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ORIGINAL PAPER

Vibrational spectra analysis, NBO, HOMO–LUMO, and nonlinear optical behavior studies on 3-(3,4-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one

Mahesh Pal Singh Yadav[1] · Anuj Kumar[1] · A. Jayarama[2]

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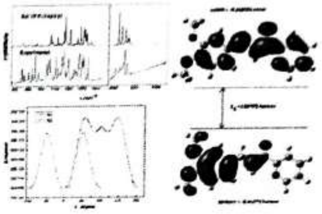
Abstract A combined experimental and theoretical study on molecular structure, vibrational spectra, HOMO–LUMO analysis, and hyperpolarizability of organic non-linear optical crystal 3-(3,4-dimethoxyphenyl)-1-(pyridin-2-yl)prop-2-en-1-one is reported. Vibrational wavenumbers with Raman intensities and infrared absorption intensities have been calculated in the ground state by the density functional theory method using 6-31G(d,p) basis set and Becke's three-parameter hybrid functional (B3LYP). Finally, the calculation results were applied to simulate infrared and Raman spectra of the title compound which showed good agreement with the observed spectra. The assignments of the vibrational spectra have been carried out with the aid of normal coordinate analysis. The natural bond orbital analysis was performed to study the intramolecular bonding, interactions among bonds, and delocalization of unpaired electrons. Electrostatic potential surface and HOMO–LUMO are reported along with global reactivity descriptors. First, hyperpolarizability of the molecule was also calculated and nonlinear behavior of the molecule analyzed using computed data.

Graphical abstract



Keywords Nonlinear optical crystal · Hyperpolarizability · DFT · Natural bond orbital analysis · HOMO–LUMO

Introduction

Chalcones are aromatic ketones that form the central core for a variety of important biological and nonlinear optical (NLO) compounds. Chalcones are abundant in edible plants [1], have relatively low redox potentials and have a greater probability of undergoing electron transfer reactions [2]. These compounds have attracted increasing attention due to numerous pharmacological applications [3–6]. These compounds exhibit good second harmonic generation (SHG) efficiency, excellent blue light transmittance [7, 8], good crystallizability [9–12], better optical limiting behavior with nanosecond laser pulses at 532 nm wavelength [13], and ultrafast optical nonlinearities at 780 nm [14]. Studies on chalcones suggest that the second-order molecular nonlinearity can be enhanced by large delocalized π-electron systems with strong donor and acceptor groups [15]. The basic strategy of using electron

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Third-order NLO property of thienyl chalcone derivative: Physicochemical analysis and crystal structure determination

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ABSTRACT

Good-quality single crystals of an efficient nonlinear optical (NLO) chalcone derivative 1-(5-chlorothiophen-2-yl)-3-(2,3-dichlorophenyl)prop-2-en-1-one (CTDCP) which meets many of the physicochemical requirements like transparency in the entire visible region, thermal stability, mechanical hardness have been achieved. The crystal belongs to orthorhombic system with the centrosymmetric space group Pbca. The third-order NLO properties were investigated using a single beam Z-scan technique with nanosecond laser pulses at 532 nm. The nonlinear refractive index is found to be of the order of 10^{-11} cm^2/W. The magnitude of third-order susceptibility is of the order of 10^{-13} esu. The compound exhibits good optical limiting at 532 nm. The mechanical property of the crystals showed load dependent hardness. The static and frequency dependent molecular hyperpolarizabilities were computed using MOPAC 2012. Thermal study confirms that the crystal is dimensionally stable up to 179°C. The influence of direction of charge transfer on the nonlinearity of the molecule has been discussed in detail.

