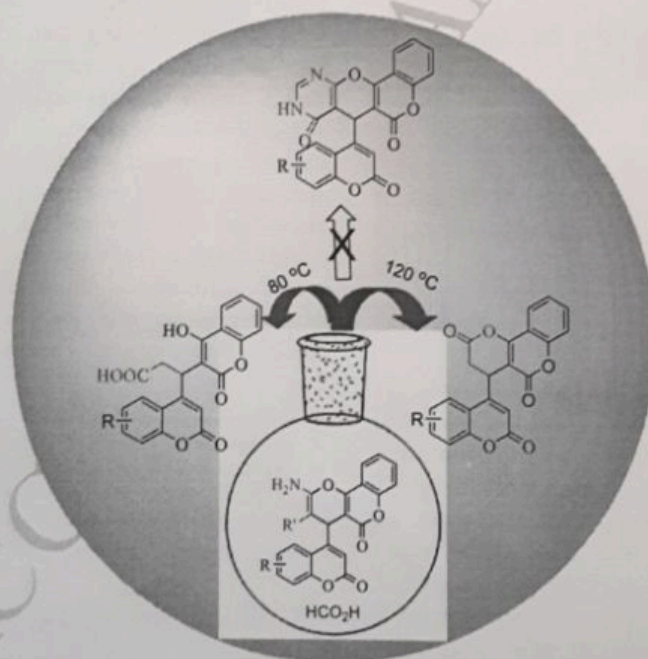
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Design and synthesis of coumarin–imidazole hybrid and phenyl-imidazoloacrylates as potent antimicrobial and antiinflammatory agents

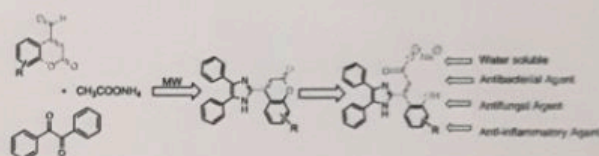
Megharaja Holiyachi¹ · S. Samundeeswari¹ · Bahubali M. Chougala¹ ·
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Abstract An improved one pot, multi-component synthesis of tri- and tetrasubstituted coumarin–imidazole hybrid has been synthesized at C4 position in good to excellent yield. The reaction was performed under various catalysts and optimization condition results obtained are satisfactory. Wherein, trisubstituted coumarin–imidazole hybrid compounds were converted into phenyl-imidazole acrylates. Further, all the newly synthesized compounds were screened for their antimicrobial activity against Gram-positive *Bacillus flexus* and Gram-negative *Pseudomonas* spp. bacterial strains and two strains of fungi studies having *Scopulariopsis* spp. and *Aspergillus terreus* organisms. Similarly, antiinflammatory activity of all the compounds was screened against MMP-2 and MMP-9. Both antimicrobial and antiinflammatory results are excellent, among all compounds, sodium acrylate compounds are quite promising against microbial strains and matrix

metalloproteins (MMPs). All the isolated compounds were characterized by IR, NMR, and mass spectral analysis.

Graphical abstract



Keywords Enzymes · Multi-component reaction · Gelatinase · Histidine · Matrix metalloproteins

Introduction

There are increasing antibiotic resistance properties among pathogens and on the other hand decreasing rate of new novel drug discovery is common drawback in medicine. Thus, multidrug resistance can cause infections as they are no longer response to most of the usual antibiotics [1, 2]. Moreover, imidazole is the integral part of the some naturally occurring molecules and is known for active scaffold in biomolecules, such as histidine, histamine, component of DNA base and Vitamin B₁₂ imidazole derivatives exhibiting broad range of biological activities, such as antimicrobial [3–5], anticancer [6], antiinflammatory [7, 8], and analgesic activities [9].

Coumarin is also one of such natural product which has been isolated from a variety of plant sources to assess their potential therapeutic uses [10]. Coumarin derivatives comprise a vast array of biological activities and have been used in traditional medicine since long time. Thus, the

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Identification of Landslide Susceptible Villages around Kalsubai Region, Western Ghats of Maharashtra using Geospatial Techniques

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ABSTRACT

Heavy rainfall triggered landslides are on the rise along the Western Ghats making it a matter of priority to identify landslide-prone areas well in advance. The present effort is aimed at identifying landslide susceptible villages (LSV) around the Kalsubai region of Deccan volcanic province (DVP), Maharashtra, India from 8 weighted landslide parameters- rainfall, slope, lithology, land use and land cover (LULC), soil properties, relative relief, aspect and lineament. These parameters were combined with advanced remote sensing (RS) data and processed in geographical information system (GIS) as well as in image processing software, which are an integral part of geospatial techniques. Out of the total 59 villages, the study identified 9 villages are situated in very high, 13 in high, 12 in moderate, 11 in low and 14 in very low risk zones. Our data reveals incessant heavy rains and steep slopes are the dominant factors in triggering landslides, exacerbated by anthropogenic activity prevalent in the study area. The spatial and non-spatial database created will help to take effective steps in preventing and/or mitigating landslide disasters in the study area. The methodology can be applied to identify other landslide prone areas in a cost effective way.

INTRODUCTION

Global incidences of landslides are on the rise putting property and life at intense risk that inflicts heavy economic burden on the governments. Landslides manifest through movement that ranges over a wide spectrum, from barely discernible to catastrophic avalanching. This in itself is a reason to initiate landslide susceptibility mapping aimed at identifying potential areas at risk for this menace. In India the Western Ghats, Nilgiris and Himalayas are landslide-prone areas, wherein the Himalayas can experience landslides anytime of the year, while the Western Ghats mostly during the rainy season. These landslides are predominantly controlled by the physiographic and tectonic setting of the region. Landslides also occur because of rising population, which is hard to control; and unplanned settlement, whose relocation is becoming problematic by the day. According to our assessment, the effects can be mitigated by installing warning systems that depend on real time observation of hydrological variables like rainfall severity, intense precipitation that continues for two days or more, ambient temperature and humidity, water holding capacity of soil and other parameters to evaluate landslide triggering mechanism and its impact.

