Received: 23 October 2020 | Revised: 23 December 2020 | Accepted: 27 December 2020

DOI: 10.1002/htj.22058

RESEARCH ARTICLE

HEAT TRANSFER WILEY

Two-dimensional Darcy–Forchheimer flow of a dusty hybrid nanofluid over a stretching sheet with viscous dissipation

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Abstract

The main objective of the present examination is to design a stable mathematical model of a two-phase dusty hybrid nanofluid flow over a stretching sheet with heat transfer in a porous medium, and the Darcy–Forchheimer flow is taken into account with viscous dissipation and melting effect. The equations of motion are reduced to nonlinear ordinary differential equations by considering suitable similarity variables. These dimensionless expressions are solved by a well-known numerical technique known as Runge–Kutta–Fehlberg fourth–fifth order method. The behavioral study and analysis of the velocity and thermal profile in dual phases (fluid phase and dust phase) for diverse values of parameters are estimated using graphs and tables. The result outcome reveals that the velocity gradient declines in the fluid phase and increases in the dust phase for a rise in values of the velocity interaction parameter. Also, the velocity gradients of the both phases diminish for increasing values of the porosity parameter. Furthermore, it is determined that the increase in the value of melting parameter leads to a decline in the thermal gradient of both phases.

KEYWORDS

Darcy–Forchheimer, dusty hybrid nanofluid, melting heat transfer, stretching sheet, viscous dissipation

Received: 12 March 2021 | Accepted: 22 May 2021

DOI: 10.1002/htj.22197

RESEARCH ARTICLE

HEAT TRANSFER WILEY

Significance of thermal radiation on dusty fluid flow over a stretching rotating disk with convective boundary condition

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Abstract

This paper explores the flow of dusty fluid over a stretching rotating disk with thermal radiation. Further, the convective boundary condition is considered in this modeling. The described governing equations are reduced to ordinary differential equations by using apt similarity transformations and then they are numerically solved using Runge–Kutta–Fehlberg-45 scheme. To gain a clear understanding of the current boundary layer flow problem, the graphical results of the velocity and thermal profiles, shear stresses at the disk, and Nusselt number are drawn. Results reveal that the increase in the value of the porosity parameter reduces the velocity of both particle and fluid phases. The increase in the value of the Biot number improves the temperature gradient of both particle and fluid phases. The rise in the value of the radiation parameter advances the heat transference of both phases. The rise in the value of the Biot number improves the rate of heat transfer. Finally, increasing the value of the radiation parameter improves the rate of heat transfer.

KEYWORDS

convective boundary conditions, dusty fluid, stretchable and rotating disk, thermal radiation

INTERNATIONAL JOURNAL FOR COMPUTATIONAL METHODS IN ENGINEERING SCIENCE AND MECHANICS
https://doi.org/10.1080/15502287.2021.1920645

Carbon nanotubes suspended dusty nanofluid flow over stretching porous rotating disk with non-uniform heat source/sink

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ABSTRACT

The current paper explores the flow of dusty nanoliquid over a rotating and stretchable disk with non-uniform heat sink/source. Further, we have done a comparative study on Single wall carbon nanotubes (SWCNT)-water and multi wall carbon nanotubes (MWCNT)-water based dusty fluid flows. By means of apt similarity variables, the governing equations are converted to set of nonlinear ordinary differential equations and then they are numerically tackled using Runge–Kutta–Fehlberg's fourth fifth order (RKF45) method by adopting shooting technique. The influence of non-dimensional parameters on the heat transfer fields are incorporated and extensively discussed by means of appropriate graphs. Further, the reduced shear stresses at the disk in the tangential direction, in the radial direction and the heat transference rates of the fluid and particles are deliberated graphically. Results reveal that, the escalating values of space and temperature dependent heat source/sink parameters improves the heat transference of both liquids. The SWCNT-water based fluid shows improved shear stress in tangential and radial direction when compared to MWCNT-water based fluid for both the phases. The SWCNT-water based fluid shows enhanced heat transfer rate than MWCNT-water based fluid for both fluid and dust phases.

KEYWORDS

Dusty fluid; SWCNT/MWCNT; non-uniform heat source/sink; stretchable and rotating disk; numerical solution

1. Introduction

The investigation on the fluid flows with the suspension of particles has received substantial consideration because of its various applications in several problems related to physiological, atmospheric and engineering fields. Flow of blood in arteries, transport of suspended powdered materials through pipes, propulsion–combustion in rockets and motion of aerosols in the upper atmosphere are some of the renowned examples. In order to solve some complications found in the flow of dusty fluids, many researchers have considered some assumptions. The dust particles are expected to be spherical in shape and are undeformable. The scrutiny of fluids flow with particles suspension would benefit to examine the accumulation and impingement of dust particles close to the walls. Recently, Datta and Mishra [1] examined the boundary layer flow of dusty liquid on a flat geometry. Manjunatha et al. [2] expounded the non-linear heat sink/source impact on dusty liquid flow past a stretchy surface. Turkyilmazoglu [3] delineated the dusty liquid stream past a stretch disk with rotation. Kumar et al. [4] elucidated the non-Fourier heat flux impact on dusty hybrid nanofluid stream past a stretchy surface. Radhika et al. [5] inspected the dusty liquid stream between dual stretchable rotating disks. Mondal et al. [6] expounded the radiation effect on dusty nanoliquid over a permeable stretchy sheet. Reddy et al. [7] elucidated the flow of dusty liquid with nanoparticles suspension above a stretchy surface. Ramzan et al. [8] elucidated the magnetohydrodynamic dusty Casson nanofluid flow with non-linear heat source/sink over a stretching cylinder. Anuar et al. [9] explicated the heat transfer analysis in dusty hybrid nanoliquid flow instigated by a stretchy sheet. Eid and Mabood [10] deliberated the carbon nanotube (CNT) based dusty nanoliquid flow past a surface.

The flow of nanoliquids with the suspension of nanoparticles having pure carbon has gained much attention in the research area. Some of the nanoparticles having pure carbon are the pure chain of carbon particles while others are the combination of carbon

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2021. 2022
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ISSN 1063-7745, Crystallography Reports, 2022, Vol. 67, No. 2, pp. 201–208. © Pleiades Publishing, Inc., 2022.

STRUCTURE OF ORGANIC COMPOUNDS

Dedicated to the Masters N. S. Vedha Karthik, Hassan, and T. S. Ojas Teja, Bangalore

Structural, Computational and 3D Interaction Energy Calculations of the Compound 2-chloro-3-(1-napthyl)-5,5-dimethyl-2-cyclohexenone

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Received November 19, 2020; revised April 29, 2021; accepted May 10, 2021

Abstract—The molecular structure of 2-chloro-3-(1'-napthyl)-5,5-dimethyl-2- cyclohexenone was determined by single crystal X-ray diffraction The compound crystallized in a monoclinic system, space group $P2_1/c$. The Cg1 ring in the molecule was puckered and showed an envelope (^1E) conformation. The crystal packing of molecules, stabilized due to a weak intermolecular C–H···O interaction, is built into an independent infinite one-dimensional polymeric chain along [001] direction. Intermolecular interactions were explored using Hirshfeld surfaces with different mapped properties. The enrichment ratios (E_{XY}) were calculated to understand the crystal packing propensity. In addition, the energy of intermolecular interaction was determined using three-dimensional models of the interaction energy density and wave functions MP2/6-311G(*d*,*p*), DFT/6-31G(*d*) and B3LYP/6-31G(*d*,*p*) of the monomer.

DOI: 10.1134/S1063774522020080

INTRODUCTION

The development of organic compounds with new molecular structures is vital to comply with social demands in the light of various biological activities. Naphthalene is one such important organic compound consisting of a pair of benzene rings. It was obtained from coal tar and was discovered by Alexander Garden in 1819 [1]. Derivatives of naphthalene exhibit the most remarkable clinical activity, including anticancer [2], tubulin inhibitor [3], antidiabetic [4], antipsychotic, anticonvulsant [5], antineurodegenerative [6], antidepressant [7], antitumour [8], antiangiogenic [9], antimicrobial [10]. Rifampicin is an antibiotic and also contains a naphthalene moiety [11]. In the title molecule, the cyclohexenone ring is substituted at the meta-position of the naphthalene ring system. The literature studies show that cyclohexenone is also one of the organic compounds with promising therapeutic effects, such as fungicidal, antimicrobial [12], antibacterial, etc. [13]. A literature review on organic compounds with medicinal values shows that the incorporation of oxygen/nitrogen/sulphur-like nuclei into the ring system enhances the biological potency through proper binding affinity for host candidates [14]. Thus, the presence of two different nuclei, along with the hetero- and halogen-functional

South East Asian J. of Mathematics and Mathematical Sciences
Vol. 17, No. 1 (2021), pp. 233-244

ISSN (Online): 2582-0850
ISSN (Print): 0972-7752

A NOTE ON SIGN BALANCED INDEX SET OF A GRAPH

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(Received: *Dec. 25, 2019* **Accepted:** *Nov. 20, 2020* **Published:** *Apr. 30, 2021*)

Abstract: Let G be a graph with vertex set V and edge set E. Let g be a labeling from E to $\{+,-\}$. The edge labeling g induces a vertex labeling $h : V \to \{+,-\}$ defined by $h(v) = \prod g(uv)$ for u in $N(v)$, where $N(v)$ is the set of vertices adjacent to v. Let $e(+) = card\{e \in E : g(e) = +\}$, $e(-) = card\{e \in E : g(e) = -\}$ and $v(+) = card\{v \in V : h(v) = +\}$, $v(-) = card\{v \in V : h(v) = -\}$. A labeling g is said to be sign friendly if $\mid e(+) - e(-) \mid \leq 1$. The sign balanced index set $(SBIS)$ of a graph G is defined by $\{\mid v(+) - v(-) \mid :$ the edge labeling g is sign friendly$\}$. In this paper we completely determine the sign balanced index sets of some important family of graphs.

Keywords and Phrases: Edge labeling, sign-friendly, sign balance index set.