KEYWORDS
Chalcone derivative; crystal growth; X-ray diffraction; nonlinear optical material

Introduction

The molecular design of novel organic materials exhibiting third-order optical nonlinearity has attracted the attention of vast majority of researchers due to their potential applications in the field of information technology such as optical communication, optical computing, data storage, and optical limiting (OL) [1–2]. Among the organic compounds, chalcone and their derivatives have received significant interest due to the greater and faster response, synthetic flexibility, a strong acceptor-donor intermolecular interaction when properly substituted and a delocalized π electron system which enhances two photon absorption (TPA), facilitating nonlinear optical activity. In addition to this it has lower dielectric constant, high thermal stability, transparency, good crystallizability from cheaper organic solvents, excellent second harmonic generation (SHG) efficiency, promising third-order NLO susceptibility, and OL behavior with nanosecond laser pulse at 532-nm wavelength [3–5]. The microscopic hyperpolarizability (β) of NLO chromophores at molecular level can be improved by enhancing the charge transfer through the molecule by placing a strong electron donor and acceptor

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Structural, thermal, linear and nonlinear optical studies of an organic optical limiter based on reverse saturable absorption

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ABSTRACT

A new derivative of chalcone, 3-(4-bromophenyl)-1-(pyridin-4-yl) prop-2-en-1-one (4BP4AP), crystallizing in centrosymmetric structure has been synthesized using the Claisen–Schmidt condensation reaction method. The FTIR and FT-Raman spectral studies were carried out on 4BP4AP for structural conformation. The single crystals were grown using slow evaporation solution growth technique. The single crystal XRD of the crystal shows that the crystal system of 4BP4AP is triclinic with space group P-1. Scanning electron microscope images enunciate the surface smoothness and the two dimensional growth mechanisms in the crystal. The crystal is transparent in the entire visible region as indicated by the UV-VIS-NIR spectrum. The thermal stability and phase transition of the compound was studied by thermogravimetric and differential scanning calorimetric analysis and found to be stable up to 200 °C. By performing the open aperture z-scan experiment, nonlinear absorption and optical limiting behavior of the crystal were studied. The crystal can be used for optoelectronic application due to its excellent photo-physical properties.

1. Introduction

Currently nonlinear optical (NLO) materials exhibiting strong two photon absorption (TPA) are of great interest due to their wide range of applications. Among the variety of molecular and bulk materials studied for NLO properties, organic materials are of particular importance due to their optical and electronic properties, which are tunable through structural modifications [1]. Organic materials with large third order NLO coefficients are attractive for various photonic applications such as optical communication, signal processing, optical modulation, optical disc data storage, electro-optic modulation, optical switching and optical limiting [2,3]. Chalcone and its derivatives are one of the important classes of optically nonlinear organic materials. These are open chain flavonoids with two aromatic rings joined by a carbonyl group and two α,β-unsaturated carbon atoms [4]. The presence of extensive conjugation in these molecules provides a charge transfer axis. Also one can tune one of the aromatic rings of chalcones as donor and the other as acceptor by incorporating suitable functionalities on the aromatic rings so that the charge transfer takes place from the donor to the acceptor through the charge transfer axis [5,6]. Due to the overlapping of π orbital in these molecules, delocalization of electronic charge distribution increases the mobility of the electron density which in turn enhances the optical nonlinearity [7].

Heterorings such as furan, pyridine and thiophene, due to their lower aromatic stabilization energy than benzene have been reported to provide more effective π-conjugation between donors and acceptors, resulting in larger nonlinearities [8]. Recently our research group has reported a number of pyridine based chalcone molecules with efficient NLO response [9–14]. Among them BPP [14] showed a SHG efficiency of 1.4 times that of urea. In this compound a bromo group is substituted at the para position of phenylene moiety seeing that para substitution is more effective in forming noncentrosymmetric crystal structures [13]. Moreover, BPP is designed by just replacing the benzene ring of 4-bromochalcone (4BC) by the pyridine ring in which a nitrogen atom is placed at the meta position to the carbonyl group and this results in the

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ALUMINUM MMCS REINFORCED WITH HBN - REVIEW

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ABSTRACT

A composite material is a combination of two or more different materials, it gives superior quality than its constituents. Composite materials can be used not only for structural applications but also in various other applications such as automobiles, aerospace, aircraft and marine etc. More recently particle reinforced metal materials are widely used in various engineering industries because of their superior performance and tailor made properties. For replacing existing material we can use a composite material with improved properties in comparison to existing one. In the present scenario, we generally preferred light weight metal mainly for aerospace application. So metal matrix composite (MMCs) act as a revolutionary idea in manufacturing. Various fabrication techniques have been used to know the morphology characteristic and strength of metal matrix composites material. One of the major problems is a uniform distribution of the reinforcing agent in the matrix phase during fabrication of composite material, which directly affects the properties of the composite material. Aluminum metal matrix is widely used due to their good mechanical properties, wear resistance, low thermal coefficient of expansion and better corrosion as compared to other metal. The addition of hexagonal boron nitride (hBN) reinforcement in aluminum present influential properties. In this review, we summarized the effect of boron nitride reinforcement and aluminum-based metal matrix composites with different particle size, weight percentage and various approach for sintering. Different characterization techniques for properties investigation is also studied with remarks.