Landslides are commonly occurring natural hazards (Ahmad et al., 2014) damaging property and leading to loss of lives (Gutiérrez et al., 2010). Cruden and Varnes (1996) classified landslides based on types of movement (slide, flow, fall, topple and spread) and types of material (rock, debris, earth), such as rock slide, debris slide, debris flow, earth flow and rock fall. Topple is a rotational forward movement and spread is movement mostly on a flat ground. According to them, landslides can travel over long distances, though their movement can change during the process, which can be expressed as debris slide-debris flow and rock fall-debris flow. The rock and soil flow, or the sludge flow can be triggered by shear failure, when shear stress is equal to or greater than shear resistance on a slope. Consequently, these can be caused by either increase of shear stress, or decrease of shear resistance on the slope. Earthquakes, tectonic movement, volcanic activity, erosion and deposition and anthropogenic activity can cause an increase in shear stress. Decrease in shear resistance can be brought about by pressure exerted by water infiltrating into pores. Such a situation can develop on natural slopes by intense fall of precipitation which can act as catalyst in destabilizing the slopes. Hungr et al. (2001) and Kuriakose et al., (2009) have also defined landslides, whereas International Geotechnical Societies' UNESCO working group on world landslide inventory (WP/WLI), contributed to the definition of international standards in landslide investigation (Brabb, 1991; Dikau et al., 1996). Baum et al. (2002) deciphered shallow landslides, often referred to as mudslides or debris flows, move downhill at speeds of 55 km per hour or more, killing people and destroying infrastructure. Terlien (1998) determined the role of weathering process, considered a conditioning mechanism, which has direct bearing on the occurrence of landslides. Wilson and Wieczorek (1995) feel rainfall to be the main trigger of landslide occurrence, whereas Coe et al. (2004) and Faubri et al. (2003) found topography was the dominant control on occurrences of landslide. Dai and Lee (2002) and Lee and Min (2001) consider slope steepness has a dominant influence on shallow landslide, followed by soil texture and soil types. Other factors such as land cover (Larsen and Torres Sanchez, 1998), elevation (Coe et al., 2004) and lineament occurrences (Aher et al., 2014) can play a significant role in landslide prediction. The losses due to low-magnitude and high-frequency landslides are on the rise because of anthropological interference along hill slopes (Pasuto and Soldati, 1996) killing approximately 61,000 people worldwide from 1900 to 2009 (EM-DAT, 2010). Ho et al. (2012) used spatial distribution of soil thickness to predict shallow landslides. Hong and Adler (2008) proposed a system



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Data article

Green synthesis of coumarin-pyrazolone hybrids: *In vitro* anticancer and anti-inflammatory activities and their computational study on COX-2 enzyme



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ABSTRACT

A series of novel quinoline-2-carboxamides **4(a–l)** were synthesized using different 2-oxo-2H-chromene-4-carbaldehyde and 3-methyl-1H-pyrazole-5(4H)-one with excellent yield under eco-friendly condition. All the compounds were confirmed on the basis of their IR, ¹H NMR, ¹³C NMR and mass analysis. Newly synthesized compounds were screened for their anti-inflammatory by using protein denaturation method and anticancer activities at NCI60. Anti-inflammatory results are found to be promising. Further, molecular docking studies were performed for all the synthesized compounds with the active site of COX-2 enzyme and results obtained are quite promising. Compounds **4e** and **4h** exhibited highest potency and selectivity for COX-2 inhibitory activity.

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Specification table

Subject area	Organic chemistry.
Compound	coumarin-pyrazolone
Data category	Spectral, Biological data.
Data acquisition format	Spectral
Data type	Analysed
Procedure	A series of twelve new coumarin derivatives of pyrazolone are synthesized via condensation of 4-formylcoumarin with 3-methyl pyrazolone without using any catalyst. The targeted compounds were characterized by spectral studies and evaluated for their <i>in vitro</i> biological activity and performed molecular docking study.

1. Rationale

Pyrazolone derivatives have taken a leading position in the medicinal chemistry and are also being used as influential pharmacophores in the field of drug design. The pyrazolone analogous possess promising antimicrobial, anti-inflammatory, analgesic, antipyretic and anticancer activities [1–3].

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Biological Chemistry & Chemical Biology

Synthesis of 2,3-Dihydro Flavone Coumarins as a Class of Potent Antifungal and Anti-inflammatory Agents

Farzanabi Shaikh,^[a] Samundeeswari Shastri,^[a] Bahubali M. Chougala,^[a] Megharaja Holiyachi,^[a] Lokesh A. Shastri,^{*,[a]} Shrinivas D. Joshi,^[b] and Vinay A. Sunagar.^[c]

An efficient, mild and environmentally benign method has been developed for the synthesis of 2,3-dihydroflavonecoumarins. The reaction of 2-hydroxyacetophenones 2 with 4-formylcoumarin 3 using anhydrous potassium carbonate as a mild base. All the synthesized compounds were evaluated for their antifungal activity against *Candida albicans*, *Aspergillus flavus* and *Aspergillus niger* fungal strains by broth dilution method. The tested compounds have exhibited promising *in vitro* potency with low MIC values ranges from 0.4 to 3.12 $\mu\text{g}/$

mL. The *in vitro* anti-inflammatory potency of synthesized compounds by gelatin zymography is comparable to tetracycline and is found to be excellent against Matrix metalloproteinase (MMP-2). Molecular docking study was performed for all the synthesized compounds with binding site of Cytochrome P450 14 alpha-sterol demethylase (CYP51) from *Mycobacterium tuberculosis* in complex with fluconazole PDB (1EA1) and results obtained are quite promising.