2020 Mathematics Subject Classification: 05C78.

1. Introduction

A graph labeling is an assignment of integers to the vertices or edges or both, subject to certain conditions. Graph labelings were first introduced in the mid 1960's. Graph labeling was used in many applications like coding theory, x-ray

Malaya Journal of Matematik, Vol. 9, No. 1, 204-207, 2021

https://doi.org/10.26637/MJM0901/0035

On 1-edge balance index set of $C_n \times P_4$, DSC and RC

H . N. Shwetha[1*], B. Shanmukha[2], A.S. Shrikanth[3] and A.R. Nagalakshmi[4]

Abstract

For a simple graph $G = E(G), V(G)$ and $Z_2 = \{0,1\}$. Let f be labeled from E to Z_2,ie $f: E \longrightarrow Z_2$so that the the edge tags are 0 or 1. Edges labeled 1 are known as 1-edges labeled 0 are known as 0-edges. Labeling of the edges f leads to labeling of the vertex $f^* : V \longrightarrow Z_2$ defined by

$$f^*(v) = \begin{cases} 1 & \text{number of 1-edges incident on } v \text{ is odd,} \\ 0 & \text{number of 1-edges incident on } v \text{ is even.} \end{cases}$$

For $i \in Z_2$ let $e_f(i) = e(i) = card\{e \in E : f(e) = i\}$ and $v_f(i) = v(i) = card\{v \in V : f^*(v) = i\}$. if $| e(0) - e(1) | \leq 1$ then a labeling f is said to be edge-friendly. The 1- edge balance index set ($OEBI$) of a graph G is defined by $\{| v_f(0) - v_f(1) | :$ the edge labeling f is edge-friendly$\}$. This paper deals with the existence of the 1-edge balance index sets of $C_n \times P_4$, DSC and RC.

Keywords

Edge-friendly, 1-edge balance index set , Edge labeling.

AMS Subject Classification

05C78.

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Article History: Received 23 October 2020; Accepted 19 January 2021

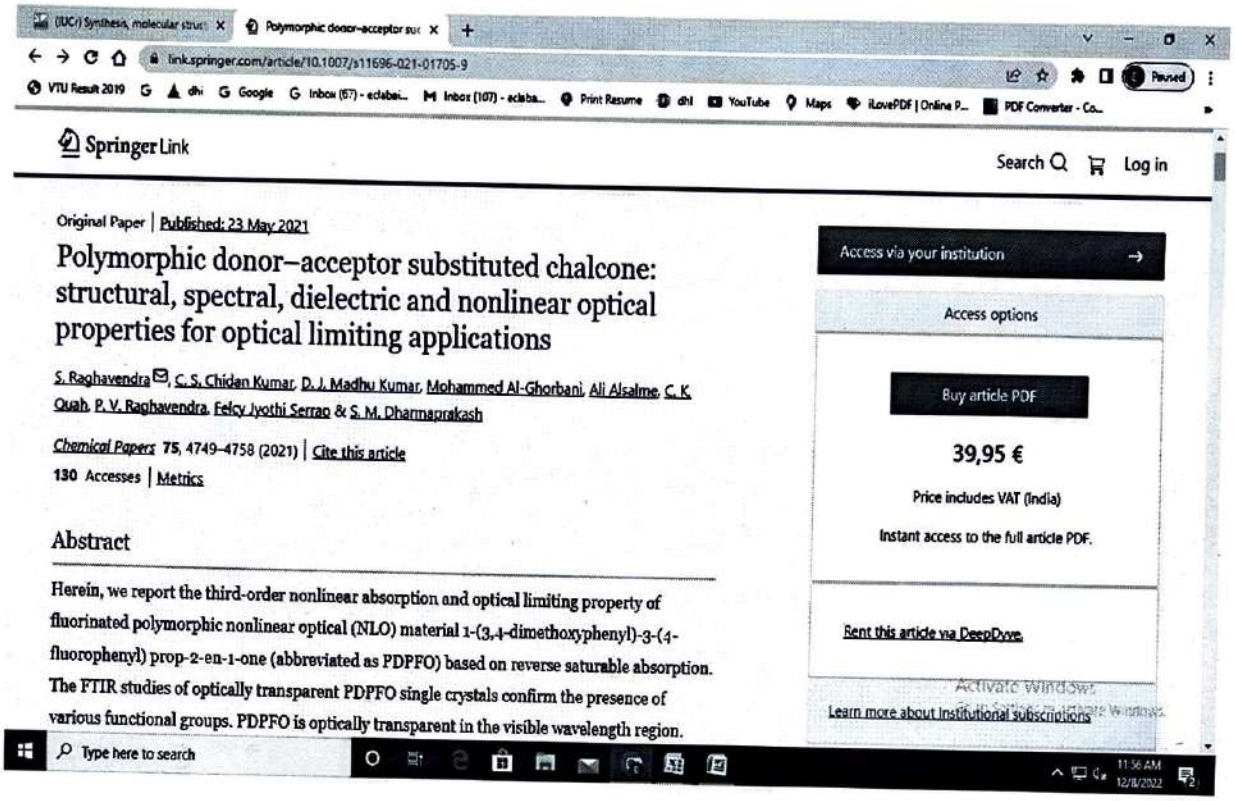
Contents

1. Introduction

A graphical label is an allotment of integers at the vertices or edges or both, subject to certain conditions.Graphical labeling Varieties have been studied by many authors [5, 15] and serve as useful templates for wide range of applications.

Cahit [5] has introduced a cordial labeling as a variation of both graceful and smooth labeling. He [6] proved that every tree is cordial, K_n is cordial if and only if $n \leq 3$, $K_{m,n}$ is cordial for all m and n, the friendship graph $C_3^{(t)}$ is cordial if and only if $t \not\equiv 2(mod 4)$, all fans are cordial. Chartrand, Lee and Zhang [7] introduced the notation of uniform cordiality. They proved that if $n = 3$ and $G = K_3$, or n is even and $G = K_{1,n-1}$ if and only if a connected graph of order $n \leq 2$ is uniformly cordial. Prajapathi and Gujjar [14] provided results about existence of cordial labeling of graphs obtained from paths, cycles, flower graphs, sunflower graphs, flower snarks, lotus inside a circle graph, helms, closed helms, armed helms and webs by the duplication of vertices and edges. Seoud et al. [16] proved that following graphs are cordial: $K_{1,1,m,n}$ when mn is even; $P_m + K_{1,n}$ if n is even or n is odd and $(m \neq 2)$; the conjunction graph $P_4 \wedge C_n$ is cordial if n is even; and the join of the one-point union of two copies of C_n and K_1. Modha and Kanani [13] prove the following graphs are k-cordial: $P_m \times C_k$, $P_m \times C_{k+1}$, $P_m \times C_{k+3}$ for all odd k and $m \geq 2$ and $P_m \times C_{2k-1}$ for all odd k, $m \geq 2$ and $m \neq tk$. Hovey [10] has introduced a k-cordial as simultaneous generalization of harmonious and cordial labeling. He proved that the following graphs are k-cordial: caterpillars for all k, all trees for $k = 3,4,5$, odd cycles with pendent edges attached for all k, cycles for all odd k, for k even, C_{2mk+j} when $0 \leq j \leq \frac{k}{2} + 2$ and when $k < j < 2k$; k_{mk} if and only if $m = 1$ and k_m is 3- cordial.

Lee and Ng [11] introduced a friendly index set and obtained



(IUCr) Synthesis, molecular struc | Polymorphic donor-acceptor su | link.springer.com/article/10.1007/s11696-021-01705-9

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Original Paper | Published: 23 May 2021

Polymorphic donor–acceptor substituted chalcone: structural, spectral, dielectric and nonlinear optical properties for optical limiting applications

S. Raghavendra, C. S. Chidan Kumar, D. J. Madhu Kumar, Mohammed Al-Ghorbani, Ali Alsalme, C. K. Quah, P. V. Raghavendra, Felcy Jyothi Serrao & S. M. Dharmaprakash

Chemical Papers 75, 4749–4758 (2021) | Cite this article

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Abstract

Herein, we report the third-order nonlinear absorption and optical limiting property of fluorinated polymorphic nonlinear optical (NLO) material 1-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl) prop-2-en-1-one (abbreviated as PDPFO) based on reverse saturable absorption. The FTIR studies of optically transparent PDPFO single crystals confirm the presence of various functional groups. PDPFO is optically transparent in the visible wavelength region.

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Contents lists available at ScienceDirect

Heliyon

journal homepage: www.cell.com/heliyon

Research article

Synthesis, structural characterization, and DFT studies of anti-cancer drug *N*-(2-Aminophenyl)-2-(4-bromophenoxy)acetamide

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ARTICLE INFO

Keywords:
XRD
Docking analysis
3D-interaction energies
Hirshfeld surface
DFT

ABSTRACT

Drug design is an integrated and developing system that portends an era of a novel and safe tailored drugs. It involves studying the effects of biologically active synthetic, semi-synthetic, and natural compounds based on molecular interactions in terms of molecular structure with activated functional groups or its unique physico-chemical properties involved. The title compound, *N*-(2-aminophenyl)-2-(4-bromophenoxy) acetamide (**c**), was synthesized in a good yield and characterized by different spectroscopic techniques (FT-IR, ^{1}H/^{13}C-NMR, and LC-MS) and finally, the structure was confirmed by X-ray diffraction (XRD) studies. The XRD data confirms that the crystal structure is orthorhombic with space group of $Pca2_1$. The intermolecular interactions (N–H ... O and N–H ... Cg) inside the molecule stabilizes the crystal structure. The existence of this intermolecular interactions are computed by the Hirshfeld surfaces (HS) and two-dimensional (2D) fingerprints plot analysis. In addition to this, Energy frame work analysis is performed to quantify the interaction energies between the molecular pairs in a crystal by incorporating new version of CrystalExplorer17 using the energy model of HF/3-21G. Also to calculate the HOMO and LUMO energies, DFT calculations were carried out.

1. Introduction

In chemotherapy, an effective drug molecule should be capable of interacting with a target protein in the body to reach the target receptor and achieve the goal of the treatment [1, 2]. Systematically, the medicinal chemist has to observe the exact contributions in which each functional group makes to the relative physical and chemical properties of the molecule to determine how these modifications impact biological actions to design better medicinal agents to meet the growing challenges in finding selective drugs [3, 4, 5]. As a result, growing knowledge and understanding of the nature of diseases and drugs has progressively resulted in the intentional design, synthesis, and evaluation of candidate drug molecules. Matrix metalloproteinase (MMP) are recognized biological objectives involved in tumor progression, innate immunity, homeostatic regulation, destroy pro-apoptotic ligand delivery, and cell-surface receptor release as well as the cleavage [6]. MMPs as inhibitors play significant roles in tumor treatment by promoting the degradation of the extracellular matrix. Therefore, the design and development of effective and specific inhibitor agents that target these enzymes are still highly pursued. Acetamide nucleus and its derivatives are important drugs classes in medicinal chemistry, and many compounds containing benzamide show significant biological activities [7]. Significant attention has also been given to acetamide molecules because of their broad applications as pharmaceutical agents. From both the theoretical and a practical perspective, their great results are highly encouraging to study these compounds in deeply [8]. The natural and synthetic compounds with acetamide nucleus exhibited diverse pharmacological activities such as anti-cancer [9], anti-angiogenic [10], anti-oxidant [11], anti-metastasis [12], anti-inflammatory [13], anti-microbial [14], tranquilizer [15], analgesic, anti-convulsant etc.