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A REVIEW ON HUMAN CERVICAL FATIGUE MEASUREMENT TECHNOLOGIES AND DATA ANALYSIS METHODS

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ABSTRACT

Fatigue and its analysis are very important for the overall productivity of any system in which man and machine is participating. High rate of Work Related Muscular Skeleton Disorder (WMSD) among workers simply explain high risk, fatigue and ignorance of ergonomics factors in workplace. The main reason of this negligence is the high cost and non-portability of fatigue assessment devices. Many assessment techniques are available, but Surface Electromyography (sEMG) is much more reliable and the best method to measure and analyze the fatigue in work place. Overhead loads are often observed as primary reason for cervical related disorders among daily wagers. Using small, portable and cheap device for measuring and analyzing SEMG signals for fatigue measurement will help evaluate the risk earlier and possibly avoid permanent and irrecoverable disorder. Such economical devices would mass spread in industries, while ensuring safety of its workers over long term and proliferating industrial production rates. This communication reviews all such available devices, applications while detailing limitations of each. A novel device is proposed which answers most of the current drawbacks.

Key words: WMSD, Fatigue, Ergonomics, Surface Electromyography (sEMG), Cervical muscle.

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Characterizing Radicals

Bipyridinium-bis(carboxylate) Radical Based Materials: X-ray, EPR and Paramagnetic Solid-State NMR Investigations

Oksana Toma,[a] Maxime Leroux,[a] Nicolas Mercier,*[a] Magali Allain,[a] Abdel Hadi Kassiba,[b] Shashi Kumar Kumara Swamy,[b,c] and Jens Dittmer*[b]

Abstract: The zwitterionic 1,1′-bis(4-carboxyphenyl)-4,4′-bipyridinium (bp4pc) has been synthesized and crystals of its hydrated form bp4pc·$2H_2O$ and of its protonated reduced form H-bp4pc have been obtained. Upon heating, bp4pc·$2H_2O$ undergoes partial dehydration, leading to bp4pc·H_2O at 160 °C, together with a color change from yellow (room temperature) to green (140 °C) and finally to brown (160–180 °C). Analysis of bond lengths in the solid state reveals the expected short (d = 1.425 Å) and long (d = 1.485 Å) C–C central bond lengths in the all-radical salt H-bp4pc and bp4pc·$2H_2O$, respectively, whereas the distance of 1.475 Å in bp4pc·H_2O does not allow a conclusion to be drawn regarding the presence of radicals in this compound. EPR and solid-state paramagnetic NMR experiments of H-bp4pc and the hydrated zwitterion bp4pc·$2H_2O$ at different temperatures, however, show that the color change of the latter upon heating is due to the presence of bipyridinium radicals, the concentration of which, although low, increases with increasing temperature. The nature of the electron donor involved in this thermal-induced electron transfer is not fully understood. Most plausible is the possibility that it is the carboxylate group with an intramolecular electron-transfer process; on the other hand it, cannot be excluded that the electron stems from the water molecule, which decomposes into O_2, H^+, and e^- giving H-bp4pc entities.