Introduction

The prevalence of fungal infections has steadily increased over the past few decades and presents a serious threat to human health, especially in immunocompromised patients, such as those undergoing organ transplants or anticancer chemotherapy and patients with AIDS.^[1,2] *Candida albicans* (*C. albicans*) is the most common fungal pathogen in clinical settings which is responsible for infections that can affect the skin, mucosa and leading to life-threatening systemic disease.^[3] Although, several antifungal agents have recently been introduced to the clinical chemotherapy, the number of available drugs to treat life-threatening fungal infections is still limited and new alternative drugs with improved efficacy are needed.^[4]

Inflammation is due to the reaction of living tissues towards injury and it comprises systemic and local responses.^[5] Inflammation occurs widely in the process of clinical pathology and plays a significant role in the progress of many diseases,^[6] therefore the compounds holding anti-inflammatory effects will be used for the treatment of various inflammation-related diseases. The matrix metalloproteinases (MMPs) are a family of zinc-dependent endopeptidases that can selectively degrade components of the extra cellular matrix.^[7] MMPs play crucial

roles in invasion and metastasis regulating signalling pathways that control cell growth, survival, invasion, inflammation and angiogenesis.^[8] As a part of an effort to design improved antifungal and anti-inflammatory drugs, the biological evaluation of several synthesized novel coumarins has been undertaken.^[9-12]

Coumarin derivatives have numerous therapeutic applications including photochemotherapy, antitumor, anti-HIV,^[13,14] central nervous system (CNS) stimulants,^[15] antibacterials,^[16] anti-inflammatory^[17] and anticoagulants.^[18] Biological activity of coumarins has become an appealing point of studies owing to its different effects to diseases and less damage to normal cells.^[19] Previous studies demonstrated that coumarin chalcone fibrates can down-regulate the total cholesterol (TC), phospholipids (PL) and triglycerides (TG).^[20] Coumarin derivatives containing a substituted formyl group at the position 4 possess antibacterial,^[21] antiinflammatory,^[21] and anticancer activities.^[22] The incorporation of another heterocyclic moiety either as a substituent or as a fused component into coumarin has been more facile if started from 4-formyl coumarin, which alters the properties of the parent material and the resulting compounds exhibit promising biological activities.^[23,24]

Flavanones form a large and essential group of naturally occurring secondary metabolites which are important intermediates for the synthesis of biologically active flavones and isoflavones. Natural and synthetic flavanones have considerable attention because of their interesting biological activities.^[25-28] They also display activities as tyrosinase,^[29] aldose reductase inhibitors^[30] and nonsteroidal inhibitors of human aromatase.^[31] The flavones also serve as important intermediates or precursors in the synthesis of many biologically active natural products.^[32] The major and commonly reported synthetic methods for flavone usually involve the Claisen-Schmidt reaction of *o*-hydroxyacetophenones with benzaldehydes to produce chalcone intermediates using diverse catalysts.^[33,34]

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Tracking Polaron Generation In Electrochemically Doped Polyaniline Thin Films

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Abstract. Electrochemically deposited polyaniline films on ITO substrates have been studied for their optical properties. π - π transitions inducing the formation of polarons and bipolarons have been studied from the optical spectra. The generation of these quasiparticles and the corresponding quantum of energy stored has been analysed and calculated from the experimental data. The evolution of polaron with increased levels of protonation has been identified and the necessary energy required for the transitions have been explained with the help of band structure diagram.

INTRODUCTION

Of late, conducting polymers have been attracting considerable attention because of their exceptional magnetic, electric and optical properties. Charge carrier transport in such polymers akin to those in metals has thus become a subject of keen interest as well as intensive research. Charge carriers formed on doping dominates the electronic properties and the conduction mechanism has been satisfactorily explained in terms of solitons, polarons and bipolarons. While solitons are found to occur in polymers with a degenerate ground state, theoretical and experimental results suggest that polarons and bipolarons are responsible for charge transport in chains with a non-degenerate ground state.

The control over electrical conductivity of (Polyaniline) PANI makes it an interesting material for further research. It varies from 10^{-10} to 10^2 S cm⁻¹ depending on its oxidation or protonation degree, morphology and method of synthesis. The transition from semiconducting through critical to metallic states can be reached for instance by increased doping by various methods like chemical, electrochemical or photoinduced doping. In the present work, thin films of (PANI) have been deposited on ITO substrates by electropolymerisation of acidified Aniline monomer. Here, optical behaviour has been studied in a binary electrolyte and the allowed transition energies for transition of quasiparticles have been calculated. The conjugated molecular structure of PANI enables effective charge transport along chain provided that charge carriers are available. The introduction of the charge carriers into the polymer system is referred to as doping in analogy with inorganic semiconductors, although its nature is different, this term is commonly used in the literature.