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https://doi.org/10.1016/j.heliyon.2021.e06464
Received 19 September 2020; Received in revised form 23 October 2020; Accepted 5 March 2021

Journal of Molecular Structure 1243 (2021) 131492

Contents lists available at ScienceDirect

Journal of Molecular Structure

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

Crystal structure elucidation, experimental and computational optical properties of novel acceptor-donor-acceptor organic material: A suitable candidate for nonlinear applications

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ARTICLE INFO

Article history:
Received 26 April 2021
Revised 27 August 2021
Accepted 12 September 2021
Available online 13 September 2021

Keywords:
Acetohydrazide
Hirshfeld surface
Hydrogen bond
Z- Scan
Semi-empirical
Optical limiting

ABSTRACT

A new organic nonlinear optical (NLO) material, 2-(4-chlorophenoxy)-N'-[(1E)-1-(4-fluorophenyl) ethylidene] acetohydrazide (4CP4FPEA), has been synthesized and single crystals were grown using DMF as solvent. The compound was characterized by ^{1}H NMR and single X-ray diffraction analyses. Analysis of intermolecular interactions was carried out by mapping Hirshfeld surfaces over 2D fingerprint plots, d_{norm} and curvedness using Crystal Explorer. Open aperture Z-Scan experimental curve showed that the 4CP4FPEA molecule exhibits lower transmittance at the focus at 532 nm wavelength. 4CP4FPEA exhibits good optical limiting behavior at the wavelength 532 nm. Estimated excited state absorption cross-section (σ_{ex}) and ground state absorption cross-section (σ_g) are found to be 3.59×10^{-17}cm^2 and 1.9×10^{-21} cm^2 respectively ($\sigma_g <<< \sigma_{ex}$) indicating that nonlinear absorption is due to Reverse Saturable Absorption. Semi-empirical calculations were implemented to calculate static and frequency dependent mean polarizability, first-order hyperpolarizability and second-order hyperpolarizability using time-dependent Hartree–Fock (TDHF) method. We have observed enhancement in nonlinear optical property compared to our previous reported molecule 2-(4-chlorophenoxy)-N'-[(1E)-1-(4-methylphenyl) ethylidene] acetohydrazide (4CP4MPEA).

1. Introduction

The term nonlinear optics describes the nonlinear relationship between dielectric polarization ($\vec{P}$) and electric field ($\vec{E}$) in optical media and it has become a foundation of the emerging field of photonics, where photons are used instead of electrons for signal transmission and processing [1]. Recently, NLO materials have been identified in a variety of applications such as second harmonic generation (SHG), third-harmonic generation (THG), electro-optic switches, frequency shifting, and optical signal processing [2]. Different classes of NLO materials such as organic, inorganic, and semi organic materials have been identified for the development of practical electronic devices but still require further materials development and characterization [3–5]. Overall, these developed materials organic materials are superior to the other materials because of their extraordinary properties like easy manufacture, flexibility for structural modifications and their device applications in optoelectronics [6–8]. The prospective applications of organic materials with third-order NLO property in the field of information technology such as telecommunication, data storage, light emitting devices, optical computing, and optical limiting has created greater interest in their study [9,10]. The optimization of molecular structural properties is very essential to the design of good NLO materials. In recent years, a number of organic materials have been investigated for second and third order NLO applications [11–14]. NLO materials in general exhibits electron acceptor (A) and electron donor (D), connected through π-conjugated bridge which includes A–π–D–π–A, A–π–A, D–π–A, D–π–D and D–π–A–π–D and these structures have a certain push-pull effect on the electrons in the molecule [15,16]. Such a push-pull structure serves as electro and photoactive resources in the device applications such as dye-sensitized solar cells, organic thin film transistors, organic light-emitting diodes [17]. In order to avoid dam-

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https://doi.org/10.1016/j.molstruc.2021.131492
0022-2860/

Physica Scripta

31

PAPER

Investigation on optical switching behaviour of regenerated and non-regenerated silk by nanosecond Z-scan technique

RECEIVED
22 August 2021

REVISED
2 December 2021

ACCEPTED FOR PUBLICATION
9 December 2021

PUBLISHED
20 December 2021

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Keywords: silk, fibroin, z-scan, optical limiting, functional data analysis

Abstract

The nonlinear optical behaviour of silk, a natural fibre, is investigated in this study. We have considered silk in the cocoon, fibre and film forms of bivoltine and multivoltine breeds. The nonlinear absorption and optical limiting studies were performed using the open aperture Z-scan technique at 1064 nm. Interestingly, silk in cocoon and fibre form possess saturable absorption (SA), whereas silk in the film form exhibits reverse saturable absorption (RSA). This shift is attributed to the removal of sericin during the regeneration of silk into a film. Further, silk films exhibit optical limiting behaviour, whose limiting thresholds are in the order of 10^{12} W cm^{-2}. Functional data analysis (FDA), a statistical approach, is employed to draw correlations amongst physical parameters. FDA offers good insight into the dependencies between silk varieties and their optical parameters. This helps in identifying the sample possessing the best properties.

Introduction

Studies on biopolymers such as proteins and fibres are quite an exciting area of research. Several efforts have been made to use proteins as an effective material in bioelectronics and biomedical optics [1, 2]. Interaction between protein systems and laser light is of increased interest in recent times [3]. Silk, a natural protein, is used in textile and biomedical industries due to its remarkable optical and mechanical properties [4]. The primary silk structure consists of Alanine, Glycine and Sericin [Gly−Ala−Gly−Ala−Gly−Ser], the amino acid composition of silk fibres forming the crystalline region. The secondary structure of fibroin is of irregular coil type and antiparallel β-sheet type, which includes the polar side chains for amorphous areas [5]. Silk fibres obtained from the silkworm Bombyx mori offer strong, implantable, and biocompatible base material that can be processed to have excellent optical properties [6].

The studies on nonlinear optically active materials are growing extensively due to their potential applications in photonics. Nonlinear optics gives information about the change in the material's optical parameters when interacting with the laser beam. Change in transmitted laser light in the far-field with the focus of a Gaussian beam through the silk sample is of recent interest in searching for new NLO materials [7]. The study of nonlinear optical absorption, including saturable absorption (SA) and reverse saturable absorption (RSA), is essential for photonic applications [8]. The researcher's investigation revealed that switching between SA to RSA and vice versa is more applicable in a similar field [9]. Both the SA and RSA process depends on the comparative strengths of the ground state and excited state absorption. When the ground state absorption is larger than the excited state absorption, SA can occur, and RSA occurs when the absorption of the excited state is much better than the ground state [10]. The variation of the nonlinear absorption of a solid film is, in general, are highly advantageous in on-chip optoelectrical application [11]. NLO materials have gained incredible attention for

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Thin Solid Films 722 (2021) 138579

Contents lists available at ScienceDirect

Thin Solid Films

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

Dominance of c-axis orientation on the carrier transport properties of Sn doped ZnO thin films

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ARTICLE INFO

Keywords:
Transparent conducting oxide
Sol-gel method
Texture Coefficient
Urbach energy
Optical band gap
Grain boundary barrier

ABSTRACT

Sol-gel derived pure and Tin (Sn) doped ZnO thin films were deposited on the glass substrate by cost-effective spin-coating method. The influence of Sn incorporation on the structural, morphological, optical, and electrical properties of ZnO films was investigated by varying Sn concentration. X-ray diffraction reveals the hexagonal crystal structure with a preferential orientation of the crystallites along c-axis in ZnO film after doping with Sn. The transparency of ZnO thin film in the visible region is increased significantly from 72% to 93% after Sn incorporation into the ZnO matrix. The grain size of the film decreased from 27 nm to 20 nm after doping with Sn. The widening of optical band gap from 3.23 to 3.29 eV i.e., a blue shift of absorption edge with Sn doping is attributed to a combination of the Burstein-Moss effect and electron-impurity scattering. Urbach energy values have shown that Sn dopant decreases the width of the band tail of localized states. The electrical properties of the films revealed the decrement of the conductivity in the doped film. The decrement in the conductivity upon Sn doping is explained considering the grain-boundary conduction model and piezoelectric scattering mechanism. The Figure of Merit was calculated to assess the efficiency of the prepared film and was found that the film Sn: ZnO (3 at.%) shows the highest value. The obtained results confirm that Sn dopant has considerable effects on the properties of ZnO thin films and can be used as promising transparent conducting oxide films for optoelectronic applications.