Introduction

1,1′-Disubstituted 4,4′-bipyridinium dications [also called viologens (V^{2+}), with the most famous being the 1,1′-dimethyl-4,4′-bipyridinium or methylviologen] are a well-known class of redox couples that undergo two reversible, one-electron reductions to a radical cation and the neutral form. Viologens have afforded a great number of charge-transfer (CT) complexes and salts, but the main applications in chemistry of viologens take advantage of the first reversible reduction step involving the two stable V^{2+} and $V^{\cdot+}$ forms; in particular because of the color change during the redox process, which can occur either in solution or in the solid state because of the different absorption domains of V^{2+} (UV) and $V^{\cdot+}$ (visible).[1] The chemistry of $V^{\cdot+}$ radical cations in solution has been well documented, but to a much less extent in the solid state. Notably, crystal structures based on viologen radicals are rare.[2] Whereas the reduction process from V^{2+} to $V^{\cdot+}$ can be achieved either electrochemically or chemically, viologen radical cations can also be generated photochemically as a result of an electron transfer from an electron donor towards bipyridinium cycles.[3] This has led to the development of several families of photochromic materials based on viologens, including zeolite compounds,[4] polycyanopolycadmates chlatrates,[5] halometalate hybrids,[6] and coordination polymers (CP) with carboxylate ligands.[7–10] If the photochromic phenomenon is not completely elucidated; however, it was shown that suitable donor-acceptor intermolecular interactions are necessary to observe the photoinduced electron transfer. On the one hand, good electron donors will lead to direct charge-transfer processes whereas worse electron donors can potentially lead to PICT processes.[1] On the other hand, short contacts between N^+(pyridinium) centers and electron donors (X atoms or molecules) must occur.[3] In addition, it was shown that the process is efficient because the (N^+···X) direction is perpendicular to the pyridinium ring, as exemplified in a series of halometalate hybrids.[6] Other examples can be taken from the growing field of photoactive CP, including carboxylate ligands based on pyridinium or bipyridinium units. For instance, 1,1′-bis(4-carboxybenzyl)-4,4′-bipyridinium in the presence of 1,4-benzenedicarboxylate (BDC^{2-}) and Cd^{2+} afforded a photochromic interpenetrated network CP in which a sandwich-type stacking D···A···D (A = viologen, D = BDC^{2-}) is formed, the photochromic properties being related to the position of one carboxylate O atom, which is approximately perpendicular to the pyridinium ring at the N atom, with an O···N^+ distance of 3.57 Å.[7] In another interesting CP compound, the release of water guest molecules modifies the characteristics of the N^+(pyridinium)···O(carboxylate) contacts, and whereas the dehydrated phase is photochromic due to specific N^+···O interac-

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Synthesis and characterization of polypyrrole grafted chitin

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Abstract

Synthesis and characterization of chitin grafted with polypyrrole (PPy) is reported in this paper. Chitin is soaked in pyrrole solution of various concentrations for different time intervals and polymerized using ammonium peroxy disulphate (APS) as an initiator. Grafting percentage of polypyrrole onto chitin is calculated from weight of chitin before and after grafting. Grafting of polymer is further verified by dissolution studies. The grafted polymer samples are characterized by FTIR, UV-Vis absorption spectrum, XRD, DSC, TGA, AFM, SEM and conductivity studies. © 2017 Elsevier Ltd

Author keywords

Chitin; Conducting polymer; Grafting; Polypyrrole

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Synthesis, growth, structural characterization, Hirshfeld analysis and nonlinear optical studies of a methyl substituted chalcone

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PRINCIPAL
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Abstract

A new chalcone compound (2E)-3-(3-methylphenyl)-1-(4-nitrophenyl)prop-2-en-1-one (3MPNP) with molecular formula $C_{16}H_{13}NO_3$ has been synthesized and crystallized by slow solvent evaporation technique. The Fourier transform infrared, Fourier transform Raman and nuclear magnetic resonance techniques were used for structural characterization. UV–visible absorption studies were carried out to study the transparency of the crystal in the visible region. Differential scanning calorimetry study shows thermal stability of crystals up to temperature 122°C. Single crystal X-ray diffraction and

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Synthesis, spectral characterization, optical and crystal structure studies of (2*E*)-1-(4'-bromobiphenyl-4-yl)-3-(2-methoxyphenyl)prop-2-en-1-one

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Abstract

The title compound, (2*E*)-1-(4'-bromobiphenyl-4-yl)-3-(2-methoxyphenyl) prop-2-en-1-one (BDCP) was synthesized, characterized using UV-Visible, FT-IR, FT-Raman, Mass spectrometry and ^{1}H NMR. In addition, powder XRD and thermal studies of the BDCP was carried out. The optical studies of the compound using SHG method are performed. The crystal has shown good SHG property with SHG conversion efficiency 1.36 times that of Urea.

