3.4. RESEARCH PUBLICATIONS AND AWARDS

3.4.5.2 Publications

PG & RESEARCH DEPARTMENT OF MATHEMATICS
Dr.N.MAHESWARI

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A COST ANALYSIS ON MULTI-ITEM INVENTORY MODEL FOR FACTORY OUTLETS WITH TWO CONSTRAINTS UNDER RANKING ASTEROID FUZZY SET

N.MAHESWARI, DR. K.DHANAM & DR. K. R. BALASUBRAMANIAN

ABSTRACT

Inventory for factory outlet problems without shortage is discussed as a special case of conventional inventory problem. The proposed procedure was programmed with MATLAB (R2009a) version software .the output of the model is affected in its input parameters in demand rate. Numerically we ventured to compare the crip model with fuzzy model .A multi-item inventory model for factory outlets in crisp and fuzzy sense are formulated in the fuzzy environment with stowage space and conveyance cost constraints have been considered. In this model, demand is constant and is related to the unit stowage space and conveyance. The asteroid fuzzy set is defined and is properties are given. The parameters involved in this model represented by asteroid fuzzy set. The average total cost is defuzzify by ranking method. The analytical expressions for maximum inventory level and average total cost are derived for the proposed model by using nonlinear programming technique. A numerical example is presented to illustrate the results.

Keywords: Factory outlets, Asteroid fuzzy set, Multi items, Stowage space constraint, Conveyance constraint, Maximum conveyance cost, Maximum stowage space, Ranking Asteroid fuzzy set.

1. INTRODUCTION

In manufacturing, services, and business operations in general, inventory issues are frequent. In some inventory models, the demand is assumed to be constant in a state environment. Cost parameters, objective functions, and decision makers' constraints are all imprecise in most real-world situations. The classical (EOQ) inventory problem is defined as the problem of determining the optimal order quantity under relatively stable conditions. This EOQ problem with varying variance had been solved for several years and published since 1915 by a number of researchers. F.W.Harries (1913) [1], E.W. Taft (1918) [2], and G.Hadley & T.M. Whitin (1958) [3] discussed two major assumptions in the classical EOQ models: the demand rate is constant and deterministic. Uncertainties are treated as randomness in conversional inventory models, and they're dealt with using probability theory. However, in some cases, uncertainties are caused by fuzziness, and the fuzzy set theory can be used in these situations. The fuzzy inventory model with storage space and budget constraints was discussed by Shuo-yan Chow and Peterson C. Julian (2009)[4]. Kun-Jen Chang (2012)[5] discussed the integrated inventory model with the transportation cost and two – level trade credit in supply chain management.

A factory outlet is outlined as a factory shop and it is a store where manufacturers sell their products directly to the public at steep discounts. Because not all of a company's products are of high quality, they cannot be sold in retail stores. But they are still usable. Moreover, in such a dynamic market, a product that is fashionable today will become obsolete tomorrow, and given the finite space in retail stores, will be undesirable once again. If that's the case, what about all the products that are no longer available, irregular or redundant? The factory sales centres are approaching. All of the above types that are not found in retail stores

Product of (λ, μ)-Multifuzzy Subgroups of A Group

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Abstract

In this paper, the concept of Cartesian Product of t-intuitionistic multi fuzzy set, t-intuitionistic multi fuzzy Subgroup of a group are defined and discussed some of their properties.

Key Words : Fuzzy set, Multi fuzzy set, (λ, μ)-fuzzy set, Multi fuzzy subgroup , (λ, μ)- multi fuzzy subgroup, Cartesian product of (λ, μ)-multi fuzzy subgroup.

1 Introduction

In 1965, L.A. Zadeh[20] introduced the notion of fuzzy set of any non empty set. In 1996, Bhakat [5] and Das[7] proposed the concept of an $(\in, \in \vee q)$-fuzzy subgroup. In 2003, Yuan et al. and Yuying Li ed al. [18,19] defined the notion of (λ, μ)-fuzzy subgroups, which is an extension of $(\in, \in \vee q)$-fuzzy subgroup. As in the case of fuzzy group, some counterparts of classic concepts can be found for (λ, μ)-fuzzy subgroups. For instance, (λ, μ)-fuzzy normal subgroups and (λ, μ)-fuzzy quotient groups are defined and their elementary properties are investigated, and an equivalent characterization of (λ, μ)-fuzzy normal subgroups was presented in [18,19]. However, there is much more research on (λ, μ)-fuzzy subgroups if we consider rich results both in the classic group theory and the fuzzy group theory in the sense of Rosenfeld[11]. After several years, S.Sabu and T.V.Ramakrishnan[12,13] proposed the theory of multi fuzzy sets in terms of multi dimensional membership functions. Aktas. H and Cagman. N[1] proposed the product of fuzzy subgroups of a group[2]. The notion of (λ, μ)-multi fuzzy subgroup was introduced by the author[4]. R.Muthuraj ed al.[9] Proposed anti product of multi fuzzy subgroups of a group. In this paper we define product of (λ, μ)-multi fuzzy subgroups of a group and study some of their related properties.

2 Preliminaries

In this section, we site the fundamental definitions that will be used in the sequel.

Definition 2.1[20]

Let X be a non-empty set. A fuzzy subset A of X is defined by a function A:X→[0,1].

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DOMINATION PARAMETERS IN TOTAL GRAPH $T(G)$ OF A GRAPH G

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Abstract

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The Total Graph $T(G, L(G), NIC)$ of G is a graph with vertex set $V(G) \cup E(G)$ where two points are adjacent if and only if they are adjacent points of G or they are adjacent lines of G or one is a point of G and another is a line of G incident with it. For simplicity, this graph is denote by $T(G)$. In this paper, we have studied some bounds for domination number of Total graph of a graph. Also, we have found the exact value the domination number of $T(G)$ for some graphs G.

Introduction

Graphs discussed in this paper are undirected and simple graphs. For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set respectively. For two vertices u and v in a connected graph G, the distance $d(u, v)$ from u to v is the length of a shortest $u - v$ path in G. A vertex and an edge are said to cover each other if they are incident. A set of vertices which covers all the edges of a graph G is called a point cover for G, while a set of edges which

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Research Article

Total Eccentricity Indices Of A Graph

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Abstract: We have defined and evaluated total eccentricity indices of polyhex nanotubes $TUAC_6(p, q)$ and $TUZC_6(p, q)$. In thispaper, we compute First Total Eccentricity Index, Second Total Eccentricity Index, First Multiplicative Total Eccentricity Index, Second Multiplicative Total Eccentricity Index, First Hyper Total Eccentricity Index, Second Hyper Total Eccentricity Index, First Multiplicative Hyper Total Eccentricity Index and Second Multiplicative Hyper Total Eccentricity Index of a graph using Total graph of a graph. We evaluate the value of these indices for some standard graphs.

Keyword: Eccentricity Index, Total graph of a graph.

1.Introduction:

Let G be a simple, finite graph with n vertices and m edges with vertex set V(G) and edge set E(G). The edge connecting the vertices u and v∈ V(G) is denoted by e = uv. The vertices and edges of a graph are called elements of G.The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. If e = uv is an edge of G, then the vertex u and edge e are incident as are v and e. Let $d_G(e)$ denote the degree of an edge e in G, which is defined by $d_G(e) = d_G(u) + d_G(v) - 2$ with e = uv.

Let G be a connected graph and v be a vertex of G. The eccentricity e(v) of v is the distance to a vertex farthest from v. Thus, $e(v) = \max\{d(u, v); u \in V\}$. The radius r(G) is the minimum eccentricity of the vertices, whereas the diameter diam(G) is the maximum eccentricity.

The Total graph T(G) of G is the graph whose vertex set is $V = V(G) \cup E(G)$ where two elements are adjacent if and only ifthey are adjacent vertices of G or they are adjacent edges of G or one is a vertex of G and another is an edge of G incident with it. Elements of V which are in V(G) are known as point vertices and are in E(G) are known as line vertices. Let $e_{T(G)}(u)$ and $e_{T(G)}(e)$ denote the eccentricity of vertex u and edge e in T(G) respectively.