1. Introduction

The increasing demand for transparent conducting oxide (TCO) thin films for various optoelectronic devices is stimulating the researchers to develop an inexpensive, flexible and stable TCO film with high optical transmittance with low resistivity. TCO thin films have a tremendous interest in the industry and are extensively studied because of their demand for various devices such as solar cells, surface acoustic devices, flat panel displays, gas sensors etc., [1-4]. Majority of the TCO materials exhibiting optical transmittance and electrical conductivity are ternary or binary compounds, containing one or two metallic elements [3]. Further, the wide band gap nature of the TCO materials suppresses the extinction coefficient significantly in the visible region. Among different TCO materials, II-IV semiconductor ZnO and ZnO based compounds are most promising non-toxic and inexpensive TCO materials and are favourable alternatives to high-cost Indium tin oxide (ITO) and SnO_2 films [5]. The wide band gap (~3.3 eV) and the large exciton binding energy (~60 meV) of ZnO are the encouraging entities for the researchers to explore the properties of undoped and doped ZnO thin films which lead to several optical and optoelectronic devices. The intrinsic ZnO further shows n-type conductivity in its intrinsic condition. This unintentional conducting behaviour originates mostly by the native defects induced in ZnO as predicted by different authors [3,6]. Additionally, the conductivity and transparent properties of the films can be effectively tuned with the active involvement of the dopants into the host matrix. Various research studies have explored that the properties of ZnO can be enhanced by adding of appropriate dopants [7-9]. Srinivasulu et al. [10] performed Fe doping into ZnO thin films using a simple spray pyrolysis technique. A transition of preferential crystallites orientation in ZnO films from (002) plane to (101) is noticed upon Fe incorporation into the host matrix. Further, at optimal doping concentration, larger values of transmittance and band gap are also noticed. Along with optoelectronic properties, dopants can also influence other parameters for various applications. For instance, W. Vallejo et al. have

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https://doi.org/10.1016/j.tsf.2021.138529
Received 17 October 2020; Received in revised form 10 February 2021; Accepted 11 February 2021
Available online 16 February 2021

ScienceDirect

Journal of Molecular Structure
Volume 1225, 5 February 2021, 129116

Structural characterization, computational, charge density studies of 2-chloro-3-(2'-methoxy)-5,5-dimethyl-2-cyclohexenone

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https://doi.org/10.1016/j.molstruc.2020.129116

Highlights

- Single crystal X-ray diffraction studies and its analysis.
- Intermolecular interactions are addressed by Hirshfeld surfaces.
- 3D-Interaction energy studies to understand crystal packing.
- Charge density distributions are studied.

Abstract

The title compound ($C_{15}H_{17}ClO_2$), was crystallized in monoclinic system with $P2_{1/c}$ space group. The Cg1 ring in the compound was puckered and displayed a *half-chair* conformation. In the crystalline solid of title compound the molecules are held together through cationic and anionic synthons of the type C-H...O. The qualitative evaluation of these interactions were performed by Hirshfeld and its related fingerprint plots. The propensity of the crystal packing was determined by enrichment ratios. Three dimensional architecture of the crystal packing was stabilized by interaction energies hence, it was carried out by using the accurate

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Journal of Molecular Structure
Volume 1210, 15 June 2020, 127979

Crystal, spectral characterization, molecular docking, Hirshfeld computational studies and 3D-energy framework analysis of a novel puckered compound ($C_{14}H_{15}Cl\ O$): 2-Chloro-3-phenyl-5,5-dimethylcyclohex-2-en-1-one

N.R. Sreenatha [a, b], A.S. Jeevan Chakravarthy [c], B. Suchithra [d, e], B.N. Lakshminarayana [a] ✉, S. Hariprasad [f], D.P. Ganesha [a]

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https://doi.org/10.1016/j.molstruc.2020.127979

Highlights

- The novel compound was synthesized and characterized by FT-IR, GC-Mass, ^{1}H and ^{13}C NMR.
- The single crystal XRD of 2-chloro-3-phenyl-5,5-dimethylcyclohex-2-en-1-one was studied and analyzed.
- Molecular docking studies of the molecule was performed on different proteins, to screen its properties.
- Analysis of intermolecular interactions by Hirshfeld surfaces and its related 2D fingerprint plots are reported.
- Interaction energies between the molecular pairs was studied and analyzed.

(48)

Abstract

Published: 17 September 2020

Electrochemical Detection of Paracetamol by Voltammetry Techniques Using Pure Zirconium Oxide Nanoparticle Based Modified Carbon Paste Electrode

Santhosh Bullapura Matt, S. Raghavendra, Manjunatha Shivanna, Manjappa Sidlinganahalli & Dharmaprakash Mallenahalli Siddalingappa

Journal of Inorganic and Organometallic Polymers and Materials **31**, 511–519 (2021)

Abstract

The central theme of this work is Synthesis of zirconium oxide nanoparticles (ZrO_2NPs) through solution combustion technique as well as their structural and morphological characterization using XRD, SEM and TEM. Electrochemical detection of paracetamol (PA) is described using ZrO_2NPs Modified Carbon Paste Electrode (ZMCPE). From the XRD analysis confirms that the particles are crystalline nature and in tetragonal phase, the average particle size found to be 35 nm. From SEM analysis it is observed that, whatever materials formed is porous in nature and these particles were appears to be uniform. HRTEM discloses that, the

(50)

J. Chem. Sci. (2020)132:70
https://doi.org/10.1007/s12039-020-01764-7

REGULAR ARTICLE

Novel acentric D-π-A-π-D nonlinear optical (2E, 4E)-[dimethylamino) phenyl]-1-(4methylphenyl)penta-2,4-dien-1-one crystal for second and third order nonlinear applications

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MS received 26 September 2018; revised 23 August 2019; accepted 19 December 2019

Abstract. A novel organic crystal namely (2E, 4E)-[dimethylamino) phenyl]-1-(4methylphenyl) penta-2, 4-dien-1-one has been grown successfully from the slow evaporation method. The single-crystal X-ray diffraction study revealed that the compound belongs to the orthorhombic crystallographic system with non-centrosymmetric P_{212121} space group with lattice parameters $\alpha = 7.1354(3)$ Å, $\beta = 11.2112(7)$ Å and 20.0744(11) Å. The thermal properties have been studied by using Thermo Gravimetric (TG) and Differential Scanning calorimetry (DSC). The second harmonic generation (SHG) efficiency of the compound is 2.9 times that of urea for Nd-YAG laser operating at wavelength 1064 nm. We also report the results of thermally induced third-order nonlinear optical (NLO) properties of NLO material investigated by Z-scan technique using continuous wave (CW) laser. The calculated values of $\chi_R^{(3)}$ (esu), $\chi_i^{(3)}$ (esu) and $\chi^{(3)}$ are of the order of 10^{-7}esu, 10^{-8} esu and 10^{-7} esu, respectively. The estimated value of the non-linear refractive index is found to be -4.21×10^{-8} cm^2/W. The compound also exhibits promising optical limiting properties at 532 nm wavelength.

Keywords. Acentric; nonlinear; crystal growth; Z scan; optical limiting.

1. Introduction

In the recent years, non-linear optics plays an important role in the recognition and development of many photon related applications such as optical data storage, optical signal processing, harmonic generators, optical limiting and optical switching, etc.[1–5] The nonlinear optical (NLO) property of organic material is governed by the delocalization of the electrons present in individual molecular chromophores with donor-π-acceptor conjugation and delocalization of these π-electron systems connecting the donor and

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Electronic supplementary material: The online version of this article (https://doi.org/10.1007/s12039-020-01764-7) contains supplementary material, which is available to authorized users.

Published online 29 May 2020

Journal of Molecular Structure 1225 (2021) 129116

Contents lists available at ScienceDirect

Journal of Molecular Structure

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

Structural characterization, computational, charge density studies of 2-chloro-3-(2'-methoxy)-5,5-dimethyl-2-cyclohexenone

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ARTICLE INFO

Article history:
Received 1 June 2020
Revised 14 August 2020
Accepted 18 August 2020
Available online 19 August 2020

Keywords:
Cyclohexenone
Puckering parameters
Hirshfeld & fingerprint graphs
Interaction energies
Charge density analysis

ABSTRACT

The title compound ($C_{15}H_{17}ClO_2$), was crystallized in monoclinic system with $P2_{1/c}$ space group. The C ring in the compound was puckered and displayed a *half-chair* conformation. In the crystalline solid title compound the molecules are held together through cationic and anionic synthons of the type C-H... The qualitative evaluation of these interactions were performed by Hirshfeld and its related fingerpri plots. The propensity of the crystal packing was determined by enrichment ratios. Three dimension architecture of the crystal packing was stabilized by interaction energies hence, it was carried out using the accurate energy density model of B3LYP/6-311G(d,p). The electron density $\rho(r)$ studies was al carried out to describe the nature of chemical bonding between the critical bond points. Laplacian of t electron densities $\nabla^2\rho(r)$ were calculated to identify the points where the charges are appearing to concentrated in the title compound.

1. Introduction

Halogenated compounds are widely used in the manufacture of pharmaceutical products, agrochemicals and fine chemicals. They serve as potent intermediates in organic transformations. In this regard, Suzuki-Miyaura cross coupling reactions have gained immense recognition worldwide, due to the simple reaction conditions, less reaction duration and easily removable by products formed during the reaction. Suzuki-Miyaura cross coupling reactions facilitate the synthesis of a wide range of organic molecules which are otherwise difficult to synthesize. The coupling reaction has gained immense recognition over a short period of time and attributed to the wide applicability of the reaction.

Aryl substituted cyclic compounds belong to an important class of organic compounds, forming precursors for the synthesis of a wide range of natural products [1–8].

Our laboratory, over the past four decades has dealt with the synthesis of some novel unsymmetrical dihalogeanted vicinal cyclic halides, which serve as potent precursors in regioselective, metal catalyzed cross coupling reactions. In this regard, we have been successful in optimizing reactions such as: Buchwald [9]; Suzuk Miyaura-[10]; Heck-; Negeshi-; Sonagashira-; [11] and Wurtz-Fitt cross coupling reactions [12]. In our previous work we had r ported the synthesis of two novel unsymmetrical dihalo- cor pounds by sequential halogenations, using simple reagents a their coupling with boronic acids to obtain novel aryl- substitut chloro-5,5-dimethyl-2-cyclohexenones [13].

Cyclohexenone is one of the popular organic compound, bei a multi dimensional starting material mainly used in the synth sis of different chemical products like pharmaceuticals and fr grances [14]. In the title compound, cyclohexenone bears -hete and -halo functional groups. Hence, the presence of these ator may add relatively more potency towards binding of a molecu to the host candidate. Also, designing of drugs requires some b sic knowledge on the nature of chemical bonding, electrostatic p tentials and crystal structure of the molecule which reveals the a rangement of atoms and packing of molecules in a crystalline sol This is quite essential to relate the structure with its biological a tivity [15]. Presence of intermolecular hydrogen bonding, electr static and short or weak van der Waal's interactions also plays a major role in drug binding at the active site of protein recept [16]. Hence it may be noted that, in the year 1989 Gautham R D siraju also described crystal engineering as "the understanding intermolecular interactions and utilization of such understandi

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https://doi.org/10.1016/j.molstruc.2020.129116
0022-2860/

2018 - 19.