Keywords: NLO crystal, Optical property, Chalcone, SHG, Hydrogen bond. NMR spectroscopy

1. INTRODUCTION

Nonlinear optical (NLO) materials play a major role in fast developing fields like photonics and optoelectronics [1-2]. The NLO properties like second harmonic generation (SHG) and third harmonic generation (THG) exhibited by many materials have been reported in the literature. Among many materials, organic materials are highly attractive due to their high damage resistance, high nonlinearities and ultra fast response [3-4]. The advantages of using organic molecules as NLO materials are that they can be designed to optimize the desired NLO property by having different donor and acceptor groups in the molecules [5-6]. A number of organic materials have been identified and synthesized, showing considerable NLO effects. However only a few of

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ANALYSIS OF THE BARRIERS FOR IMPLEMENTING GREEN SUPPLY CHAIN MANAGEMENT (GSCM) PRACTICES ON ORGANIC IRRIGATION: AN INTERPRETIVE STRUCTURAL MODELLING (ISM) APPROACH

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ABSTRACT

From the last 5-8 years in academia, industries and irrigationsector, green supply chain management (GSCM) has took up significant consideration and being used for optimization of resourses. Nowadays consumers are attractive toward further ecological surrounding and administrations are creating severer ecological protocols, and farmers are opting to decrease the ecological affect being caused by agriculture. The key purpose stated by this paper is to define the connection between the 10 barriers and recognize also the utmost important barrier amongst the listed 10 barriers. Sorting of barriers has been recognized out based on two powers (driving power and dependence power) using MICMAC analysis. Interpretive Structural Modelling (ISM) method is used for creating a structural model of barriers to implement GSCM in organic irrigation. The nature of the recognized barriers is multifaceted and inter-reliant which demands the request of a structural model like Interpretive Structural Modelling (ISM) method. The research is taken into 3 different parts/level, first identifying the barrier, second defining the barrier and last sorting of

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MICROSTRUCTURE CHARACTERISTICS & MECHANICAL PROPERTIES OF DISSIMILAR TIG WELD BETWEEN STAINLESS STEEL AND MILD STEEL

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ABSTRACT

In this experiments, TIG welding parameters influence on weld-ability of both stainless steel304 and mild steel 1018 specimens with dimension of 150 mm long x 75 mm wide x 3 mm thick is investigated. This paper investigated the microstructure and mechanical properties of dissimilar materials such as SS and MS joints by tungsten inert gas (TIG) welding. Tungsten inert gas welding techniques is wildly used for joining both ferrous and non-ferrous metals. Performance of Tungsten inert gas (TIG) welding on between stainless steel 304 and Mild steel 1018 plate have been studied by optical microscope. The work aims at joining of dissimilar material are stainless steel and mild steel done by TIG welding with the various parameters like voltage, welding speed and gas flow rate. The filler metal grade ER309 employed for joining of these dissimilar metals. Optical Microscopic examination was carried

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SURFACE SEGREGATION OF CHROMIUM CARBIDE IN STAINLESS STEEL AND ITS THERMODYNAMIC STABILITY STUDY BY CYCLIC HEAT TREATMENT

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ABSTRACT

Steels are heat-treated to yield a great range of microstructures and properties. Generally, heat treatment uses phase transformation during heating and cooling to change a microstructure in a solid state. In heat treatment, the processing is most often entirely thermal and modifies only structure. Thermomechanical treatments, which change component shape and structure, and thermochemical treatments which modify surface chemistry and structure, are also important processing approaches which fall into the domain of heat treatment. Present work is the analysis of the mechanical properties and microstructural changes that occur after the cyclic heat treatment of 316L stainless steel. Here during heat treatment of stainless steels chromium carbides will be formed, any type of stainless steels which are heated in the temperature range of 400^{O}C to 800^{O}C will subject to formation of chromium carbides.