The topological indices are one of the mathematical models that can be defined by assigning a real number to the chemical molecule. The physical-chemical characteristics of the molecules can be analyzed by taking benefit from the topological indices. Properties such as boiling point, entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation. Acetic factor, etc can be predicted using topological indices..

In 2016, Kulli introduced K Banhatti indices [6].

In 2016, Bhanumathi and Easu Julia Rani introduced K-eccentric indices [2, 4]

In 2020, Bhanumathi and Mariselvi defined and evaluated total eccentricity indices of polyhex nanotubes $TUAC_6(p, q)$ and $TUZC_6(p, q)$ [5].

2.Some Eccentricity based indices of a graph G using Total graph T(G)

Here, we evaluate the First and Second Total Eccentricity Index and First and Second Multiplicative Total Eccentricity Index, First and Second Hyper Total Eccentricity Index and First and Second Multiplicative Hyper Total Eccentricity Index of some particular graphs.

In [5], we define, the First and Second Total Eccentricity Index as

$$BT_1(G) = \sum_{uv} [(e_{T(G)}(u) + e_{T(G)}(e)]$$

$$BT_2(G) = \sum_{uv} [(e_{T(G)}(u).e_{T(G)}(e)]$$

The First and Second Multiplicative Total Eccentricity Index are defined as

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Personalized Medical Information Filtering using Evidence Phrases

Mu. Annalakshmi, A. Padmapriya

Abstract: ***Finding the required information in the field of medicine from the World Wide Web has been a challenging task for the users since large number of medical research documents are added to it every day. Personalization of web search would help the professionals or beginners in medicinal field in retrieving the relevant information. The proposed method gathers the users' browsing patterns from the browser and builds evidence phrases based on factors like visit count, bookmarks or downloads. These evidence phrases determine the rank of the websites in the search results. The proposed method is evaluated with the relevance data collected from allied medical professionals. Evaluation shows that the proposed method ranks the user preferred pages in the top of the search results. It helps the users from the field of medicine to find their information needs more quickly without surfing all the search results of the query.***

Keywords: User Personalization, User Profiling, Evidence Phrases, Information Filtering, Relevance

I. INTRODUCTION

Information filtering is an essential tool used by web searchers to find the desired information in the web which is rapidly expanding. The need for information filtering is more in the fields like marketing, sociology, economics and medicine. As far as the field of medicine is concerned, a large number of research documents are added to Internet every day. This makes information access for medical professionals even more difficult. Google [19] is the most popular and widely used general search engine and this can be used for medical search also. There are several specialized search engines for medical search but they are more suitable for experts in the field rather than the beginners or novice users. Searches by Google can be used by all kinds of users but they are of greater help to beginners, allied healthcare professionals and novice users.

In general different search engines use several factors to rank the web pages [12]. They have to be more intelligent to identify the users' real search intent by resolving the ambiguity in query terms. This is possible only if the information about the user is available to the search engines.

User profiling or Personalization which has emerged as a significant area of research interest in the recent years is a strategy that aids the search engines in this context. The user profiles can be built either explicitly or implicitly. Explicit profiling requires the users to explicitly specify their preferences or ratings which they are reluctant to do because of the increased effort and time. Also the users view more pages than they rate. But the user preferences can be recorded implicitly by examining the user search history or bookmarks which is far easier due to lesser or no effort from users. The research work [5] lists out some of the interest indicators including both implicit and explicit that helps in preparing user profiles. User profiles can be automatically obtained by many approaches which include using a proxy server to trace the browsing history or desktop bots to record the activities on the personal computer. But both these approaches require that the user has to install the proxy servers or bots.

WordNet [9] is a lexical database for English language which mainly stores the synonyms of a word (when used as noun, verb, adverb or adjective) along with its related words hypernyms, hyponyms, holonyms, meronyms and their corresponding meanings. It can be viewed as both dictionary and thesaurus, and is mainly used in text analysis and artificial intelligence applications. The UMLS, or Unified Medical Language System [8], is a set of files and software that brings together many health and biomedical vocabularies and standards to enable interoperability between computer systems. The UMLS can be used to enhance or develop applications, such as electronic health records, classification tools, dictionaries and language translators. One powerful purpose of the UMLS is linking health information, medical terms, drug names, and billing codes across different computer systems. The UMLS has many other purposes that include search engine retrieval, data mining, public health statistics reporting, and terminology research. Personalization of user profiles and use of UMLS and WordNet serve as the motivating factor for the proposed work.

The rest of the paper is organized as follows. The related works which act as motivating factor for the proposed work are described in section 2. The proposed method is explained in section 3. The experimental study is summarized in section 4. Section 5 concludes the research work.

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Research article

In vitro micropropagation of *Tinospora cordifolia* (Willd.) Miers from shoot tip explants

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Young shoot tip

Abstract

An efficient *in vitro* micropropagation protocol from shoot tip explants was established for *Tinospora cordifolia* (Willd.) Miers. Young and mature shoot tip (YST and MST, respectively) explants from two different-aged plant sources (15 d and 3 yr) were treated simultaneously to develop and compare their efficacy in the micropropagation protocol. Among the cytokinins and synergetic treatments, 6-benzyladenine (BA; 2.0 mg/L) and kinetin (KN; 1.0 mg/L) responded better in bud break and shoot development, at both individual concentrations and in combination. Addition of the auxin indole-3-acetic acid (IAA; 0.5 mg/L) to the optimal cytokinin concentrations of BA (2.0 mg/L) with KN (1.0 mg/L), enhanced multiple shoot induction and shoot growth. Further supplementation of gibberellic acid (0.1 mg/L) and an antioxidant (ascorbic acid at 100 mg/L) significantly enhanced the shoot bud induction, shoot number and shoot length. Assessment of different basal media using the best plant growth hormone complex confirmed that the Murashige and Skoog (MS) medium best supported shoot bud break and shoot development in both the shoot tip explants. The best rooting response was from half-strength MS medium fortified with indole-3-butyric acid (0.5 mg/L), resulting in approximately 80% of the plantlets successfully acclimatized both at *in vitro* and *in vivo* conditions. In conclusion, the YST explants responded better than the MST explants in all aspects of growth and development and proved that the age of explants was an important determinant for efficient micropropagation in *T. cordifolia*.

Introduction

Medicinal plants have been used fundamentally in all cultures from ancient times, as remedies and cures for humans. An increasing reliance on the use of medicinal plants in the industrialized societies has been traced to the extractions and development of several drugs and chemotherapeutics from these plants as well as from several traditionally used herbal remedies (UNESCO, 1994). In the interim, medicinal plant reserves in developing countries are decreasing and in danger of extinction due to increasing trade demands for cheaper healthcare products to more target specific drugs and biopharmaceuticals (Debnath et al., 2006). Micropropagation or tissue culture technology can provide a continuous, reliable source of pharmaceuticals and could be used for the large-scale culture of plant cells from which important metabolites can be extracted (Hussain et al., 2012).

Tinospora cordifolia (Willd.) Miers. (Menispermaceae), a large glabrous climbing shrub, is distributed throughout tropical India upto an altitude of 300 m (Pradhan et al., 2013). It has been used

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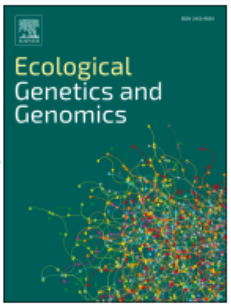

Mycorrhizal and endophytic fungal association in *Paphiopedilum druryi* (Bedd.) Stein - A strict endemic and critically endangered orchid of the Western Ghats

Selvaraju Parthibhan, Raju Ramasubbu

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NEIGHBORHOOD CONNECTED DOMINATION AND ECCENTRIC DOMINATION OF BOOLEAN GRAPH $BG_3(G)$ OF A GRAPH G

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Abstract

Let G be a simple (p, q) graph with vertex set $V(G)$ and edge set $E(G)$. $BG_3(G)$ is a graph with vertex set $V(G) \cup E(G)$ and two vertices are adjacent if and only if they correspond to a vertex and an edge incident to it in G or two non-adjacent edges of G. In this paper, we study the concept of neighborhood connected domination and eccentric domination in Boolean graph $BG_3(G)$.