Experimental Methods

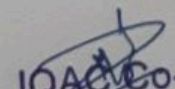
PANI films were potentiostatically deposited on a glass ITO substrate by cyclic voltammetry within a potential window of ± 0.9 V. The deposition solution consisted of 1.5 ml of Aniline in 3ml of HClO₄ dissolved in 50 ml of double distilled water. The solution was stirred well for 5 minutes using a magnetic stirrer. This solution was used as the bath solution for deposition of PANI thin films. The films were studied by measuring the UV-Visible absorption

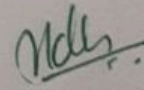
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Core–Shell Novel Composite Metal Nanoparticles for Hydrogenation and Dye Degradation Applications

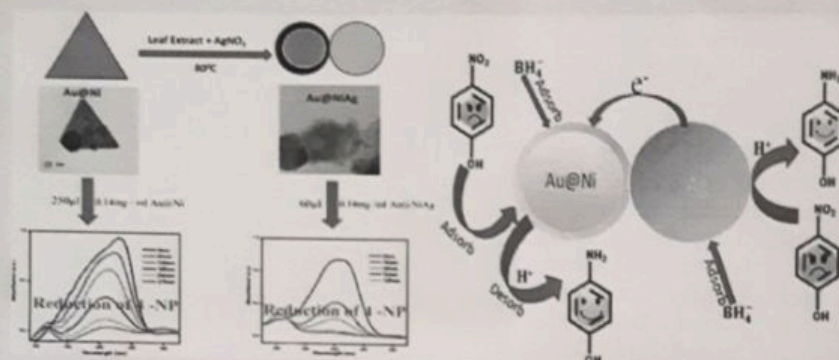
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Supporting Information



ABSTRACT: Biofriendly green sustainable nanocatalyst Au@NiAg with high catalytic activity was prepared for hydrogenation and degradation of aquatic contaminants such as 4-nitrophenol (4-NP), Methyl Orange (MO), and Orange G (OG). Synthesized Au@Ni nanoparticles have a triangular shape while the Au@NiAg nanoparticles are of spherical shape and of smaller size, attributed to the digestive ripening of the Au@Ni where silver ion was deposited on the host Au@Ni nanoparticle surface. The Au@NiAg nanoparticles catalyzed hydrogenation of 4-nitrophenol and reduction of organic dyes follow Langmuir–Hinshelwood kinetics. The Au@NiAg nanoparticles have shown excellent catalytic activity with activity factors of $3167\text{ s}^{-1}\text{ g}^{-1}$, $5476\text{ s}^{-1}\text{ g}^{-1}$, and $3810\text{ s}^{-1}\text{ g}^{-1}$ for 4-NP, MO, and OG, respectively. Silver nanoparticles act as cocatalyst for overall improvement of the performance of Au@NiAg. Above all the involvement of leaf extract mediated synthesis will open up an area to the production of sustainable, ecofriendly and nontoxic core–shell nanocatalysts with exemplary catalytic activity.

1. INTRODUCTION

Today as the population of world increases, the use of harmful chemicals in the textile industry and other industries is now an inevitable commodity which has become a global concern. Due to industrialization industrial wastewater management is a major ecological problem, posing a threat to aquatic life and society at large. Some of the organic pollutants soluble in water are toxic in nature. For instance, compounds such as 4-nitrophenol and organic dyes such as Methyl Orange and Orange G are not biodegradable. 4-Nitrophenol interacting with blood forms methemoglobin, which is responsible for methemoglobinemia, causing cyanosis, confusion, and unconsciousness.¹ Plenty of research work has been happening in recent years to have 4-aminophenol from hydrogenation of 4-nitrophenol by using sodium borohydride as reducing agent with the help of nanocatalysts such as core–shell noble metal nanoparticles which are chemically viable.^{2–5}

Noble metal nanoparticles such as Au and Ag show higher catalytic activity but tend to agglomerate due to their high surface energy, by virtue of which eventually there is a large

reduction in the catalytic performance of the metal nanoparticles. To circumvent this problem, surface functionalization by organic molecules or by other inorganic chemically active metal or metal oxides is necessary, resulting in the formation of noble metal core and shell formation.⁶

The core–shell nanoparticles based on noble metals have gained considerable importance because the knowledge of the core–shell thickness, shape, and size plays a crucial role in catalytic,⁷ surface enhanced Raman spectroscopy (SERS),⁸ and antimicrobial⁹ applications. The metallic core–shell alloy nanoparticles are garnering significant interest from the scientific fraternity because of their unique optical, chemical, and physical properties. Various core–shell nanoparticles have been proposed as catalysts for reaction such as Ni@PtNi nanoparticles supported on reduced graphene oxide (rGO),¹⁰

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Influence of Cadmium Substitution on Structural and Mechanical Properties of Co-Ni Nano Ferrite Synthesized by Co-Precipitation Method

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The objective of this work is to synthesize cadmium doped cobalt nickel ferrite ($\text{Co}_{0.5}\text{Ni}_{0.5}\text{Cd}_{1-2x}\text{Fe}_{2-2x}\text{O}_4$) series with $x = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5$ by co-precipitation method and analysis of structural properties using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM) characterization. The XRD characterization of the samples confirms the cubic spinel structure. Grains in the samples are granular in nature as depicted by SEM images. The FTIR spectra of synthesized ferrites show two strong absorption bands (ν_1 and ν_2) in the range $400\text{--}600\text{ cm}^{-1}$ belonging to tetrahedral (A) and octahedral (B) interstitial sites. Williamson Hall and size-strain plot results show the variation in the grain size with change in doping concentration. Crystallite size D , lattice constant a , micro strain ϵ , x-ray density $\Delta\rho$, dislocation density ρ_D , hopping lengths (L_A and L_B), bond lengths (A–O and B–O), ionic radii (r_A and r_B), texture coefficients $[TC_{(hkl)}]$, and mechanical properties are also reported.