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Journal of Molecular Structure 1194 (2019) 177–184

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: http://www.elsevier.com/locate/molstruc

Nonlinear reverse saturation absorption, self-defocusing behavior and structure-property relationship of a novel 2,3,4-trimethoxy-4'-nitrochalcone single crystal

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ARTICLE INFO

Article history:
Received 3 November 2018
Received in revised form
22 March 2019
Accepted 24 April 2019
Available online 7 May 2019

Keywords:
Crystal growth
Single crystal XRD
Hirshfeld analysis
Z-scan
Optical limiting

ABSTRACT

The present work describes the crystal structure, third-order nonlinear optical (NLO) properties and Hirshfeld Surface (HFs) analysis of 1-(4-nitrophenyl)-3-(2, 3, 4,-trimethoxyphenyl) prop-en-1-one (**2, 3,4TMNC**). The synthesized material was characterised by FT-IR, FT-Raman, UV–Visible, NMR [^{1}H, ^{13}C (^{1}H)] and single crystal X-ray diffraction techniques. TGA-DTA analysis revealed that crystal has higher thermal stability. HFs analysis is performed to visualize intra and intermolecular interactions (C–H···O). The third-order NLO properties were studied using standard open and closed aperture Z-Scan technique with a continuous wave (CW) DPSS laser ($\lambda = 532$ nm). The calculated values of nonlinear refraction coefficient (n_2), third-order nonlinear susceptibility ($\chi^{(3)}$) and nonlinear absorption coefficient (β) were found to be of the order of $\sim 10^{-9}$ cm^2/W, 10^{-7} esu and 10^{-5} cmW^{-1} respectively. Normalized transmittance is decreased with increased input intensity of laser i.e. **2, 3, 4 TMNC** showed good optical limiting property. The optical limiting threshold was found to be 3.36 kJ/cm^2. Thus, the title chalcone derivative is a potential material for optical limiting applications.

1. Introduction

In the field of nonlinear optics, organic materials have gained greater attention because of their importance in optical communication, laser frequency conversion, optical limiting, all-optical switching and optical data storage [1–4]. Nonlinear optical (NLO) materials having strong two-photon absorptions are very much useful due to their tremendous applications [5,6]. In conjugated organic materials (containing alternative single and double bond), the delocalization property of the π electrons makes their distribution highly deformable, which gives rise to enhancement of optical nonlinearities and hence the organic systems shows better NLO response than inorganic counter part [7,8]. Recently, researchers have recognized organic NLO materials containing Nitro group as a most possible candidates for both second and third-order nonlinear applications because of their high NLO coefficients [9,10]. Also Nitro groups are well identified for their good acceptor strength and high melting points which is crucial parameters for NLO device applications [11,12]. Chalcone is the organic material having π conjugated system and due to the overlap of π orbital, delocalization of electrons leads to a high mobility in the electron [13]. One could expect high NLO activity from the donor-acceptor substituted chalcone derivatives due to

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https://doi.org/10.1016/j.molstruc.2019.04.102
0022-2860/

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Proceedings of the Jangjeon Mathematical Society
22 (2019), No. 3. pp. 427 - 436

www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2019.22.3.427

1-EDGE BALANCE INDEX SETS OF $C_n \times P_3$ AND $K_{n,n}$

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Abstract

Let G be a graph with vertex set V, edge set E and $Z_2 = \{0, 1\}$. Let f be a labeling from E to Z_2, so that the labels of the edges are 0 or 1. The edges labelled 1 are called 1-edges and edges labelled 0 are called 0-edges. . The edge labeling f induces a vertex labeling $f^* : V \longrightarrow Z_2$ defined by

$$f^*(v) = \begin{cases} 1 & \text{if the number of 1-edges incident on } v \text{ is odd,} \\ 0 & \text{if the number of 1-edges incident on } v \text{ is even.} \end{cases}$$

For $i \in Z_2$ let $e_f(i) = e(i) = card\{e \in E : f(e) = i\}$ and $v_f(i) = v(i) = card\{v \in V : f^*(v) = i\}$. A labeling f is said to be edge-friendly if $| e(0) - e(1) | \leq 1$. The 1- edge balance index set $(OEBI)$ of a graph G is defined by $\{| v_f(0) - v_f(1) | :$ the edge labeling f is edge-friendly$\}$. The main purpose of this paper is to completely determine the 1-edge balance index sets of $C_n \times P_3$, $K_{n,n}$.

2010 AMS Subject Classification:05C78
Keywords: Edge labeling, Edge-friendly, 1-edge balance index set.

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Three-Dimensional Boundary layer Flow and Heat Transfer of a Fluid Particle Suspension over a Stretching Sheet Embedded in a Porous Medium

https://doi.org/10.1515/nleng-2018-0008
Received January 10, 2018; revised October 20, 2018; accepted December 28, 2018.

Abstract: This article presents the effect of nonlinear thermal radiation on three dimensional flow and heat transfer of fluid particle suspension over a stretching sheet. The combined effects of non-uniform source/sink and convective boundary condition are taken into consideration. The governing partial differential equations are transformed into ordinary differential equations using similarity variables, which are then solved numerically by using Runge Kutta Fehlberg-45 method with shooting technique. The influence of various parameters on velocity and temperature profiles are illustrated graphically, and discussed in detail. The results indicate that the fluid phase velocity is greater than that of the particle phase for various existing parameters.

Keywords: Convective boundary condition; Fluid particle suspension; nonlinear thermal radiation; Stretching sheet; Three dimensional flow

1 Introduction

Heat transfer phenomenon due to suspended particles into the fluid has important role in recent and advanced processes of industrial and engineering problems concerned with powder technology, sedimentation, rain erosion in guided missiles, combustion, atmospheric fallout, fluidization, nuclear reactor cooling, electrostatic precipitation of dust, waste water treatment, acoustics batch settling and so forth. A study on fundamentals of dusty fluid was made by Saffman [1]. Vajravelu and Nayfeh [2] have investigated the hydromagnetic flow of a dusty fluid over a porous stretching sheet. Some more investigations on heat transfer process with fluid particle suspension can be seen in the Refs [3–9]. Al-Rashed et al. [10] report the influence of surface waviness on natural convection boundary layer flow of the two-phase dusty fluid having compressible nature. Recently the effect of thermal stratification on MHD flow and heat transfer of dusty fluid over a vertical stretching sheet embedded in a thermally stratified porous medium in the presence of uniform heat source and thermal radiation has been numerically investigated by Gireesha et al. [11].

Thermal radiation plays an important role in manufacturing industries for the design of nuclear power plants and several engineering applications. Due to its vital applications, numerous researchers have paid their attention to thermal radiation effect [12–17]. Mahanthesh et al. [18] investigated the Marangoni transport of dissipating SWCNT and MWCNT nanofluids under the influence of magnetic force and radiation. Further, it is worth to notice that the linear radiation is valid for small temperature difference. But, for the larger temperature difference nonlinearized Rosseland approximation is to be considered. Hayat et al. [19] initiated the tangent hyperbolic nanofluid flow in the presence of nonlinear thermal radiation. The idea of nonlinear thermal radiation along with heat transfer phenomenon has recently been presented by so many researchers (see [20–23]). Recently, Prasannakumara et al. [24] studied the effect of nonlinear thermal radiation on slip flow and heat transfer of fluid particle suspension with nanoparticles over a nonlinear stretching sheet immersed in a porous medium.

Three dimensional flow has many applications in solar collectors, aeronautical engineering, science and technology, crude oil purification, magnetic material processing, geophysics and controlling of cooling rate, insulation engineering, grain storage devices, ground water pollution, purification process and petroleum reservoirs.

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International Journal of Mathematical Archive-9(5), 2018, 191-202
IJMA Available online through www.ijma.info ISSN 2229 - 5046

MAGNETOHYDRODYNAMIC TWO-PHASE DUSTY FLUID FLOW AND HEAT MODEL OVER RIGA PLATE WITH DEFORMING ISOTHERMAL SURFACES IN THE PRESENCE OF NONLINEAR THERMAL RADIATION

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(Received On: 02-01-18; Revised & Accepted On: 25-04-18)

ABSTRACT

The present work deals with the study of MHD viscous two-phase dusty flow and heat transfer over a Riga plate with permeable stretching body in the presence of non linear thermal radiation. The wall boundary is subjected to a linear deformation as well as to a quadratic surface temperature. Similarity transformations are utilized to reduce the governing partial differential equations into a set of nonlinear ordinary differential equations. The reduced equations were numerically solved using Runge-Kutta-Fehlberg fourth-fifth order method along with shooting technique. The impact of various pertinent parameters for the velocity and temperature fields are profiles are analyzed through graphs in detail. Also, friction factor and Nusselt numbers are discussed and presented through graphs.

Keywords: *Two phase flow; Dusty fluid, Riga plate, Nonlinear thermal radiation, Runge-Kutta-Fehlberg fourth-fifth order method.*

1. INTRODUCTION

The analysis of the flow of fluids with gas–particle mixture or suspended particles has received notable attention due to its practical applications in various problems of atmospheric, engineering, and physiological fields. Typical examples occurring in nature are forest-fire smoke, dust storms and the dispersion of the solid pollutants in atmosphere. In addition, solid rocket exhaust nozzles, blast waves moving over the Earth's surface, fluidization in chemical reactors with gas–solid feeds, fluidized beds, petroleum industry, environmental pollutants, physiological flows, purification of crude oil and other technological fields are some of the practical problems where the dusty viscous flow found its applications. Other important applications involving dust particles in boundary layers include soil salvation by natural winds, lunar surface erosion by the exhaust of a landing vehicle and dust entrainment in a cloud formed during a nuclear explosion. Two-phase particulate suspension flows containing discrete particle phase and the continuous fluid phase have several engineering applications. Study of boundary layer flow and heat transfer in dusty fluid is very constructive in understanding of various industrial and engineering problems concerned with powder technology, nuclear reactor cooling, sedimentation, atmospheric fallout, rain erosion in guided missiles, fluidization, combustion, electrostatic precipitation of dust, acoustics batch settling, aerosol, waste water treatment and paint spraying and etc. Saffman [1] initially formulated the basic equations for the flow of dusty fluid, who derived the motion of gas equations carrying the dust particles. Vajravelu and Nayfeh [2] investigated the hydromagnetic flow of a dusty fluid over a porous stretching sheet. Since then many researchers have discussed and observed the phenomena of the mass and heat transfer of dusty fluid flow between parallel plate and over a stretching surface under different thermal conditions. Gireesha *et al.* [3] described the boundary layer flow and heat transfer analysis of dusty fluid past a stretching sheet in the presence of non-uniform heat source/sink. Manjunatha *et al.* [4] numerically investigated the steady two dimensional flow and heat transfer analysis of dusty fluid towards a stretching cylinder embedded in a porous media under the influence of non-uniform source/sink. Prasannakumara *et al.* [5] analyzed the effect of thermal radiation, nonuniform heat source/sink on the flow of two-dimensional incompressible viscous dusty fluid over a

*Corresponding Author: Jayaprakash M.C**

Outline

Cited By (18)

Figures (16)

ELSEVIER
Optical Materials
Volume 86, December 2018, Pages 138-147

Crystal structure, Hirshfeld and third-order nonlinear optical properties of 3-(4-dimethylamino)phenyl)-1-(4-methoxyphenyl)prop-2-en-1-one: A potential material for optical limiting applications

T. Chandra Shekhara Shetty [a], S. Raghavendra [b], C.S. Chidan Kumar [c], S. Naveen [d], Shivaraj R. Maidur [e], Parutagouda Shankaragouda Patil [e], Siddegowda Chandraju [f], G.S. Ananthnag [g], S.M. Dharmaprakash [h]

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https://doi.org/10.1016/j.optmat.2018.10.007

CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure and Hirshfeld surface analysis of (*E*)-1-(3,5-dichloro-2-hydroxyphenyl)-3-(5-methylfuran-2-yl)prop-2-en-1-one

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Received 21 August 2018
Accepted 28 August 2018

Edited by P. McArdle, National University of Ireland, Ireland

Keywords: crystal structure; chalcones; furan; hydrogen bonding; Hirshfeld surfaces; fingerprint plots.