1. Introduction

Graphs discussed in this paper are undirected and simple graphs. For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set respectively. Let $v \in V$. The open neighborhood $N(v)$ of a vertex v is the set of all vertices adjacent to v in G. $N[v] = N(v) \cup \{v\}$ is called the closed neighborhood of v. If $S \subseteq V$, then $N(S) = \bigcup v \in sN(v)$ and $N[S] = N(S) \cup S$.

A vertex and an edge are said to cover each other if they are incident. A

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DOMINATION PARAMETERS IN TOTAL GRAPH $T(G)$ OF A GRAPH G

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Abstract

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The Total Graph $T(G, L(G), NIC)$ of G is a graph with vertex set $V(G) \cup E(G)$ where two points are adjacent if and only if they are adjacent points of G or they are adjacent lines of G or one is a point of G and another is a line of G incident with it. For simplicity, this graph is denote by $T(G)$. In this paper, we have studied some bounds for domination number of Total graph of a graph. Also, we have found the exact value the domination number of $T(G)$ for some graphs G.

Introduction

Graphs discussed in this paper are undirected and simple graphs. For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set respectively. For two vertices u and v in a connected graph G, the distance $d(u, v)$ from u to v is the length of a shortest $u - v$ path in G. A vertex and an edge are said to cover each other if they are incident. A set of vertices which covers all the edges of a graph G is called a point cover for G, while a set of edges which

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PG & RESEARCH DEPARTMENT OF PHYSICS

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Abstract

Green synthesis of nanoparticles is a facile method as they are eco-friendly and cost-effective and also the resources are easily available. Nowadays, the demand for magnetic nanoparticles has increased around 13% and they are used in magnetic sensing, medical imaging, wastewater treatment and antibiotic drugs. In this report, the eco-friendly green synthesis of magnetic iron nanoparticles was efficiently synthesized by using *Murraya koenigii* leaves extract. The UV–visible spectrum revealed the presence of a surface Plasmon resonance band at 240 nm and analyzed the formation of iron nanoparticles. X-ray diffraction pattern determined the crystallinity of nanoparticles. Fourier-transform infrared spectrum illustrated the functional groups of iron nanoparticles. The particle size distribution graph showed that the formed particles were in the range of nanometer. High-resolution transmission electron microscopy spectrum realized the spherical-shaped iron nanoparticles were ranging between 4 and 9 nm in size. The energy-dispersive X-ray spectrum and mapping revealed the iron, oxygen and carbon elements in the prepared nanoparticles. The vibrating sample magnetometer analysis showed the paramagnetic behavior of the prepared magnetic iron nanoparticles. The inhibition potent of magnetic nanoparticles on various human pathogens was revealed through antimicrobial assay. The

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CRYSTAL Research & Technology

Research Article

Synthesis, Growth, Physicochemical Characterization, and Computational Studies on Aminopyridinium Chloronicotinate Single Crystal

G. Amudha, R. Santhakumari, D. Chandrika, S. Mugeshini, N. Rajeswari, Suresh Sagadevan

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Abstract

Aminopyridinium chloronicotinate (APCN) single crystals are grown using a slow evaporation solution growth method. The APCN crystal belongs to the monoclinic crystal system with a centrosymmetric space group $P2_1/c$, resulted from the X-ray diffraction analysis. Powder X-ray diffraction analysis is used to determine the crystallinity nature of grown crystals. Various functional groups in the grown crystal were identified using Fourier transform infrared spectroscopy. The optical transmittance, energy bandgap of the crystal is analyzed through UV–vis–NIR spectroscopy. The thermal stability of APCN crystal is studied by using thermogravimetric and differential thermal analysis. The mechanical property of the grown crystal is determined by the Vickers microhardness test. The density functional theory method at B3LYP with 6–31+G(d,p) basis set is used to perform the theoretical investigations in order to get the information regarding the HOMO-LUMO, global chemical reactivity descriptors, natural bond orbital, Mulliken

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Synthesis, growth, experimental, and theoretical characterization of 6-amino-1H-pyrimidine-2,4-dione dimethylacetamide single crystal

S. Mugeshini [a], R. Santhakumari [a], N. Rajeshwari [a], G. Amudha [a], D. Chandrika [a], Suresh. Sagadevan [b]

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Highlights

- Good quality single crystals of 6APDDA were grown from an aqueous solution.
- Their crystal state structures were characterized by single crystal X–ray diffraction.
- Optical properties of the studied compounds were carried out.
- DFT calculation by DFT/B3LYP/3-21G(d,p) method.
- Hirshfeld surfaces and 2D fingerprint plots were performed to confirm intermolecular interactions in the crystals.

Abstract

The single crystals of nonlinear optical organic compounds are essential for their use in optical devices. With this purpose, this research presents the formation of good quality single crystals of 6-amino-1H-pyrimidine-2,4-dione dimethylacetamide from an aqueous solution at room temperature by following the slow evaporation solution growth technique. While single crystal X-Ray Diffraction (SXRD) analysis was used to examine the structural properties of the grown crystal, Powder X-Ray Diffraction (PXRD) was employed toconfirm its crystalline nature and phase purity. The presence of the various functional groups was verified using Fourier Transform Infrared (FTIR) spectral analysis. The UV-vis-NIR spectrum was recorded to investigate the optical transparency of the grown crystal.Hirshfeld surface analysis was carried out to further examine the possibly present intermolecular interactions. Finally, the structure of the crystal was optimized using the DFT/B3LYP/3-21G(d,p)level combined with the DFT/B3LYP/6-311++G(d,p) level to study the molecular properties of the grown crystal such as stable configuration, dipole moment, polarizability, hyperpolarizability Nuclear Magnetic Resonance (NMR), Natural Bond Orbital (NBO) theory, and Mulliken's atomic charges in the gaseous state.

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Dr.G.AMUDHA, Dr.R.SANTHAKUMARI

Journal of Molecular Structure
Volume 1257, 5 June 2022, 132606

Growth, spectroscopic and Hirshfeld surface analysis on pyridine urea single crystal

G. Amudha [a], R. Santhakumari [a], D. Chandrika [a], S. Mugeshini [a], N. Rajeswari [a], Suresh Sagadevan [b]

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Highlights

- Pyridine urea crystal was grown from slow evaporation method.
- The FTIR spectral studies on pyridine urea have been compared with
- The HOMO-LUMO energy gap, the GCRD parameters have been calculated.
- The strong intramolecular interactions were revealed by NBO analysis.
- Hirshfeld surface analysis was used to quantify the intermolecular interactions.

Abstract

Organic single crystal pyridine urea (PYUA) was synthesized using the slow evaporation solution growth method at room temperature. Structural characteristics of the crystal were studied through crystal X-ray diffraction, Fourier transform infrared (FT-IR), and UV-vis-NIR spectral analyses. The thermogravimetric analysis (TGA) and differential thermal analysis (DTA) techniques was used to investigate the thermal stability of the PYUA crystal. The Vickers hardness study confirmed the PYUA as a soft crystal constructed by H-bonds and π…π interactions of average strength. The DFT calculations with the B3LYP method and Gaussian 09 software were used to perform computational analyses in a gaseous state. Hirshfeld investigations reveal H-H interactions demonstrating the largest contribution in the molecular packing.