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Morphology and miscibility of chitin- polyaniline blend

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In this article, we discuss the blending of chitin with polyaniline (PANI) and its miscibility. Miscibility of the chitin-PANI blend has been studied by solution viscometry, Fourier transform infrared (FTIR) spectrum and scanning electron microscope (SEM) techniques. From viscosity measurement Krigbaum and Wall polymer-polymer interaction parameter (Δb) is calculated; it is found to be positive for all compositions of the blend. From FTIR analysis, probable interaction is predicted. Viscosity measurement of chitin and PANI blends shows a linear relationship between intrinsic viscosity and blend composition with a positive deviation from the theoretical value and positive value of Δb refers to the miscibility of the blend system. From SEM studies, blends having 5% lithium chloride (LiCl) show a homogeneous and continuous structure. Blends having less than 5% LiCl show a homogeneous and fibrillar structure, which is further supported by atomic force microscopy studies. Fibrous structure improves as the amount of PANI increases. FTIR analysis confirms the interaction between chitin and PANI. Further, this result is supported by DSC, TGA, XRD and dissolution studies of the blend.

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Author keywords

Biopolymer; Blending; Chitin; Miscibility; Polyaniline

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Synthesis, single crystal structure and spectroscopic aspects of chalcone 2(2E)-1-(4′-bromobiphenyl-4-yl)-3-(2, 3-dimethoxybenzaldhyde) prop-2-ene-1-one

Vinutha P.R.[a] ✉ , Jayarama A.[b], Kaliprasad C.S.[c], Narayana Y.[c], Byrappa K.[d], Kumar M.S.[e], MR S.K.[f]

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Abstract

The title compound, (2E)-1-(4′-bromobiphenyl-4-yl)-3-(3,4-dichlorophenyl)-3-hydroxypropan-1-one (BDCP) was synthesized, spectrally characterized (IR, UV, FT-IR, ^{1}H NMR, and FT-Raman), and its three-dimensional structure was confirmed by single crystal diffraction studies. In addition, Second Harmonic Generation (SHG) efficiency of the crystal, thermogravimetric analysis (TGA), and powder XRD were performed. The bromo phenyl ring makes a dihedral angle of 50.8 (2)^0 and 34.5 (2)° with the methoxy phenyl ring and central phenyl moiety. The dihedral angle between the methoxy phenyl ring and the central phenyl moiety is 17.1(2)^0. The short contacts C9—O1…Cg1 and C3—H3…Cg3 are

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Synthesis, crystal structure and Hirshfeld surface analysis of a novel chalcone derivative: (2E)-3-(2,3-dimethoxyphenyl)-1-(3-nitrophenyl)prop-2-en-1-one

Prabhu S.R.[a, b], Upadhyaya V.[b] ✉, Jayarama A.[c]

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Abstract

A novel chalcone derivative (2E)-3-(2,3-dimethoxyphenyl)-1-(3-nitrophenyl)prop-2-en-1-one(3DMNP) has been synthesized and crystals have been grown by slow solvent evaporation solution growth technique. The crystals were characterized by FTIR, ^{1}H NMR, DSC, TGA and single crystal X-ray diffraction methods. The crystals are thermally stable up to 143.5 °C. The compound crystalizes in the monoclinic system, in centrosymmetric space group $P2_1/n$ with unit cell parameters a == 8.6125(3) Å b == 12.3005(4) Å c == 14.8416(5) Å α == γ == 90.00° β == 103.97(2)° Z == 4, V == 1525.79(9) Å^3. The C–H...O intermolecular hydrogen bonding interactions stabilizes the crystal structure. Further the Hirshfeld surface analysis facilitates the study of the nature of intermolecular interactions and fingerprint plots provide the information about the percentage contribution from each individual contact. © 2017 Elsevier B.V.

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Sampathkumar Dhanalakshmi, Punyamoorthy Ramadevi and Bennehalli Basavaraju*

A study of the effect of chemical treatments on areca fiber reinforced polypropylene composite properties

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Abstract: Areca fibers have a great prospect in the polymer composite field since they possess superior properties like being light weight, strong and having high strength-to-weight ratio. In addition, areca fibers are biodegradable, non-toxic and eco-friendly and have low maintenance cost. In this research work, areca fibers were subjected to chemical treatments such as NaOH, $KMnO_4$, C_6H_5COCl and $H_2C{=}CHCOOH$ to reduce the hydrophilic nature of areca fibers and to improve interfacial adhesion between areca fibers and thermoplastic polypropylene matrix, so that areca-polypropylene composites with improved properties can be obtained. The untreated and all chemically treated areca-polypropylene composites with 30%, 40%, 50%, 60% and 70% fiber loadings were fabricated by the compression molding technique. Investigations of tensile, flexural and impact properties of areca fiber reinforced polypropylene composites were done under given fiber loadings by following American Standard for Testing Materials (ASTM) standard procedures. Amongst all untreated and chemically treated areca-polypropylene composites, acrylated areca-polypropylene composites with 60% fiber loading showed higher tensile and flexural strength values and with 50% fiber loading showed higher impact strength values. Hence, chemically treated areca-polypropylene composites can be considered as a very promising material for the fabrication of lightweight material industries.