resistively, mechanical hardness, magnetic permeability, chemical stability, low dielectric loss and high Curie temperature. On the other hand, Mn–Zn ferrites with low resistivity and high power losses, have distinctive magnetic properties.^[3]

The ferrite materials are categorized by hexagonal ferrites (Pb, Ba, and Sr ferrites) and spinel ferrites (such as Ni, NiZn, NiZnCu, MnZn, etc.). In recent years, the synthesis process and properties of nano crystalline Ni–Zn-ferrites has been investigated extensively due to their potential applications in non-resonant devices, radiofrequency circuits; high-quality filters, rod antennas, transformer cores, read write heads for high speed digital tapes, and operating devices.^[4–8] Cobalt and nickel ferrites are under extensive research due to their important magnetic properties like, high coercivity, good

1. Introduction

The low eddy current loss is of primary importance for applications related to high-frequencies. Ferrites are particularly good for high-frequency applications because of their high resistivity.^[1] In fact, the ferrites with very high resistivities in bulk state make them useful magnetic material for application at microwave frequencies.^[2] The two series Ni–Zn and Mn–Zn ferrites are widely used in devices such as magnetic heads, converters, inductor cores, high frequency transformers and electromagnetic wave absorbers because they have important properties for these technological applications. Nickel zinc ferrites possess a unique combination of desirable properties such as high electrical

remnant magnetization and moderate saturation magnetization. They also exhibit high electrical resistivity very good chemical and thermal stability.^[9,10] Based on these properties the ferrites are used in many diverse range important application such as magnetic permanent magnets,^[11] magnetic tape,^[12] transformer core,^[13] radiofrequency circuits and high quality filters,^[14] data storage,^[15] high frequency integrated inductors,^[16] controlled drug delivery^[17] catalysis,^[18,19] gas sensors,^[20] and microwave absorbing paints.^[21]

There are several different synthesis methods used to fabricate ferrites as reported in literatures including sol-gel,^[22] coprecipitation,^[23] mechano-chemical,^[24] refluxing,^[25] precursor,^[26] auto-combustion and microwave,^[27] and ultrasonic cavitation^[28] methods.

In spite of enormous studies cadmium substituted $\text{Co}_{0.5}\text{Ni}_{0.5}\text{Fe}_2\text{O}_4$ has been paid less attention. In this work, Cd doped Co–Zn ferrites synthesized by coprecipitation method and structural properties were studied using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM) analysis.

2. Experimental Section

2.1. Materials

All of the starting materials $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$, and $\text{CdCl}_2 \cdot \text{H}_2\text{O}$ were of analytical grade

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Synthesis and Structural Studies of $Zn_{0.95}Cu_{0.05}Mn_2O_4$ Ceramics

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The fabrication of $Zn_{0.95}Cu_{0.05}Mn_2O_4$ ceramic material is obtained by simple chemical route (co-precipitation method) at 600°C. The sample is characterized by X-ray diffraction (XRD) and scanning electron microscope (SEM). The diffraction pattern in comparison with the JCPDS card #96-901-2843, confirms the spinel tetragonal structure with lattice parameters $a = 5.9365 \text{ \AA}$ and $c = 8.6422 \text{ \AA}$, unit cell volume of 304.573 \AA^3 . The other possible parameters like crystallite size, X-ray density, dislocation density, micro strain, and texture co-efficient are reported using XRD analysis. The micro strain and crystallite size are correlated with the respective values got from Williamson–Hall and size-strain analysis method. The SEM image showed the clouds like algae structure with grain size 3.934 \mu m . The effect of copper doping on structure and morphology of zinc manganite is evidenced.

The general formula of spinels is AB_2O_4 , where the valences of A and B can be 2 and 3 as in $ZnMn_2O_4$, where Zn^{2+} is located in tetrahedral sites and Mn^{3+} in octahedral sites. This kind of elemental distribution is known as normal spinel, the corresponding general formula can be written as $A^{tet}B^{oct}_2O_4$. Manganese oxides, zinc oxides, and manganese–zinc oxide spinel have attracted much attention owing to their excellent structural, chemical, and physical properties.^[7–12] As one of the important manganese spinel oxides is nanocrystalline $ZnMn_2O_4$ with general formula AB_2O_4 , have attracted a great attention to their electronic, optoelectronic, mechanical, electrochemical and

1. Introduction

Nanoparticles have been investigated intensively in recent years because of their size-dependent properties. The synthesis of inorganic structures with nanoscale dimensions and morphological specificity is of a great importance and interest in material science and nanotechnology.^[1–5] The high surface to volume ratio of the grains, small size, enhanced contribution from grains and grain boundary regions, quantum confinement of charge carriers, band structure modification, and possibility for defects in grains are some of the factors which contribute to the electrical properties of nano-structured materials.^[6] This difference between nano and bulk materials has immense theoretical and technological importance.

semiconducting properties resulting in the prospective applications owing to the field of sensors, specific memory devices, NTC thermistor, lithium ion batteries as an anode and so on.^[13–18] Doping these materials can be used to induce and improve their properties.

Intention of our work is to prepare copper substituted zinc manganite $Zn_{0.95}Cu_{0.05}Mn_2O_4$ by co-precipitation method and to study their physical properties using X-ray diffraction (XRD) and scanning electron microscope (SEM) characterization. The micro strain and crystallite size are correlated with the respective values got from Williamson–Hall (W–H) and size-strain plot (SSP) method.