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Dr.S.MUGESHINI, Dr.R.SANTHAKUMARI

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Journal of Molecular Structure
Volume 1249, 5 February 2022, 131600

Growth, computational studies, and docking analysis on α-pyrrolidinopentiophenone hydrochloride monohydrate single crystal

S. Mugeshini [a], R. Santhakumari [a], N. Rajeswari [a], G. Amudha [a], D. Chandrika [a], Suresh Sagadevan [b]

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Highlights

- An organic single-crystal α -pyrrolidinopentiophenon hydrochloride monohydrate was grown by a solvent evaporation method.
- The investigations on FTIR and FT-Raman were also carried out to analyze all the vibrational modes present in the title compound.
- The MEP map was examined, for analyzing electrophilic and nucleophilic attack sites.
- Molecular docking was used to determine the lengths of hydrogen bonds and binding energy with various antifungal proteins.

Abstract

The title compound, α -pyrrolidinopentiophenone hydrochloride monohydrate (α-PVP) was grown using the solvent methanol through solution growth technique at room temperature. The crystalline nature and its parameters were confirmed by single and powder X-ray diffraction (XRD) studies. The Fourier Transform Infrared Spectroscopy was used to identify the presence of vibrational frequencies for the title compound. UV–vis-NIR spectral and fluorescence analyses were carried out in order to ascertain its optical properties. Through 3D molecular Hirshfeld surface analysis, the crystal with multi inter contacts was pictured while its total surface area was quantified using a 2D fingerprint generated by DFT/B3LYP/6–311++*G* (d,p) in the standard basis set method, and the bandgap energy was measured. The MEP map was examined, for analyzing electrophilic and nucleophilic attack sites. The molecular NLO properties such as static dipole moment, mean polarizability, anisotropy of polarizability, and first-order hyperpolarizability were calculated. To investigate the biological activity of the α-PVP molecule, molecular docking was used to determine the lengths of hydrogen bonds and binding energy with various antifungal proteins.

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Dr.R.SANTHAKUMARI, Dr SURESH SAGADEVAN

3-D Supramolecular, quantum computational, and vibrational spectroscopic investigation on L-cysteinium methanesulfonate single crystals

P. Koteeswari, Solhe F. Alshahateet, R. Santhakumari, Is Fatimah & Suresh Sagadevan

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Abstract

This article reports on molecular modeling using density functional theory (DFT) performed on L-cysteinium methanesulfonate (L-CMS). Calculations were performed on the B3LYP/LanL2DZ level with 6-31 G(d,p) basis set using the Gaussian 09 program package. The optimized structure, HOMO-LUMO, energy gap, electronic properties, MEP, dipole moment, first-order molecular hyperpolarizability (β), chemical potential, global hardness, softness, global electrophilicity, and natural bond orbital analysis of this compound were studied by computational procedures. Intermolecular O-HO, N-HO, and S-HO hydrogen-bonding interactions with different motifs were observed in the crystal structure. Hirshfeld surface analyzes were also performed. Energy frameworks have been constructed to understand the packing of molecules by examining the different intermolecular interaction energies.

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Dr.S.PARTHIBAN

ell, Tissue and Organ Culture (PCTOC) › Article

# of seaweeds extract and plant growth ors on high-frequency in vitro ration and ex-vitro rooting of *gia maculata* Bedd.: an endemic s of Southern Western Ghats

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Rengasamy Anbazhakan, Selvaraju Parthibhan & Thiruppathi Senthil Kumar

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Abstract

Indirect organogenesis system was used to develop a successful protocol for in vitro plant regeneration of *Ceropegia maculata*. Organogenesis was attained through callus derived from internode and leaf explants of 6 months old mature plants. Organogenic callus were induced from internode and leaf explants on MS medium fortified with 2,4-D at 0.5 mg L^{-1} (97.0%) and 0.7 mg L^{-1} (93.3%), respectively. Callus proliferation was achieved on 0.5 mg L^{-1} 2,4-D with 0.5 mg L^{-1} NAA combination from both the explants. Adventitious shoot regeneration from callus was attained on MS medium augmented with TDZ 0.5 mg L^{-1} from internode and leaf derived callus (92.6% and 92.3%), respectively. In vitro rooting was observed on medium fortified with IBA 0.5 mg L^{-1} (5.93 shoot per roots). Callus derived shoots (about 4 cm) shifted to MS medium augmented with different concentration (10—30%) of *Ulva lactuca*, *Caulerpa scalpelliformis* and *Sargassum wightii* seaweed extracts, produced maximum shoot elongation (14.56 cm in length and 12.26 cm in length) from both internode and leaf explant derived shoots. Prolific rooting (7.33 root per shoot) was observed on the medium augmented with 20% *S. wightii* extract. Ex vitro rooting on in vitro derived shoots with IBA 100 mg L^{-1} produced maximum number of roots (10.36) and root length (7.33 cm) and grew normally. All the plantlets were successfully hardened and acclimatized upon transferred to the greenhouse condition

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Somatic embryogenesis from stem thin cell layers of *Dendrobium aqueum*

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Abstract

An efficient *in vitro* regeneration protocol through somatic embryogenesis was established from stem transverse thin cell layers (tTCLs) of *Dendrobium aqueum* Lindley, an imperiled orchid. This study outlines the induction and successive maturation stages of *D. aqueum* somatic embryos (SEs). The tTCLs (~ 0.5 mm thick) cultured on half-strength Murashige and Skoog (MS) medium containing cytokinins and auxins, either individually or in combination, produced embryogenic callus (EC). Treatment with 0.5 mg dm^{-3} zeatin induced EC in 41.42 % of tTCLs. As many as 42.66 globular SEs per tTCL were formed in the presence of 1.5 mg dm^{-3} N^6-(2-isopentyl) adenine (2iP) but only on 10.33 % of explants. The combined treatment of 2iP (1.5 mg dm^{-3}) and 0.5 mg dm^{-3} 6-benzyladenine resulted in 34 globular SEs on 14.7 % of tTCLs whereas the combination of 2iP and 1.0 mg dm^{-3} indole-3-butyric acid (IBA) induced 7.4 globular SEs on 52.33 % of tTCLs. Supplementation of activated charcoal, amino acids, and antioxidants alleviated browning at all the concentrations tested, but the EC response declined. The addition of 0.5 mg dm^{-3} polyvinylpyrrolidone to 1.5 mg dm^{-3} 2iP and 1.0 mg dm^{-3} IBA produced 24 SEs on 19.89 % of tTCLs suggesting that the EC and SEs can be effectively induced by individual cytokinins whereas the synergistic treatments with other compounds can only enhance the induction of EC. Histological observations of EC showed the formation of globular SEs from sub-epidermal regions. Successive developmental stages of globular SEs and the intermediate stage of protocorm like bodies until the formation of plantlets were observed. The plantlets obtained through SEs showed no morphological variations, and inter simple sequence repeat profiles also confirmed the genetic fidelity of *in vitro*-derived progeny with high monomorphism (97.78 %). In conclusion, the use of stem tTCLs is an effective method to produce SEs through indirect somatic embryogenesis in *D. aqueum*.

Additional key words: auxins, cytokinins, epiphyte, embryogenic callus, *in vitro* culture, ISSR, protocorm like bodies.