Keywords: areca fibers; chemical treatments; composite properties; polypropylene; SEM image analysis.

1 Introduction

In recent years, interest in the powerful use of biopolymeric materials has expanded significantly. Specifically, the thought of utilizing biopolymer-based materials as one of the components in advanced green composite materials has become more intriguing both in the educated community and in industry. Biologically degradable polymers are referred to as biopolymers and they are sustainable materials which can be produced from renewable resources. Bioplastics can be incinerated without the outflow of lethal deposits that can harm the earth. Biofiber reinforced biopolymer composite materials largely have attractive properties. They are renewable, recyclable (partially or completely), relatively cheap, biodegradable and thus eco-friendly.

In general, the hydrophilic nature of natural fibers and the hydrophobic nature of polymer matrix results in incompatibility between the fibers and matrix and further leads to poor interfacial bonding between the fibers and matrix. This, in turn, causes inferior properties to the natural fiber reinforced polymer composites. This defect can be remedied by chemical modification of natural fibers, as chemical modification will make the natural fibers become less hydrophilic and give strong compatibility between the fibers and matrix. Several studies have shown the influence of various types of chemical treatments on the performance of natural fibers and natural fiber reinforced polymer composites. The different surface modifications of natural fibers, such as mercerization, isocyanate treatment, acrylic acid treatment, latex coating, potassium permanganate treatment, acetylation, silane treatment, benzoyl chloride treatment and peroxide treatment have achieved various levels of success in improving the moisture resistance property of natural fibers, fiber strength, fiber fitness and fiber-matrix adhesion in natural fiber reinforced polymer composites. Further,

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Corrosion Behaviour and Characterisation of Ni–Nb_2O_5 Composites Prepared by Pulse Electrodeposition[1]

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Abstract—The Ni–Nb_2O_5 composites were prepared by pulse electrodeposition method. Operating variables were optimized for getting a good deposit. The quantity of Nb_2O_5 particles in the coating was analyzed by an energy-dispersive X-ray diffraction spectrometer. X-ray diffraction and scanning electron microscopy were used to analyze the structure and surface morphology of the coatings. Texture coefficient and hardness of the deposits were determined and discussed. The corrosion behavior of the coatings was analyzed by traditional weight loss and electrochemical methods. Comparisons of the corrosion behaviour of coatings obtained by direct current (DC) and pulse current (PC) were investigated.

Keywords: Ni–Nb_2O_5 composites, pulse electrodeposition, SEM, EDAX, XRD, electrochemical measurements

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INTRODUCTION

Electrodeposition is a technology for the coating of metals, alloys or composite films, characterized by a unique simplicity of implementation, low capital cost and high versatility. This technique has been in use since the nineteenth century for the deposition of decorative films as well as coatings that impart better corrosion resistance or improved mechanical or wear properties [1–3]. During the last 40 years however, electrodeposition has been applied to various aspects of manufacturing in electronics leading to revolutionary advances. Hence this is one of the methods to produce metal matrix composite coatings, where an insoluble material is suspended in a conventional plating electrolyte bath and which is going to be incorporated in the growing metal matrix [4, 5]. The inserted material can be powder, fiber or an encapsulated particle and its incorporation rate is affected by several parameters such as the electrolyte, concentration of metal ions and particles, pH, applied current density or potential, agitation, organic additives, particle size, etc. These produced composite coatings combine the advantages of metal electroplating with those of composite materials. Now a days the use of second phase particles in their nano size is in more practice because these particles will impart their special properties to the composite coatings like higher corrosion and wear resistance, hardness, super conduction and magnetic properties, semiconductor properties, photo catalytic properties compare to pure metal or alloy coatings and also the insertion of these into the metal matrix is somewhat trouble free compare to the use of micro or macro sized particles in the metal matrix composite and those are known to be the nano composite coatings.