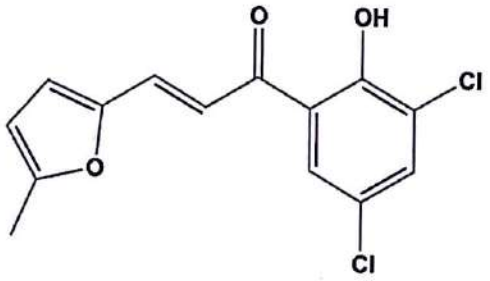
CCDC reference: 1852049

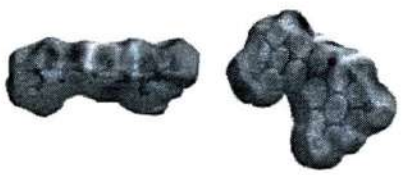
Supporting information: this article has supporting information at journals.iucr.org/e

The title chalcone derivative, $C_{14}H_{10}Cl_2O_3$, is almost planar, with a dihedral angle of 7.0 (2) ° between the 3,5-dichloro-2-hydroxyphenyl and 5-methylfuran rings. There is an intramolecular O—H···O hydrogen bond present forming an $S(6)$ ring motif. In the crystal, molecules are linked by bifurcated C—H/H···O hydrogen bonds, enclosing an $R_1^2(6)$ ring motif, forming a 2_1 helix propagating along the *b*-axis direction. The intermolecular interactions were quantified using Hirshfeld surface analysis.

1. Chemical context

Chalcone derivatives are an important class of organic compounds comprising two aromatic rings connected *via* an α,β unsaturated carbonyl system. They belong to the flavonoid family, which are basically found in fruits and vegetables (Hijova 2006). Chalcones occupy an important place in the pharmaceutical industry since their derivatives serve as the core structures for many organic compounds possessing various biological activities such as antibacterial (Vibhute & Baseer, 2003), anti-microbial (Prasad *et al.*, 2006), anti-inflammatory (Lee *et al.*, 2006), anti-hyperglycemic (Satyanarayana *et al.*, 2004), anti-malarial (Syahri *et al.*, 2017) and anti-oxidant (Cheng *et al.*, 2008). Chalcones also exhibit some non-linear optical (NLO) properties and also find applications in laser technologies such as optical communications, data storage and signal processing because of the α,β unsaturated functionality (Shobha *et al.*, 2017). Based on the above importance, we report here the crystal structure of (*E*)-1-(3,5-dichloro-2-hydroxyphenyl)-3-(5-methylfuran-2-yl)prop-2-en-1-one.





2. Structural commentary

The title molecule comprises 5-methylfuran and 3,5-dichloro-2-hydroxyphenyl rings connected *via* an unsaturated α,β carbonyl system as shown in Fig. 1. The molecule is relatively

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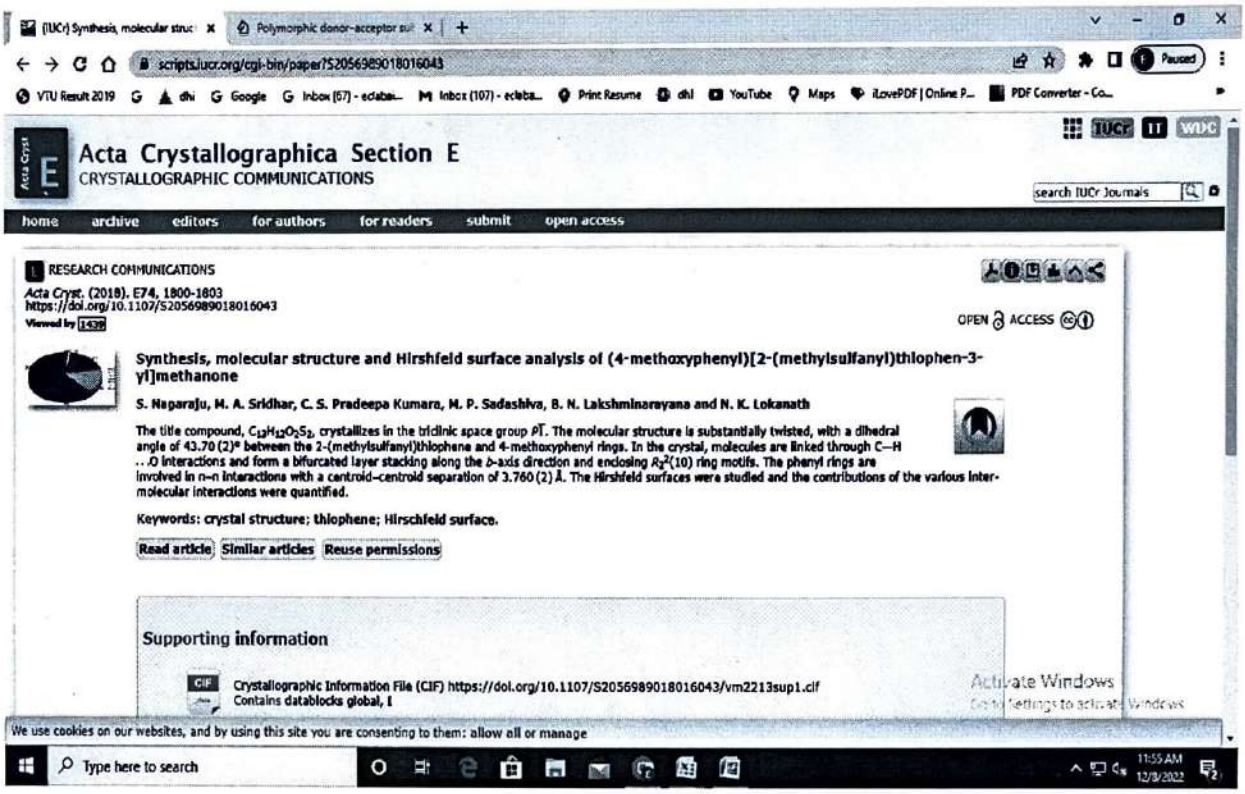

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RESEARCH COMMUNICATIONS

Acta Cryst. (2018). E74, 1800-1803
https://doi.org/10.1107/S2056989018016043

Viewed by 1439

OPEN ACCESS

Synthesis, molecular structure and Hirshfeld surface analysis of (4-methoxyphenyl)[2-(methylsulfanyl)thiophen-3-yl]methanone

S. Naparaju, H. A. Sridhar, C. S. Pradeepa Kumara, M. P. Sadashiva, B. N. Lakshminarayana and N. K. Lokanath

The title compound, $C_{13}H_{12}O_2S_2$, crystallizes in the triclinic space group $P\overline{1}$. The molecular structure is substantially twisted, with a dihedral angle of 43.70 (2)° between the 2-(methylsulfanyl)thiophene and 4-methoxyphenyl rings. In the crystal, molecules are linked through C—H . . .O interactions and form a bifurcated layer stacking along the *b*-axis direction and enclosing $R_2^2(10)$ ring motifs. The phenyl rings are involved in π–π interactions with a centroid–centroid separation of 3.760 (2) Å. The Hirshfeld surfaces were studied and the contributions of the various intermolecular interactions were quantified.

Keywords: crystal structure; thiophene; Hirschfeld surface.

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Data Article

Structural and Hirshfeld surfaces of thiophene based isoxazole derivatives: 3-(3-Methylthiophen-2-yl)-5-(3,4,5-trimethoxyphenyl)isoxazole and 5-(3-Methylthiophen-2-yl)-3-(3,4,5-trimethoxyphenyl)isoxazole

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ARTICLE INFO

Article history:
Received 5 October 2018
Revised 24 October 2018
Accepted 30 October 2018
Available online 1 November 2018

Keywords:
Crystal structure
Isoxazole
Thiophene
Hirshfeld surfaces
Electrostatic potentials

ABSTRACT

The title compounds $C_{17}H_{17}NO_4S$ (I) and $C_{17}H_{17}NO_4S$(II) crystallized in the mono tem with the space group of $P2_{1/c}$. The dihedral angles of 8.88(2)° and 10.5 observed between their terminal rings for I and II, respectively. Intramolecular bonds form a pair of S(6) ring motifs in (I) and three S(6) ring motifs in (II). T structure is stabilized by short intermolecular hydrogen bonds generating ring the type $R_2^2(12)$ (I) and $R_1^2(5)$ (II). Overall packing form a 3D supramolecular n (I) and layer stacking along *b* axis in (II). The intermolecular interactions and centage of contributions were quantified for both the compounds using Hirshfeld

Specifications Table

Subject area	*Crystallography*
Compounds	*3-(3-Methylthiophen-2-yl)-5-(3,4,5-trimethoxyphenyl)isoxazole 5-(3-Methylthiophen-2-yl)-3-(3,4,5-trimethoxyphenyl)is*
Data category	*Crystallography*
Data acquisition format	*Single crystal X-ray diffraction method*
Data type	*Process and analysis*
Procedure	*The title compound was characterized by spectral studies, single crystal X-ray diffraction, Hirshfeld surfaces studies.*
Data accessibility	*CCDC-969823*
	CCDC-1576454