Introduction

The *Orchidaceae*, one of the largest, most highly evolved, and diverse families of flowering plants, contains about 35 000 species belonging to 850 genera (Hossain *et al*. 2013). *Dendrobium* is a large genus of the *Orchidaceae* with about 1 600 species worldwide, and 116 can be found in India (Misra 2007). *Dendrobium aqueum* Lindley is an endemic orchid distributed in the Kolli hills (Namakkal) and Shervarayans (Salem) of Eastern Ghats, Tamil Nadu, India (Matthew 1983). Natural *D. aqueum* populations are declining due to anthropogenic activities such as the collection of orchids and habitat destruction. This species was categorized as near threatened in 2000 by the International Union for Conservation of Nature and Natural Resources (Kumar *et al*. 2001), and subsequent field studies at the Kolli hills have recorded a continual decline of this natural population (Sudhakar Reddy *et al*. 2005). Studies on the phenology and *in vitro* propagation through asymbiotic seed germination and protocorms have been already achieved in *D. aqueum* (Parthibhan *et al*. 2012,

Submitted 13 June 2017, *last revision* 22 November 2017, *accepted* 4 December 2017.
Abbreviations: 2iP - N^6-(2-isopentyl) adenine; AC - activated charcoal; BA - 6-benzyladenine; DSE - direct somatic embryogenesis; EC - embryogenic callus; IAA - indole-3-acetic acid; IBA - indole-3-butyric acid; ISSR - inter simple sequence repeat; KN - kinetin; MS - Murashige and Skoog; NAA - 1-naphthalene acetic acid; PGR - plant growth regulator; PLB - protocorm-like body; PVP - polyvinylpyrrolidone; SE - somatic embryo; tTCL – transverse thin cell layer; TDZ - thiadiazuron; ZEA - zeatin.
Acknowledgements: We sincerely acknowledge the financial assistance from the Ministry of Environment, Forest and Climate change, New Delhi, Government of India, and the Rajiv Gandhi National Fellowship (UGC). The corresponding author thanks the University Grants Commission (UGC), New Delhi, for providing an Emeritus Fellowship.
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Dr.S.PARTHIBAN

In Vitro Cellular & Developmental Biology - Plant
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PLANT TISSUE CULTURE

In vitro micropropagation, flowering, and tuberization of *Ceropegia maculata* Bedd.—an endemic plant of Southern Western Ghats

Rengasamy Anbazhakan[1] · Chinnaiyan Rajasekar[2] · Mariappan Muthukumar[3] · Selvaraju Parthibhan[1] · Thiruppathi Senthil Kumar[1]

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Abstract
Ceropegia maculata Bedd. is an endemic plant of Southern Western Ghats, Tamil Nadu, India. It has important medicinal properties, edible tubers, and ornamental flowers. *In vitro* propagation protocol of this plant is required and is established by using nodal explants. Sterilized nodal explant was inoculated on Murashige and Skoog (MS) medium supplemented with various plant growth regulators (PGRs) and additives for *in vitro* shoot multiplication. Maximum shoot induction (86%) with an average of 2.43 shoots per explant was obtained on MS medium supplemented with 1.5 mg L^{-1} of N6-benzyl adenine (BA). The highest number of shoots (6.66) per explant was observed on MS medium containing combination of 1.5 mg L^{-1} BA and 0.5 mg L^{-1} indole-3-butyric acid (IBA). In this study, *in vitro* flowering (93.33% and 4.86 flowers per mature shoot) on MS medium plus 0.5 mg L^{-1} BA and tubers (95.33%) on MS medium plus combination with 2.0 mg L^{-1} BA with 0.5 mg L^{-1} naphthalene acetic acid (NAA) were observed. The highest number of roots (9.33) per shoot was recorded on half-strength MS medium supplemented with 0.5 mg L^{-1} IBA. The rooted plantlets were hardened with sand and coconut coir mixed with red soil 1:1:1 (w/w/w) ratio. Acclimatized plants were transferred to field and survival rate was 90%. For the first time, developed this protocol allows an efficient method for *in vitro* plant regeneration and conservation of this endangered species.

Keywords *Ceropegia maculata* · Node explant · Micropropagation · Rooting · Hardening

Introduction

Ceropegia maculata Bedd. is an ethnomedical plant which belongs to the family Apocynaceae. The genus *Ceropegia* comprising twiners, herbs, and occasionally subshrubs is distributed in tropical and subtropical regions of Asia, Africa, Australia, Malaysia, and the Canary and Pacific Islands (Nayar and Sastry 1988; Anonymous 1992). The plant names are universally called as the lantern flower, Christensen, parasol flower, parachute flower, bushman's pipe, the string of hearts, snake creeper, wine-glass vine, rosary vine, necklace vine flower, Chinese lantern, lantern plant, trap flowers, and pitfall trap flowers (Yadav 1996; Quattrocchi 2000). The six recognized centers of diversity of the genus are East Africa, Africa of the West, Southern Africa, the Indian subcontinent, the Arabian Peninsula, and Madagascar (Chavan *et al.* 2018). The maximum variety of flowers of the *Ceropegia* spp. is found in subtropical Africa on the eastern side of the African continent (Dyer 1983; Bruyns 2003; Bruyns *et al.* 2015). The Indian *Ceropegia* was first updated with 44 species, of which 28 were endemic; after 13 new additions, the genus now comprises 57 species, 3 varieties, and 2 subspecies in which 35 species are endemic to the Western Ghats (Karthikeyan *et al.* 2009). The Indian *Ceropegia* species are present in limited, inaccessible pockets of the Himalayas and the Western Ghats due to over exploitation for medicinal purposes. The edible sweet–sour leaves of *Ceropegia* are known to be digestive tonic. *Ceropegia* tubers are also edible as they contain starch, sugar, gum, albumin, carbohydrates, fats, and raw fiber (Mabberley 1987; Jain and Defillips 1991). Tubers of some *Ceropegia*

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Dr.M.SAHAYA SOFIYA

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ARTICLES

The Struggle for Survival and Identity in Cormac McCarthy's The Road

PDF

M.L. Eileen Brisha, Dr. M. Sagaya Sophia

Published 2021-07-30

Abstract

McCarthy's novel *The Road* (2006) is known for its setting which deviates McCarthy's readers from 'far from the madding crowd' setting to the city life which has been at present destructed by an unknown catastrophe which shatters the lives of the people of America. In such a setting the author makes his leading character wander along with his son in search of safety and a better future for his son while travelling in challenging weather surrounded by cannibals. The author makes the readers wonder at the survival skill of the father and his concern for his son in an era where people devour their own children. This paper focuses thus on the father's struggle to cope up with his dying spirit which he fuels up to live only with the help of his memory about his wife and his father and with this spirit, he becomes the bridge between his lost world and his son's unknown 'New' world where cannibalism has become the order of the day, to survive and safeguard his son from the moral less life and inculcate moral values and a better future for him.

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Dr.R.ROHINI

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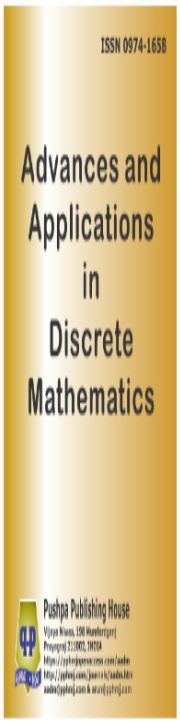

SOME STATUS INDICES OF BINARY TREE GRAPHS

R. Rohini, P. Gladyis and G. Srividhya

Abstract:

In this paper, the status of binary tree and status based some indices of binary tree graphs are computed.

Keywords and phrases:

status index, binary tree, perfect binary tree.

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Dr.N.MAHESWARI

Journal of Mathematical Control Science and Applications
Vol. 7 No. 2 (July-December, 2021)

Submitted: 27th August 2021 *Revised: 30th September 2021* *Accepted: 24th November 2021*

A COST ANALYSIS ON MULTI-ITEM INVENTORY MODEL FOR FACTORY OUTLETS WITH TWO CONSTRAINTS UNDER RANKING ASTEROID FUZZY SET

N.MAHESWARI, DR. K.DHANAM & DR. K. R. BALASUBRAMANIAN

ABSTRACT

Inventory for factory outlet problems without shortage is discussed as a special case of conventional inventory problem. The proposed procedure was programmed with MATLAB (R2009a) version software .the output of the model is affected in its input parameters in demand rate. Numerically we ventured to compare the crip model with fuzzy model .A multi-item inventory model for factory outlets in crisp and fuzzy sense are formulated in the fuzzy environment with stowage space and conveyance cost constraints have been considered. In this model, demand is constant and is related to the unit stowage space and conveyance. The asteroid fuzzy set is defined and is properties are given. The parameters involved in this model represented by asteroid fuzzy set. The average total cost is defuzzify by ranking method. The analytical expressions for maximum inventory level and average total cost are derived for the proposed model by using nonlinear programming technique. A numerical example is presented to illustrate the results.