2. Experimental Section

The co-precipitation method was used to prepare the sample $Zn_{0.95}Cu_{0.05}Mn_2O_4$. All the chemical reagents used in the experiment were of A.R. grade and used without further purification and treatment. A stoichiometric ratio of zinc chloride, copper chloride, and manganese chloride (0.95:0.05:2) were dissolved in distilled water. The solution was added with ammonia (NH_3) to get a desired pH value and filtered to get precipitate. Then, the paste was left to dry at room temperature overnight and the final dry powder left was powdered uniformly using agate mortar. To get final product, the dry powder was calcinated at 600 °C for 4 h in a muffle furnace, using an alumina crucible. The black powder left is the zinc copper manganite sample. The structural confirmation and different properties of synthesized sample was carried out with XRD using a Bruker AXS D8 Advance instrument ($\lambda = 1.5406 \text{ \AA}$, Detector Si(Li) PSD from STIC, Cochin) and the morphology of the samples was observed using SEM (JEOL

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Al-Doped Co-Cd Nanoferrites by Solution-Combustion Synthesis: Preparation and Structural Characterization

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Abstract—Al-doped Co-Cd ferrites $\text{Co}_{0.4}\text{Cd}_{0.6}\text{Al}_x\text{Fe}_{2-x}\text{O}_4$ ($x = 0.1, 0.2, 0.3, 0.4$) were prepared by solution-combustion synthesis (SCS) and characterized by XRD, SEM, EDAX, and FTIR. A simple cubic spinel structure of synthesized ferrites with $a = 8.496\text{--}8.545 \text{ \AA}$ was confirmed by XRD. The uniform size distribution of ferrite grains was observed in SEM micrographs. The elemental analysis confirmed the presence of all metal ions from the ferrite formula. FTIR spectra showed two absorption bands, ν_1 ($568\text{--}580 \text{ cm}^{-1}$) and ν_2 ($413\text{--}451 \text{ cm}^{-1}$), attributed to Me-O vibration modes at tetrahedral and octahedral sites, respectively. Our results may turn interesting to those engaged in combustion synthesis of ferrites.

Keywords: solution-combustion synthesis, Al-doped Co-Cd ferrites, structural characteristics

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1. INTRODUCTION

Cubic spinel ferrites AB_2O_4 [1] find wide practical applications [2]. Cobalt ferrite CoFe_2O_4 attracts much attention owing to its excellent properties such as relatively high saturation magnetization (M_s), high coercivity (H_c), magnetic anisotropy, chemical stability, and catalytic activity, some of which can also be tuned [3]. Spinel ferrites are good candidates for use in magnetic recording and microwave applications [4], permanent magnets [5], magnetic drug delivery [6], high-density information storage [7], in recording heads, antenna rods, loading coils, microwave devices, and core material for power transformers [8].

Ferrite materials can be prepared by a number of methods such as co-precipitation [9], solid-state reactions [10, 11], citrate gel process [12], solution combustion [13], ball milling [14], and hydrothermal synthesis [15].

In this communication, we report on the influence of Al doping on structural and mechanical properties of crystalline Co-Cd spinel ferrites prepared by solution-combustion synthesis (SCS).

2. EXPERIMENTAL

AR grade starting materials— $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$, $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$, and $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ —were taken in stoichiometric amounts, dissolved in double distilled water, and stirred at 60°C to get uniform solution. A suitable amount of sucrose was added into the mixture. The mixture was then heated until ignition and resultant product was sintered at 800°C [16] for 10 h. The end product was then used to prepare pellets 1 cm in diameter under 10-ton pressure using PVA as binder. These pellets were sintered again at 1000°C for 10 h. The latter ones were characterized by XRD (Bruker AXS D8 diffractometer, Cu $K\alpha$ radiation, JCPDS card 00-022-1086), SEM/EDAX (JEOL Model JSM-6390LV) and FTIR (Thermo Nicolet, Avatar 370).

3. RESULTS AND DISCUSSION

3.1. XRD Analysis

XRD patterns of synthesized ferrites are shown in Fig. 1. The peaks matched well with those from JCPDS card 00-022-1086. The reflections observed from the planes (220), (311), (400), (422), (511), (440) and (533) confirm the formation of a cubic spinel structure.

Determining the Geo-Ecological Parameters For Designing Bhumi Desha Wise Map of Belagavi District

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ABSTRACT:

The specific *Bhumi Desha* attributes specific type of geo-climatic conditions. The predominance of *Dosha* (body humors) of specific *Bhumi Desha* (geologicregions) influences the human beings and is reflected in their *Prakruti* (Health constitutions). Considering this unique contribution, one can inculcate the appropriate preventive and curative measures for an individual depending upon *Doshic* imbalance (disease). The geo-ecological parameters of each *Bhumi Desha* as per present context are not dealt anywhere. Therefore, there is a need of proper identification and mapping of such regions into different types of *Bhumi Desha* based on the Ayurvedic fundamentals so as to develop and implement the appropriate preventive and curative measures for an individual.

It is a cross sectional study consisting of 30 different geographical regions of predominance having particular type of *Bhumi Desha*. A pre-designed and semi-structured research datasheet was prepared that consisted classically explained geo-ecological parameters of different types of *Bhumi Desha*. On the basis of classical parameters of the ideal *Bhumi Desha* as *Jangala Desha* (arid land), *Anupa Desha* (marshy land) and *Sadharana Desha* (intermediate land) were identified by taking up field visit. Geo-ecological parameters like latitude-longitude, temperature, humidity, wind, vegetations, crops soil, rock type, etc., of that particular *Bhumi Desha* were collected, recorded and analyzed to develop the systematic assessment parameters. Later the mapping of such geo-geographic regions into different types of *Bhumi Desha* was prepared using Google earth, a map was prepared.