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https://doi.org/10.1016/j.cdc.2018.10.011

Available online at www.joac.info

ISSN: 2278-1862

Journal of Applicable Chemistry

2018, 7 (4): 1056-1062

(International Peer Reviewed Journal)

Crystal Structure, Molecular Docking, Hirshfeld Surfaces and Computational Studies of (2-((1H-Benzo[D]Imidazol-2-Yl) Methoxy)-5-Chlorophenyl)(4-Chlorophenyl)Methanone

B.N. Lakshminarayana[1]*, N.R. Sreenatha[2], B.K. Manuprasad[3], T.N. Mahadeva Prasad[4] and G.B. Thippeswamy[5]

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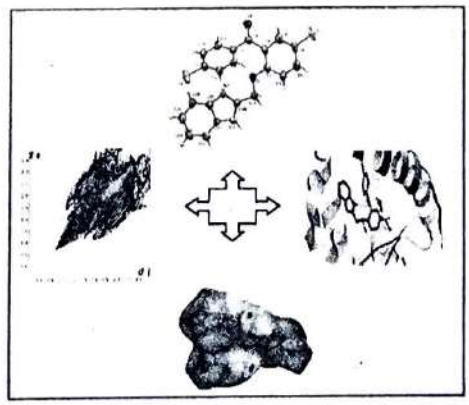
Accepted on 8th July, 2018

ABSTRACT

The title compound was synthesized and characterized by single crystal X-ray diffraction studies, molecular docking and Hirshfeld surface analysis. The title compound $C_{21}H_{14}N_2O_2Cl_2$ crystallizes in the monoclinic system with the space group of $P2_1/c$ with cell parameters a=13.5920(8)Å, b=7.4310(5)Å, c=19.6210(1)Å, β=114.554(6)°, V=1802.6(2)Å^3 and Z=4. The structure exhibited intermolecular interaction of the type C-H...O, molecular docking analysis of the title compound is executed with anti-cancerous target with hER-α protein shown high binding affinity. In addition to this Hirshfeld surface computational analysis were carried out. The major inter-contacts contributing to the Hirshfeld surface are H...H, H...Cl, H...C and H...O.

Graphical Abstract



Keywords: Benzophenone, crystal structure, anticancer, Hirshfeld Surfaces.

Journal of Chemistry and Chemical Sciences, *Vol.8(3), 493-501, March 2018* *ISSN 2229-760X (Print)*
(An International Research Journal), *www.chemistry-journal.org* *ISSN 2319-7625 (Online)*

Spectral, Optical and Structural Studies of 2-methoxybenzaldehyde

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(Received on: March 8, 2018)

ABSTRACT

The crystal structure of the title compound 2-methoxybenzaldehyde has been determined by X-ray diffraction technique. The compound crystallizes in tetragonal crystal system under the space group.

P 43 21 2 with cell parameters a = 11.0120(12) Å, b = 11.0120(12) Å, c = 23.615(4) Å, Z = 16 and V = 2863.7(7)A^{-3}. The title compound C_8 H_8 O_2 was synthesized and characterized by ^{1}HNMR, ^{13}CNMR, TGA, DSC, and UV-Vis NIR spectroscopy studies.

Keywords: Antioxidant, Antimicrobial, Nuclaer Magnetic Resonance(NMR), Nonlinear Optics(NLO).

1. INTRODUCTION

In recent years, due to growing consumer demand for food products which is free from chemical synthetic additives, solution has been paid to explore naturally occurring antioxidants, antimicrobials, and anti-fungals. Recent investigation on plant kingdom are found to have grecial interest with its variety of diversity which appears to be one of the best alternatives, as they show minimal environmental impact and danger to the consumers.

Journal of Chemistry and Chemical Sciences, Vol.8(3), 467-476, March 2018
(An International Research Journal), www.chemistry-journal.org
ISSN 2229-760X (Print)
ISSN 2319-7625 (Online)

Synthesis, Crystal Structure and Hirshfeld Surface Studies of '1-(2-hydroxy-5-methylphenyl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one'

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(Received on March 2, 2018)

ABSTRACT

This paper reports "Synthesis crystal structure and Hirshfeld surface studies of 1-(2-hydroxy-5-methylphenyl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one" the titled compound is crystallized into orthorhombic crystal class with the space group of *Pbca*, the cell parameters *a=13.6680(12)Å, b=13.3750(8)Å, c=14.5410(14)Å*, Z=*8*, the structure is solved by direct method and refined by full matrix least square method based on F^2 and reduced to *R=1.06*, x-ray diffraction study revealed that the molecule is slightly twisted, presense of hydrogen bond interaction of the type C-H...O. Intermolecular interactions are analyzed using Hirshfeld surfaces. The structure may exhibits supra molecular features of the bond type C-H...O.

Keywords: Thiophene, synthesis, crystal structure, dihedral angle, Hirshfeld surfaces.

1. INTRODUCTION

Chalcone is the basic skeleton present in all flavonoids, which are important secondary plant metabolites, reported to exhibit wide range of biological activities such as anti-oxidant[1], antibacterial[2], antifungal[3], anticancer[4-6], anti HIV[7] anti-inflammatory[8] and inhibition of various enzymes such as aldose reductase, cycloxigenase, tyrosinkinase[9-11]. The α, β unsaturated ketone group present in chalcones is believed to be responsible for the biological activity of

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Journal of Chemistry and Chemical Sciences, *Vol.8(2), 250-258, February 2018* *ISSN 2229-760X (Print)*
(An International Research Journal), *www.chemistry-journal.org* *ISSN 2319-7625 (Online)*

Synthesis, Structural, Molecular Docking and Hirshfeld Surface Analysis of (2-((6-chloropyridin-3-yl)methoxy)-5 bromophenyl) (4-chlorophenyl) methanone

B. N. Lakshminarayana[1*], T. N. Mahadeva Prasad[2], N. R. Sreenatha[3], D. P. Ganesha[4], B. K. Manuprasad[5] and S. Nagaraju[6]

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(Received on: December 14, 2017)

ABSTRACT

The title compound (2-((6-chloropyridin-3-yl)methoxy)-5-bromophenyl) (4-chlorophenyl) methanone was synthesized and characterized by spectroscopically (HRMS, IR and ^{1}NMR) single crystal X-ray diffraction studies, molecular docking and Hirshfeld surface analysis. The title compound $C_{19}H_{12}NO_2Cl_2Br$ crystallizes in the monoclinic space group with cell parameters a = 8.4160(8) Å, b = 17.191(3) Å, c =12.302(2) Å, α = 90°, β = 90.374(3)°, γ = 90°, V = 1774.7(5) Å^3 and Z = 4. The pyridine ring and the phenyl ring bridged by the central phenyl ring are nearly coplanar. The docking analysis of the title compound is executed with anti-cancer target with hER-α protein. In addition to this Hirshfeld surface computational analysis was carried out. The major intercontacts contributing to the Hirshfeld surface are H...H, H...Cl, H...C and H...Br.

Keywords: Benzophenone; crystal structure; pyridine ring; anti-inflammatory; anticancer.

Journal of Molecular Structure 1173 (2018) 300–306

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: http://www.elsevier.com/locate/molstruc

3D energy frameworks of a potential nutraceutical

S. Madan Kumar [a, *], B.N. Lakshminarayana [b], S. Nagaraju [b], Sushma [c], S. Ananda [c], B.C. Manjunath [d], N.K. Lokanath [e], K. Byrappa [f]

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ARTICLE INFO

Article history:
Received 12 April 2018
Received in revised form
29 May 2018
Accepted 20 June 2018
Available online 26 June 2018

Keywords:
Stilbene
Crystal structure
Hydrogen bond
Hirshfeld surfaces
Enrichment ratio (*E*)
3D energy frameworks

ABSTRACT

A new stilbene derivative (potential neutraceutical), 1,3-dimethoxy-5-(4-((4-nitrobenzyl)oxy)styryl) benzene (**STL**) was synthesized, characterized by spectroscopy (^{1}H, ^{13}C NMR and LC-MS) and single crystal X-ray diffraction method. The compound crystallizes in the monoclinic crystal system (space group $P2_1/c$) with unit cell dimensions $a = 32.6130(12)$ Å, $b = 7.1894(3)$ Å, $c = 16.7673(6)$ Å, $\beta = 92.539(3)$ °, $Z = 4$, and $V = 3927.5(3)$ Å^3. The asymmetric unit consists of two title molecules (A\B) and the intramolecular hydrogen bonds of the type C–H···O (A\B: *S*(5) ring motif) are observed. The crystal structure is stabilized with C–H···O (A\B: *C*9 chains) intermolecular hydrogen bonds and short contacts of the type C–H ... π (A\B). The intercontacts in the crystal packing were analyzed using Hirshfeld surfaces method using 2D finger print plots and enrichment ratio (*E*). The major intercontact contributing to the Hirshfeld surfaces are found to be from H···H, O···H and C···H (A\B). The favourable contacts responsible for crystal packing (A\B) are H···H, C···H, O···H and C···C confirmed with *E* values. In addition, the 3D-topology of the crystal packing is analyzed and visualized. The dispersion energy framework contribution is greater than the electrostatic energy frameworks.

1. Introduction

Stilbene scaffolds are one of the basic elements found in various biologically active and natural synthetic compounds [1–3]. These derivatives play a major role in the plant defence system by acting as protectants against various pathogens and abiotic stress [4,5]. Grapes and berries contain a natural stilbene, resveratrol which is a phytoalexin [6–11]. Resveratrol is used against breast cancer and is an effective inhibitor of ribonucleotide reductase that catalyzes the rate-limiting step of *de novo* DNA synthesis [12,13]. Many studies reported the evidence of resveratrol mediated in healing of intestine and colon injury [14,15], protecting against brain damage and cerebral ischemia [16]. A series of *trans*-stilbene derivatives have potentials to act as antimicrobial, antioxidant and anticancer potentials [17]. In addition, stilbene derivatives with their unique crystal structures have been reported [18–20]. (see Scheme 1)

With the above importance, we present here the synthesis, spectroscopy, crystal structure, Hirshfeld surfaces, enrichment ratio (*E*) and 3D energy frameworks of the crystal packing of a new stilbene derivative (potential neutraceutical), 1,3-dimethoxy-5-(4-((4-nitrobenzyl)oxy)styryl)benzene (**STL**). This work presents the energy frameworks in the crystal packing of **STL** molecules in terms of electrostatic energy framework, dispersion energy framework and total interaction energy.