Keywords: Factory outlets, Asteroid fuzzy set, Multi items, Stowage space constraint, Conveyance constraint, Maximum conveyance cost, Maximum stowage space, Ranking Asteroid fuzzy set.

1. INTRODUCTION

In manufacturing, services, and business operations in general, inventory issues are frequent. In some inventory models, the demand is assumed to be constant in a state environment. Cost parameters, objective functions, and decision makers' constraints are all imprecise in most real-world situations. The classical (EOQ) inventory problem is defined as the problem of determining the optimal order quantity under relatively stable conditions. This EOQ problem with varying variance had been solved for several years and published since 1915 by a number of researchers. F.W.Harries (1913) [1], E.W. Taft (1918) [2], and G.Hadley & T.M. Whitin (1958) [3] discussed two major assumptions in the classical EOQ models: the demand rate is constant and deterministic. Uncertainties are treated as randomness in conversional inventory models, and they're dealt with using probability theory. However, in some cases, uncertainties are caused by fuzziness, and the fuzzy set theory can be used in these situations. The fuzzy inventory model with storage space and budget constraints was discussed by Shuo-yan Chow and Peterson C. Julian (2009)[4]. Kun-Jen Chang (2012)[5] discussed the integrated inventory model with the transportation cost and two – level trade credit in supply chain management.

A factory outlet is outlined as a factory shop and it is a store where manufacturers sell their products directly to the public at steep discounts. Because not all of a company's products are of high quality, they cannot be sold in retail stores. But they are still usable. Moreover, in such a dynamic market, a product that is fashionable today will become obsolete tomorrow, and given the finite space in retail stores, will be undesirable once again. If that's the case, what about all the products that are no longer available, irregular or redundant? The factory sales centres are approaching. All of the above types that are not found in retail stores

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FUZZY COMPLEMENT OF G^c FOR A CONNECTED FUZZY GRAPH G

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Abstract

In a systematic way, during the year 1975, Rosenfeld introduced fuzzy graphs. Fuzzy graphs have been introduced independently by Yeh and Bang during the same time. The main objective of this paper is to define a new concept of operation namely, fuzzy complement of a complement fuzzy graph and derive its structural properties. The graphs considered are finite, connected and simple.

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Dr.M.SIVAKAMI, Dr.K.RENUKA DEVI

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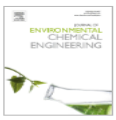

Green synthesis of magnetic nanoparticles via Cinnamomum verum bark extract for biological application

M. Sivakami [a], K. Renuka Devi [b], R. Renuka [b], T. Thilagavathi [c]

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Highlights

- The phytomediate synthesis of Fe nanoparticles have performed with Cinnamomum verum bark extract.
- Spherically 20-80 nm sized Fe nanoparticles shown better inhibition upon *E. coli*, *K. pneumonia*, *S. aureus* and *B. subtilis*.
- The antioxidant, anti-inflammatory, anti-diabetic assays shown the efficient inhibition than positive control.

Abstract

The green synthesis of magnetic Fe nanoparticles (NPs) was prepared via Cinnamomum Verum bark extract. The UV–vis analysis explained the formation of Fe NPs with SPR band at 288 nm. The powder X-ray diffraction analysis (XRD) explicated the mean crystallite size was at 36 nm. The Fourier Transform Infra-Red analysis (FTIR) revealed the functional groups in the prepared Fe NPs. The Scanning Electron Microscope (SEM) and High-Resolution Transmission Electron Microscope (HR-TEM) analyses notified the circular and spherical shaped Fe NPs with the size at 20–50 nm. The Energy dispersive X-ray spectroscopy (EDS) and mapping analyses validated the formation of Fe NPs with purity. The Vibrating Sample Magnetometer (VSM) revealed the paramagnetic behavior of prepared Fe NPs. The phytochemical analysis described the phytochemicals compounds which present in Cinnamomum Verum bark extract. The Antibacterial assay described the much higher inhibition zone of prepared Fe NPs upon human pathogenic bacteria. The Antioxidant (DPPH) assay described the efficient scavenging behavior of Fe NPs with 89 % at 80 μg/mL concentration. The Anti-inflammatory assay explicated the potential protein denaturation behavior of Fe NPs with 87 % at 500 μg/mL concentration. The Anti-diabetic assay reported the much higher potential efficiency of prepared Fe NPs with 84 % at 500 μg/mL concentration.

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Dr.A.DHANALAKASHMI

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Study on Physico-Chemical Parameters and Structural Characterization of Soils in Pudukkottai District of Tamilnadu, India.

Estudio sobre parámetros fisicoquímicos y caracterización estructural de suelos en el distrito Pudukkottai de Tamil Nadu, India.

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ABSTRACT

The soil is the most important constituent to fulfilment of all the basic needs of human beings and also is an important component of our farming. The study was conducted with the main objective to investigate the soil samples of Pudukkottai district of Tamil Nadu for its physico-chemical analysis and structural characterization. The collected soil samples were analyzed for its pH, EC, Nitrogen, Phosphorus, Potassium, Zinc and Iron. Besides, the sample was characterized by FTIR studies for structural conformation. From the study the results revealed that the collected soil was red soil and its texture was sandy clay loam. The soil pH was 9.29 which was alkaline and the EC was 0.02 dSm^{-1}. The available macro-nutrients as nitrogen, phosphorus and potassium for paddy field soil samples had 118, 11 and 160 kg/ha respectively. Micronutrients Nutrients also analyzed. FT-IR spectrum of soil was recorded spectrum of soil was shown the C-H deformation vibrations occur at 1402. The C=C Stretching vibrations occur at 1644 and the N-H Stretching vibrations occur at 2344. Management options to improve the soil fertility were discussed.

Keywords: pH, EC, Nitrogen, Phosphorus, Potassium, Zinc, FTIR, Soil fertility.

Sustainability, Agri, Food and Environmental Research, (ISSN: 0719-3726), 8(X), 2020: http://dx.doi.org/10.7770/safer-V0N0-art2080

RESUMEN

El suelo es el componentemásimportante para satisfacertodas las necesidadesbásicas de los sereshumanos y también es un componenteimportante de nuestraagricultura. El estudio se realizó con el objetivo principal de investigar las muestras de suelo del distrito Pudukkottai de Tamil Nadu para suanálisisfisicoquímico y caracterizaciónestructural. Las muestras de suelorecolectadas se analizaron para determinarsu pH, CE, nitrógeno, fósforo, potasio, zinc y hierro. Además, la muestra se caracterizó por estudios FTIR para conformaciónestructural. A partir del estudio, los resultadosrevelaron que el suelorecogido era rojo y sutextura era francoarcillosoarenoso. El pH del suelo era 9,29, que era alcalino y la CE era 0,02 dSm-1. Los macronutrientesdisponiblescomonitrógeno, fósforo y potasio para muestras de suelo de arrozalestenían 118, 11 y 160 kg / ha, respectivamente. MicronutrientesNutrientestambiénanalizados. El espectro FT-IR del suelo se registró. El espectro del suelomostró que las vibraciones de deformación C-H ocurrenen 1402. Las vibraciones de estiramiento C = C ocurrenen 1644 y las vibraciones de estiramiento N-H ocurrenen 2344. Se discutieron las opciones de manejo para mejorar la fertilidad del suelo.