Synthesis and Property Analysis of Poly-Acryl-Amide (PAM)/Poly-Vinyl-Alcohol (PVA) Blend Thin Films

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Abstract. We present a study of variation in the dielectric properties of polymeric blend films of polyacrylamide (PAM)/Polyvinylalcohol (PVA). Initially, the PAM and PVA were used to obtain apolymeric blend solution in distilled water. Preparation of blended films was conducted by a drying process. Films of pure PAM, pure PVA and blend films (w/w%) were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The characterizations revealed proper trends for the films depending upon weight percent (PAM: PVA: 20:80, 40:60, 60:40, 80:20). Variations in their dielectric property were investigated by use of a LCR (inductor capacitor resistor) meter.

INTRODUCTION

Modern manufacturing industries are in dire need of light weight, non-corrosive and inexpensive materials to increase productivity while reducing the manufacturing cost. One of the most sought-after material for this purpose is the class of polymeric blends due to their ability to form complex shapes, corrosion resistance and lighter weight [1]. Polymer blends have been used in the past few decades for numerous applications like building and construction, automotive parts, electrical and electronics components, medical devices, packaging, power tools, furniture, etc.[2]. These polymer blends are expected to survive not only under strenuous mechanical, chemical, thermal and electrical circumstances imposed by the requirements of a definite application, but also under complex atmospheric environmental conditions.

The properties of a blend are dependent on the method of their preparation and various other factors [3]. Various methods have been used to synthesize polymer blends, such as solution casting(SC), mechanical-melt mixing, latex blending, spray or freeze drying, fine powder mixing, etc. SC is a method for obtaining thin films from a solution of all ingredients in a suitable common solvent followed by drying to eliminate the solvent. It offers pinhole-free and high purity good quality films with uniform thickness and no residues [4].

Blends are physical mixtures of two or more polymers with/without any chemical bonds between them, that yield products with unique properties and lower production cost. Polyacrylamide (PAM) is a commercial polymer used in agriculture, biomedicine,[5] electrical and mechanical field due to its hydrophilicity and inertness[6]. Polyvinyl-alcohol (PVA) is a high crystalline, non-toxic and water-soluble polymer which has good film formation ability. PVA and PAM are two well-known polymers and their individual biomedical, mechanical and other properties have been thoroughly investigated [7] However, PVA suffers due to inability to resist complex loads and unfavorable properties for cell adhesion and growth. The introduction of other polymeric components into the PVA matrix has been shown to improve its electrical and mechanical properties. [8]

Isolation and Characterization of Volatile Oil Constituents From Fruit Peels of Selected Rutaceae Genotypes From India

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Abstract: The essential oil was isolated from the fruit peels of eight Rutaceae genotypes of South India by utilizing the cold pressing method and has been analyzed through GC/MS. Altogether, 28 chemical constituents were detected and grouped into seven categories based on the presence of functional groups. Among all the groups, monoterpene hydrocarbons constituted the most dominant group ranging from 86.96-100 %, followed by sesquiterpene hydrocarbons (0.32-12.27 %), other miscellaneous compounds (12.52 %), oxygenated monoterpenes (0.34-0.79 %), oxygenated sesquiterpenes (0.83 %) and aldehydes (0.46 %), respectively. Limonene was the most abundant compound found in all the samples (51.53-93.52 %), followed by γ -terpinene (19.77 % in CLMB, β -pinene (17.83 % in CLMBI; 17.02 % in CLMS; 14.58 % in CLMM; 13.11 % in CLMB), 5-Ethylidene-1-methylcycloheptene (12.52 % in CLT), sabinene (7.73% in AM) and α -pinene (5.86 % in CLMB). Principal component analysis of all the volatiles detected from the samples discriminated into two main chemotypes (limonene and γ -terpinene/ β -pinene). Further, based on the rich content of limonene, γ -terpinene and β -pinene in the genotypes CS, CLMB and CLMBI, they could be the potential sources for the commercial production of essential oil in the pharmaceutical industries.

Key words: Citrus, essential oil, GC/MS, principal component analysis, volatiles oil.

Introduction

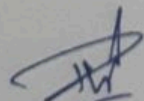
Rutaceae, the large family of angiosperms (order Sapindales), comprises 154 genera and approximately 2100 species ¹. The distribution of this family is nearly cosmopolitan, mainly in tropical and sub-tropical regions. The family is commonly known as the rue or citrus family, which is well known due to its economic importance. India, the home of several citrus species harbors a large

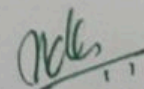
reservoir of diversified varieties and cultivars. It is believed that the citrus species have been originated in the north-eastern part of India and adjacent northern Burma ². The genetic diversity of citrus is mainly concentrated in the north-eastern and north-western parts of India. The South region of the country is not a center of origin of citrus species, but due to a long history of cultivation, enormous variability of citrus found in

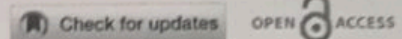
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RESEARCH ARTICLE

Documentation of algae and physico-chemical assessment of paddy field soil of Belagavi, Karnataka

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ABSTRACT

Algae are the diverse group of organisms in the soil and aquatic environment. The role of them in soil fertility enhancement has been extensively studied worldwide. Belagavi is a tropical agricultural belt in the North Karnataka region with highly fertile soil. Water and soil samples were collected randomly from the paddy field of 15-20 well-distributed spots in 4 selected locations viz Kusumali, Jamboti, Kinaye and Piranwadi. The identification revealed the presence of 94 species and 71 genera in the investigated sites. Among all, 62 species belonged to Bacillariophyceae, 14 species to Chlorophyceae, 10 species to Cyanophyceae, 3 to Xanthophyceae, followed by Trebouxiophyceae and Zygnematophyceae (2 species each) and one species of Ulvophyceae. The maximum number of 62 species was recorded from Kusumali, followed by 49 species in Kinaye, 44 in Jamboti and 35 in Piranwadi. The month of February had the highest number of species (61), decreased to 45 in March, 42 in April and 37 in May. Among the physicochemical parameters analysed for the soil samples, it was found that the pH of the soil is slightly acidic in all the study sites ranged between 5.03-5.85. Further, the electrical conductivity (EC) varied from 0.27-0.345 dS/m, found to be in a good range. Estimation of available micro and macronutrients of soil were measured, and it was found to be at low to moderate levels. The present study indicates the extensive distribution of different classes of algae in the rice fields of four study locations in Belagavi.