2. Methodology

2.1. Materials and methods

All the chemicals were purchased from Sigma Aldrich Chemical Co. The melting point (°C) was determined using the micro controller CL725 based digital melting point apparatus. The compound purity was confirmed using TLC on silica gel 60 F254. ^{1}H and ^{13}C NMR spectra were recorded on an Agilent-NMR, 400 MHz and 300 MHz, respectively. The NMR was recorded using $CDCl_3$ and the

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https://doi.org/10.1016/j.molstruc.2018.06.083
0022-2860/

X-Ray Structure Analysis Online 2018, VOL. 34

Crystal Structure and Hirshfeld Surfaces of (*E*)-1-(2-Hydroxyphenyl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one

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The title compound, (*E*)-1-(2-hydroxyphenyl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one, is crystallized into a monoclinic crystal class with cell parameters $a = 8.2530(5)$Å, $b = 13.1530(14)$Å, $c = 14.1570(11)$Å, $\beta = 125.579(6)^\circ$ and space group of $P2_1/c$. The structure is solved by a direct method, and it is refined to $R = 0.048$. The structure exhibits short C-H···O interactions. Hirshfeld surface computation studies shows that H···H, C···H and O···H are major contributions.

(Received December 30, 2017; Accepted March 13, 2018; Published on web June 10, 2018)

Chalcone is an aromatic ketone that forms the central core for many important aromatic compounds that are biologically active. These are also known as flavonoids which are found in vegetables and fruits. Chalcone exhibits attractive therapeutic activities, such as antibacterial, antifungal, antioxidant, antineoplastic, antiinflammatory and antiviral.[1] The thiophene ring attached to the chalcone, is a five-membered heterocyclic ring with sulfur as a heteroatom having the molecular formula C_4H_4S; its derivatives exist in petroleum or coal.[2] Thiophene is widely known owing to its important electronic plausibility and biological activities. Further, its derivatives are widely used in organic light-emitting diodes (OLEDs), organic field-effect transistors and in solar cells.[3] That of biological activities, such as anti-breast cancer, antimicrobial, anticancer, anti-inflammatory, anti-hypertensive further raloxifine, is a drug used for the prevention and treatment of osteoporosis in postmenopausal women. This based on the benzothiophene system.[4,5] Recently tiaprofenic acid and tenidap are drugs containing thiophene rings, used as non-steroidal anti-inflammatory drugs (NSAIDs) for pain killing and for inflammatory disorders.[6] In addition to this, the thiophene nucleus is treated being as important in the synthesis of heterocyclic compounds with the pharmalogical activities antihypertensive, diabetes mellitus, cholestorol inhibitors.[7] Considering these to be important biological activities we hereby report on the crystal structure, Hirshfeld surfaces and computational studies of (*E*)-1-(2-hydroxyphenyl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one.

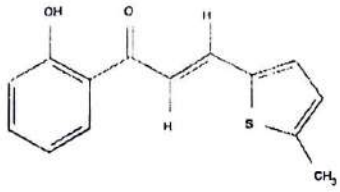

Fig. 1 Scheme of the compound (*E*)-1-(2-hydroxyphenyl)-3-(5-methylthiophen-2-yl)prop-2-en-1-one.

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2′-Hydroxyacetophenone of 0.005 mols was added to 15 ml of methanol taken in a conical flask; to this, 5 ml of aqueous NaOH was added and underwent stirring at room temperature; later, 0.005 mols of 5-methyl-2-thiophene-carboxaldehyde was slowly added while continuing stirring for 48 h. The mixture poured into ice cold water, mixed properly and acidified with dilute HCl. The title compound separates as a precipitate, which was collected by filtration and recrystallized from methanol (Fig. 1).

The X-ray intensity data for the title compound, $C_{14}H_{12}O_2S$, was collected at a temperature of 293 K on a Bruker X8 APEX II diffractometer using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073$ Å). A complete data set was processed using SAINT. The structure was solved by direct method SHELXS and refined by the full-matrix least-squares method on F^2 using SHELXL programs, respectively. Geometrical

Table 1 Crystal data and structure refinement details for the title compound

CCDC Number: 1577562	
Chemical formula: $C_{14}H_{12}O_2S$	
Molecular weight = 244.31	
$T = 293$ K	
Space group: $P2_1/c$	
Crystal system: monoclinic	
$a = 8.2530(5)$Å	$V = 1249.87(18)$Å^3
$b = 13.1530(14)$Å	$Z = 4$
$c = 14.1570(11)$Å	Radiation type : Mo $K\alpha$
$\beta = 125.579(6)^\circ$	Wavelength = 0.71073 Å
Absorption coefficient = 0.25 mm^{-1}	
Crystal size = 0.30 × 0.27 × 0.25 mm	
Diffractometer: APEX (Bruker, 1999)	
Absorption correction: psi-scan; T_{min}, T_{max} = 0.944, 0.953	
No. of reflections measured = 2072	
No of independent reflections = 2072	
No. of reflections observed = 1748	
$R_{int} = 0.021$ (sin $\theta/\lambda)_{max} = 0.595$ Å^{-1}	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S: 0.048, 0.162, 1.07	
Data/Restraints/Parameters: 2072/0/156	
H-atom treatment: H-atom parameters constrained	
$(\Delta\rho)_{max} = 0.25$ eÅ^{-3}	$(\Delta\rho)_{min} = -0.29$ eÅ^{-3}

Chemical Data Collections 11–12 (2017) 131–138

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Data Article

Spectral studies, crystal structure, molecular docking and Hirshfeld surfaces computational studies of 3-(3-Bromophenyl)-5-(4-methoxyphenyl) isoxazole

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ARTICLE INFO

Article history:
Received 20 June 2017
Revised 30 August 2017
Accepted 14 September 2017
Available online 15 September 2017

ABSTRACT

The title compound 3-(3-Bromophenyl)-5-(4-methoxyphenyl) isoxazole was characterized by spectral studies (HRMS, IR, ^{1}H NMR and ^{13}C NMR), single crystal X-ray diffraction studies, molecular docking and Hirshfeld surface analysis. The molecule, $C_{16}H_{12}BrNO_2$ crystallizes in Monoclinic lattice with space group *P21/c* with cell dimensions, *a* = 30.1462(1) Å, *b* = 5.8322(3) Å, *c* = 7.6783(4) Å, ß = 96.43(3)° and *Z* = 4. The isoxazole ring makes a dihedral angle of 24.97° with phenyl ring while the dihedral angle between isoxazole ring and bromopheny is 25.48°. The crystal structure is stabilized with C–H...π interactions and the intermolecular contacts are quantified using Hirshfeld surfaces computational method. The major intercontacts contributing to the Hirshfeld surfaces are H...H,

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http://dx.doi.org/10.1016/j.cdc.2017.09.001

Results in Physics 7 (2017) 2550–2556

Contents lists available at ScienceDirect

Results in Physics

journal homepage: www.journals.elsevier.com/results-in-physics

Structure property relationship of a new nonlinear optical organic crystal: 1-(3,4-Dimethoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one for optical power limiting applications

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ARTICLE INFO

Article history:
Received 15 May 2017
Received in revised form 14 July 2017
Accepted 15 July 2017
Available online 19 July 2017

Keywords:
Nonlinear
Optical power limiting
Z-scan
Self-focusing

ABSTRACT

A new organic potential nonlinear optical (NLO) material 1-(3,4-dimethoxyphenyl)-3-(3-fluorophenyl) prop-2-en-1-one (DMP3FP) is crystallized in acetone. The single crystal X-ray diffraction data shows that material crystallizes into centro-symmetric orthorhombic space group *Pbca with* $a = 15.6552(6)$ Å, $b = 8.5571(3)$ Å, $c = 20.7697(7)$ Å. The functional groups in DMP3FP molecule are identified by Fourier Transfer Infrared (FTIR) spectra. The thermal stability and melting point are determined using thermo gravimetric analysis/differential thermal analysis (TGA/DTA). Using UV Visible spectral studies direct band gap energy of the crystal is determined to be 3.19 eV. The nonlinear absorption coefficient and optical power limiting of the crystal was studied using Z-scan technique. The crystal exhibits a self-focusing effect at a wavelength of 532 nm showing optical limiting and reverse saturable absorption by having excited state absorption coefficient greater than ground state absorption coefficient.

Introduction

Materials exhibiting nonlinear optical (NLO) properties have potential applications in the field of photonics. Organic materials exhibiting two photon absorption (TPA) are of practical importance in applications such as frequency up lasing, multi photon microscopy, three dimensional fluorescence imaging, eye and sensor protection and optical signal reshaping etc., [1–5]. The failure of symmetry carry-over from molecule to crystal is one of the features of NLO material [6]. Also the strength of electron acceptor/donor groups, molecular symmetry, molecular planarity and conjugation length etc. are the other parameters which affect the NLO property [7]. The NLO efficiency of organic molecules can be enriched by adopting suitable design strategies discussed in the literature [8,9]. Chalcones are promising NLO materials among the organic molecules because of their good optical power limiting (OL) property and third-order nonlinearity [10,11]. Since π conjugated systems are observed in chalcones, they lead to overlapping of π orbital and delocalization of electronic charge distribution and high mobility of the electron density [12]. A. J. Kiran et al. [13] reported five derivatives of dibenzylideneacetone with very high third order optical nonlinearities of the order of 10^{-11} esu. By substituting t-butyl, t-butoxy, and dimethylamine electron donor groups to halogenated oligomers, M.B. S. Costa et al. [14]. Materials showing two photon absorption and third order optical nonlinear properties were investigated by Ting chao He et al. [15], Bing Gu et al. [16], Anthoni P. M. et al. [17]. In the process of ongoing research activity of our group [18-20] to investigate NLO materials, a new material 1-(3,4-dimethoxyphenyl)-3-(3-fluorophenyl)prop-2-en-1-one is (DMP3FP) synthesized and crystallized. The crystal exhibits third order nonlinear optical properties such as nonlinear absorption (NLA) and OL behavior.

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http://dx.doi.org/10.1016/j.rinp.2017.07.037
2211-3797/