Palabras clave: pH, CE, Nitrógeno, Fósforo, Potasio, Zinc, FTIR, Fertilidad del suelo

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Dr. A.DHANALAKSHMI

Research Article

Evaluation of Different Soil Textures in Combination with Growing Media on Growth, Yield, and Water Productivity of Blackgram

Dhanalakshmi A, K Karthikeyani Vijayakumari, Marimuthu S & U Surendran

Pages 2670-2682 | Received 10 Apr 2020, Accepted 20 May 2020, Published online: 29 Nov 2020

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ABSTRACT

The production and productivity of blackgram (*Vigna mungo*) are very poor and one of the important reasons is that it is cultivated on marginal lands having low soil fertility and under rainfed conditions without assured irrigation. The present study was aimed to evaluate the different growing media in soil types having varying soil texture and its impact on the growth and yield of blackgram. A pot culture experiment was conducted in split plot design with four texture of soils (S_1: Loamy, S_2: Clay, S_3: Sand and S_4: Pure sand) as the main plots and five growing media (G_1: Cocopeat, G_2: Vermiculite, G_3: Vermicompost, G_4: Sawdust, G_5: Hydrogel and G_6: Control) as the subplots. The results of the experiment revealed that growing of blackgram in sandy soil texture with application of cocopeat recorded significant improvement in growth parameters *viz*., plant height, root length, leaf area index (LAI), nos. of root nodules plant^{-1}. The same treatment resulted in significantly higher yield attributes such as number of pods plant^{-1} (49.3), grain yield

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ABSTRACT

The production and productivity of blackgram (*Vigna mungo*) are very poor and one of the important reasons is that it is cultivated on marginal lands having low soil fertility and under rainfed conditions without assured irrigation. The present study was aimed to evaluate the different growing media in soil types having varying soil texture and its impact on the growth and yield of blackgram. A pot culture experiment was conducted in split plot design with four texture of soils (S_1: Loamy, S_2: Clay, S_3: Sand and S_4: Pure sand) as the main plots and five growing media (G_1: Cocopeat, G_2: Vermiculite, G_3: Vermicompost, G_4: Sawdust, G_5: Hydrogel and G_6: Control) as the subplots. The results of the experiment revealed that growing of blackgram in sandy soil texture with application of cocopeat recorded significant improvement in growth parameters *viz*., plant height, root length, leaf area index (LAI), nos. of root nodules plant^{-1}. The same treatment resulted in significantly higher yield attributes such as number of pods plant^{-1} (49.3), grain yield (1126 kg ha^{-1}), water use efficiency, water productivity and benefit cost ratio over other texture

PG & RESEARCH DEPARTMENT OF PHYSICS
Dr.R.RENUKA

Solanum torvum mediated synthesis and characterization of silver nanoparticles for antibacterial activities

Original Article | Published: 02 February 2021
Volume 30, pages 596–601, (2021) Cite this article

R. Renuka, K. Renuka Devi, M. Sivakami & T. Thilagavathi

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Abstract

The silver nanoparticles (AgNPs) with biogenic synthesis employing plants have been grown to be a promising alternative to the traditional chemical synthesis method. The AgNPs were triumphantly synthesized using *Solanum torvum* (Turkey berry) fruit extract characterized by UV–Visible spectrum as a consequence of strong surface plasmon resonance peak at 442 nm. The existence of bio-molecules acting as a capping and stabilizing agent in the AgNPs with *Solanum torvum* was revealed by Fourier transform infrared spectroscopy analysis. X-ray diffraction investigation for the greener route synthesized AgNPs witnessed as face centered cubic crystalline nature along with an average crystalline size of 25 nm. Scanning electron microscope images evidenced that the nanoparticles have an irregular shape of hexagonal morphology and the presence of silver element was depicted in Energy-dispersive X-ray spectroscope profile. The AgNPs were explored against two gram-positive and negative bacteria via antibacterial activity. The results showed that biosynthesized AgNPs have a strong inhibitory effect on bacteria with a more pronounced inhibition against *Bacillus subtilis*. AgNPs with very high antibacterial activity can also be employed as an efficient material for different medicinal applications.

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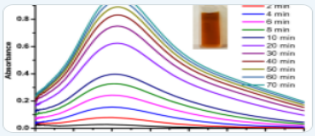

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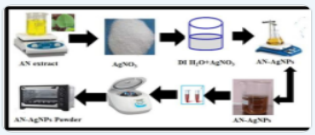

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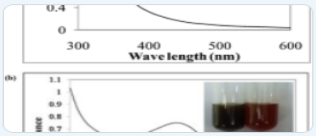

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Dr.R.SANTHAKUMARI

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Synthesis, growth and computational studies on vanillin nicotinamide single crystals

Published: 20 June 2021

Volume 127, article number 544, (2021) Cite this article

M. Buvaneswari, R. Santhakumari, R. Jayasree & Suresh Sagadevan

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Abstract

Vanillin nicotinamide (VN) has been grown by the slow evaporation method using ethanol solvent. The structural parameters and crystalline nature occurring in the crystal were analyzed by X-ray diffraction techniques. The functional groups and vibrational modes were analyzed by spectral studies. The optical absorption property of the VN crystal was analyzed using Ultraviolet–visible spectrophotometer. Thermal stability of the grown crystal was performed through thermogravimetric analysis/differential thermal analysis. The Fourier transform infrared spectrum of VN in solid-phase was recorded in order to identify the functional groups. Density functional theory computations were used by B3LYP/6−3-21G (*d*, *P*) as a standard basis set to optimize molecular geometry. The highest occupied molecular orbital (HOMO)- lowest-unoccupied molecular orbital (LUMO) energy gap and natural bond orbital of the grown VN crystal were examined using the B3LYP/3-21G (*d*, *p*) basis set.

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Dr.S,MUGESHINI

Chinese Journal of Physics
Volume 72, August 2021, Pages 229-239

Growth and computational studies on vanillin isoniazid single crystals

S. Mugeshini [a], R. Santhakumari [a], N. Rajeswari [a], G. Amudha [a], D. Chandrika [a], Suresh Sagadevan [b]

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Highlights

- Vanillin isoniazid (VIN) single crystals were grown
- The optimized structure of the VIN compound was calculated by DFT.
- The vibrational frequencies of the VIN compound were analyzed.
- The vibrational frequencies of the VIN compound were analyzed.
- The energy gap of VIN molecules is computed using HOMO-LUMO
- The Mulliken atomic charge of synthesized VIN molecule has been investigated

Abstract

In this paper, we performed the synthesis, characterization, and computational studies on Vanillin isoniazid (VIN) single crystals grown by the slow evaporation solution growth technique. The crystalline perfection and monoclinic crystal structure with space group C_c have been confirmed using single-crystal X-ray diffraction and powder X-ray diffraction method. The presence of various functional groups has been identified by FTIR and Raman spectroscopy. These data are in good agreement with theoretical and experimental values of FT-IR, FT-Raman.The optical absorption studies were carried out for the grown crystal VIN which has been analyzed by UV–Vis–NIR spectroscopy. Thermogravimetric (TG) and differential thermal analysis (DTA) were carried out to characterize the thermal stability of the VIN crystals. The quantum chemical calculations for VIN crystal are performed at the B3LYP, B3PW91, levels of theory with the 6–311++G(d,p) basis set. Finally, inter-and intramolecular charge transfer, hyper conjugative interaction of the compound is investigated from natural bond orbital (NBO) analysis. The Mulliken atomic charge of VIN single crystal has been investigated using theoretical calculations.

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Dr.R.SANTHAKUMARI

Journal of Molecular Structure
Volume 1239, 5 September 2021, 130449

Synthesis, growth, crystal structure, vibrational, DFT and HOMO, LUMO analysis on protonated molecule–4–aminopyridinium nicotinate

R. Vasanthakumari [a], W. Nirmala [b], Suresh Sagadevan [c], S. Mugeshini [d], N. Rajeswari [d], Ranjith Balu [e], R. Santhakumari [d]

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Highlights

- An organic crystal 4–amino pyridinium nicotinate (4APNA) single crystal has been grown by a slow evaporation method.
- Various functional groups in the grown crystal have been identified using Fourier-transform infrared (FTIR) spectra.
- The suitability of the crystal for optical applications was analyzed through Ultraviolet-Visible-near-IR Spectroscopy (UV–Vis-NIR)studies.
- Theoretical calculations were carried out using density functional theory (DFT).
- The intermolecular interactions that exist inside the crystal have been investigated by Hirshfeld surface evaluation.