Among the different types of composite coatings like Zn, Ni, Zn–Ni, and Ni–P etc., the Ni nano composite coatings have several special applications in air craft, gas turbines, steam power plants, chemical and petrochemical industries. From the analysis of the recent literatures it can be understood that Ni composite coatings obtained from the DC (direct current) methods will have less particle concentration and in turn will have less applicability towards the wear and corrosion resistance than the Ni composite coatings obtained from the PC (pulse current) methods [6, 7].

In this context a considerable number of literature studies cite the enhanced properties resulting from micrometer, sub micrometer and nano size particles embedded in nickel compared to pure nickel coatings. Qu et al. reported that the use of ultrasonic vibration under PC methods resulted in diminishing agglomeration, but the amount of Al_2O_3 nano-whiskers embedded in composite coatings was also reduced [8]. Wang and others fabricated Ni–ZrO_2 composite nano coatings by PC and revealed that pulse reverse current (PRC) composite nano coatings possess excellent wear resistance properties [9]. PrabhuGanesan and others developed Zn–Ni–Cd coatings by PC and

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[1] The article is published in the original.

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Numerical Investigation of Heat and Mass Transfer in Radiative Magnetohydrodynamic Flow with Chemical Reaction

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Abstract

Numerical investigation is carried out to analyze the heat and mass transfer in magnetohydrodynamic flow over a stretching sheet in the presence of thermal radiation and chemical reaction. The governing equations are transformed as ordinary differential equations using self suitable transformations, further these equations are solved numerically using shooting technique. The influence of pertinent parameters namely, magnetic field parameter, thermal radiation parameter, chemical reaction parameter, thermal and mass Grashof numbers etc., on velocity, temperature and concentration fields are discussed with the assistance of graphs. Numerical results are presented to discuss the behaviour of friction factor along with heat and mass transfer rate. Results shows that thermal radiation parameter have tendency to enhance the thermal boundary layer thickness.

1. Introduction

The hydromagnetic flow and heat exchange over a stretching surface has considered for practical applications in industrial and engineering. For instance streamlined expulsion of plastic sheet, paper creation, glass blowing, metal turning, drawing plastic films, aerodynamic expulsion of plastic sheet, condensation process of metallic plate in a cooling bath and expulsion of a polymer sheet from a colour. The MHD boundary layer flow due to an exponentially stretching sheet in presence of radiation was discussed by Ishak [1]. The MHD flow over a stretching sheet with thermal radiation and thermal conductivity was analyzed by Cortell [2]. The impacts of thermal radiation and chemical reaction on the study of two-dimensional stagnation point flow over a viscous incompressible electrically conducting fluid over a stretching surface with suction in the presence of heat generation was analyzed by Krishna *et al.*, [3]. Mansour *et al.*, [4] explored the impacts of chemical reaction, thermal stratification, Soret number and Dufour number on MHD free convective heat and mass exchange of a thick, incompressible and electrically leading fluid on a vertical stretching surface embedded in a saturated porous medium. Afify [5] explained the MHD free convective flow of viscous incompressible fluid and mass transfer over a stretching sheet with chemical reaction. The heat and mass transfer in thermophoretic radiative hydromagnetic flow over an exponentially stretching surface embedded in porous medium with internal heat generation or absorption, viscous dissemination and infusion impacts was outlined by Sandeep and Sulochana [6]. Raju and Sandeep [7] were concentrated on the influence of induced magnetic field and thermal radiation on nanofluid flow past a stretching surface. The heat transfer qualities of a two dimensional consistent of hydromagnetic characteristic convection flow of a nanofluid over a non linear stretching sheet taking in to an record the effects of radiation and convective boundary conditions has been researched numerically by Rahman and Eltayed [8]. A numerical examination of insecure magnetohydrodynamic blended convective boundary layer flow of a nanofluid over an exponentially stretching sheet in porous medium is displayed by Anwar *et al.*, [9]. The effects of aligned magnetic field, thermal radiation, heat generation or absorption, viscous

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