Introduction

Algae are one of the principal groups of soil microflora in the agricultural fields. It has been found that the growth of algae is directly correlated to the physicochemical properties of soil and water (1). Rice is commonly grown in submerged and water logged environments. The diversified physico-chemical properties of rice field aquatic habitats provide a favorable environment for the growth of various groups of algae (2). These microenvironmental habitats differ physico-chemically and biologically from each other. The heterogeneity of these paddy field ecosystems influences the structure and diversity of microbial communities, and they support a series of microbiological processes (3, 4). Cyanobacteria and diatoms play a key role in agricultural soils as they enhance fertility and they are capable of reducing 30-

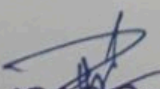
40 % urea and nitrogen requirement to paddy crops (5). The proper application of cyanobacteria and diatoms in the form of biofertilizer is increasing worldwide, due to the fact that most of them are cosmopolitan in distribution, with a wide range of ecological magnitude to inhabit in the diverse environmental conditions (6).

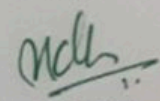
Diatoms are cosmopolitan in distribution with an estimated number of more than 100000 species (7). They are good ecological indicators of environmental conditions of specific habitats. Some of them are highly tolerant to environmental extremities, while others are highly sensitive to stresses such as freezing and heat desiccation (6). They also significantly contribute to carbon sequestration and play a major role in the recycling of silica (8). Further, they induce a fundamental link between primary and secondary production of food chains in aquatic ecosystems (9).

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Application of Remote Sensing and GIS Techniques to Study Sediment Movement along Harwada Beach, Uttar Kannada, West Coast of India

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ABSTRACT

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Beaches, the most dynamic coastal landform on Earth, show dynamic changes over different timescales such as diurnal, tidal, monthly, and seasonal changes. These changes can be constructive or destructive. The long-term studies on beaches help in understanding and planning for any coastal management programs. The present study was undertaken on Harwada Beach located in Karwar of Uttar Kannada district, on the West Coast of India, mainly to understand the morphological changes, sediment movement, and depositional environment through bimonthly beach profiles at five stations. In the present study correlation of the field data along with the remote sensing data (Sentinel 2A multispectral sensor) was carried out to understand the long-term changes. This study shows that the beach has undergone dominant erosion and exhibits cyclic movement of the sediments within the study area. The seasonal and annual study undertaken on Harwada Beach showed that the central part of the study area is most stable during the 4-year observation, while rest of the beach shows erosion.

ADDITIONAL INDEX WORDS: Beach, Morphology, Sentinel 2, DSAS model, Karwar.

INTRODUCTION

The Indian peninsula is blessed with 7352 km of coastline, and the coast here plays an important role in governing the coastal climate. The west coast of India is quite dynamic to morphological changes, especially along the beaches, which is mainly due to longshore sediment transport aided by SW (June–September) and NE (December–January) monsoons, whereas the east coast is highly dynamic owing to contribution from major east flowing rivers giving rise to significant delta formations. In addition, the east coast experiences effects of frequent cyclones modifying the morphology of the coast. Morphological studies have been carried out by many researchers along West Coast of India.


Hanamgond (1993) studied the area between Kwada Bay and Belekeri Bay beaches, situated on the central west coast of India, which include monthly, seasonal, and annual scale morphology and sedimentology including heavy minerals. Hanamgond and Chavadi (1993) carried out morphological studies of Aligadde Beach of Uttar Kannada district and report the cyclic behaviour with circulation of sediments within the beach explaining 12 possible patterns of sediment movement

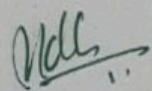
based on morphological data, aided by wind, wave, and longshore currents. Nayak *et al.* (2010) studied the geomorphic processes in the vicinity of Venkatapura estuary, which revealed that the estuary is favourable for the deposition of the sediments in and around the mouth due to interaction of high monsoon waves and river currents, forming spits and bars at the river mouth. Hegde *et al.* (2009) carried out research on the Sharavati River estuary at Honnavar to understand the small-scale morphodynamic processes and inferred that the river mouth adjustments of tropical coasts take place owing to high waves, strong winds, and a large influx of sediment from the river during monsoons. Deepika and Jayappa (2017) studied the morphology of Udupi Beach along Dakshina Kannada district, indicating most of the longshore currents were directed toward the north and the majority of the morphological changes observed were during the SW monsoon and showed cyclic behaviour of the beaches. Hanamgond and Mitra (2007) studied the evolution of Karwar Coast using remote sensing techniques and field data. Their study reports that the entire city of Karwar lies on the sand formed by the growth of spits and beach ridges at the Kali River mouth; their study also indicated several major lineaments (mean vector 224.26°) corroborating with the NE–SW trending lineaments of the west coast of India. Hanamgond and Mitra (2008) carried out similar studies along the Malvan coast, Sindhudurg District of Maharashtra, west coast of India, which indicated

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