Abstract

An organic crystal 4–aminopyridinium nicotinate (4APNA) single crystal has been grown by a slow evaporation method. The crystallinity and structural orientation of as-grown 4APNA compound was thoroughly studied using single-crystal X-ray diffraction and powder X-ray diffraction (XRD) and found to be a monoclinic crystal system with $P2_1/c$ space group. Various functional groups in the grown crystal have been identified using Fourier-transform infrared (FTIR) spectra. The suitability of the crystal for optical applications was analyzed through Ultraviolet-Visible-near-IR Spectroscopy (UV–Vis-NIR)studies. Theoretical calculations were carried out using density functional theory (DFT) to define optical geometry using B3LYP with a 6–311 G (d, p) basis set and the results have been compared with experimental data. The intermolecular interactions that exist inside the crystal have been investigated by Hirshfeld surface evaluation.

Introduction

In recent years, the interest of researchers in various natural materials has improved significantly to grow efficient organic crystals. In telecommunications, frequency doubling, and optical computing processes, organic crystals are important since they act as a source in electro-optics [1], [2], [3], [4], [5], [6], [7], [8]. Inorganic crystals, the strength of van der Waals interactions is important for the intermolecular attraction in the lattice instead of intramolecular chemical bonds. Attention has been given to the latest organic nonlinear optical materials for their advantages over the inorganic substances [9]. Several nonlinear optical complexes have been created from aminopyridine and carboxylates such as 4–aminopyridinium maleate, 4–aminopyridinium hydrogen maleate, 4–aminopyridinium succinate tetrahydrate, 4–aminopyridinium monothalate, 4–aminopyridinium picrate, 4–aminopyridinium chloride, 2–aminopyridinium 4–nitrophenolate 4–nitrophenol, 2–aminopyridinium succinate, and its derivatives are involved in hydrogen bond interactions [10], [11], [12]. This finding plays an essential function in heterocyclic chemistry. Nicotinic acid is a 3–pyridine carboxylic acid and has a pyridine ring with a carboxyl group connected to it [13], [14], [15], [16]. The structure of 4–aminopyridinium nicotinate was reported by Jebas etal. [17]. In the present study, new crystals of 4–aminopyridinium nicotinate (4APNA) have been grown by slow evaporation solution growth method and investigations with the help of FT-IR, FT-Raman, UV, single crystal XRD, DFT, and Hirshfeld analyses have been carried out.

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Dr.R.RAJESWARI

Chinese Journal of Physics
Volume 73, October 2021, Pages 746-755

Synthesis, growth, spectral and computational studies on aminomethylpyridinium trichloroacetate single crystal

N. Rajeswari [a], R. Santhakumari [a], S. Mugeshini [a], D. Chandrika [a], Suresh Sagadevan [b]

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Highlights

- AMPTA single crystals were grown using the slow evaporation technique.
- The spectral, optical, and thermal properties of the AMPTA crystals was studied.
- AMPTA crystals are subjected to quantum chemical calculations.
- The energy gap of AMPTA molecules were computed using HOMO-LUMO.

Abstract

The molecular compounds 2-amino-6-methylpyridine and trichloroacetic acid were synthesized in the ratio 1:1 and a single crystal aminomethylpyridinium trichloroacetate (AMPTA) was grown with the base compound 2-amino-6-methylpyridine (2AMP) as a donor and the acid compound trichloroacetic acid (TA) functions as an acceptor. The modes of vibration with the functional group was investigated from the analysis of FTIR spectroscopy. The existence of proton was prognosticated by ^{1}H NMR spectral analysis. The $\pi \rightarrow \pi^{*}$ transition shifted to wavelength 310nm in UV–vis-NIR spectra confirms the emergence of the AMPTA crystal. The percentage of transmittance spectrum showed the suitability of the compound for non-linear optical applications. TG-DTA analysis was done to study the thermal stability and the melting point of AMPTA crystal was assessed through thermogravimetry (TG) and differential thermal analysis (DTA). The density functional theoretical method (DFT) was carried out with the help of the B3LYP/3-21G(d,p) basis set, and the results were compared with the experimental values.

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Dr.R.SANTHAKUMARI

Journal of Molecular Structure
Volume 1243, 5 November 2021, 130856

Synthesis, growth, structural, spectroscopic, optical, thermal, DFT, HOMO–LUMO, MEP, NBO analysis and thermodynamic properties of vanillin isonicotinic hydrazide single crystal

M. Buvaneswari [a], R. Santhakumari [a], C. Usha [b], R. Jayasree [c], Suresh Sagadevan [d]

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- The vanillin isonicotinic hydrazide (VINH), an organic single crystal
- Single-crystal X-ray diffraction to determine the cell dimensions
- Powder X-ray diffraction to evaluate the planes and phase purity of the crystal
- Spectral, optical, and thermal properties were studied.
- Further, DFT, HOMO–LUMO, MEP, HOMA, NBO analysis were studied
- The dipole moment, linear polarizability, and first hyperpolarizabilities have been investigated as molecular parameters.

Abstract

The work is aimed to present the synthesis and physical analysis of vanillin isonicotinic hydrazide (VINH), an organic single crystal, produced by the method of slow evaporation at room temperature. The grown VINH crystal was subjected to (SXRD) single-crystal X-ray diffraction to determine the cell dimensions. The powder X-ray diffraction study was performed to evaluate the planes and phase purity of the crystal. The presence of functional groups were analyzed through FTIR spectroscopy. UV–Vis–NIR spectroscopy study was carried out to enumerate the cutoff wavelength. Thermogravimetric and differential thermal analysis (TGA/DTA) was done to identify the thermal properties of the grown crystal. Further, the density functional theory (DFT/B3LYP) methods with the 6-311++G(d,p) basis set were used to compute the optimized molecular structure

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Dr.G.AMUDHA

Chinese Journal of Physics
Volume 76, March 2022, Pages 44-58

Synthesis, growth, DFT, and HOMO-LUMO studies on pyrazolemethoxy benzaldehyde single crystals

G. Amudha [a], R. Santhakumari [a], D. Chandrika [a], S. Mugeshini [a], N. Rajeswari [a], Suresh Sagadevan [b]

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Highlights

- A good quality single crystal of Pyrazolemethoxy benzaldehyde (PMB) was
- Single crystal X-ray diffraction study was carried out to study the crystal structure.
- Crystal was characterized by FT-IR and UV–vis spectroscopic techniques.
- Thermal stability of the grown crystal was studied by TG/DTA analyses.
- Density functional theory was applied to obtain the optimized geometry of the crystal.

Abstract

Pyrazolemethoxy benzaldehyde (PMB) was synthesized and crystals were grown by slow evaporation solution growth method. PMB was crystallized in a monoclinic crystal system with a centrosymmetric C2/c space group, according to single-crystal X-ray diffraction analysis. The crystalline planes were identified using powder X-ray diffraction analysis. FTIR - FT-Raman spectroscopic techniques were performed to determine the vibrational modes of functional groups for the grown crystal. UV-visible spectral analysis and photoluminescence studies were taken to investigate the linear optical properties of the grown crystal. Thermogravimetric and differential thermal analysis (TG/DTA) were used to determine the thermal stability of the PMB crystal. In addition to this density functional theory (DFT) calculations such as frontier molecular orbital's (FMOs), global chemical reactivity parameters, hyperpolarizability, natural bond orbital (NBO) analysis, Mullikan atomic charge distribution, and molecular electrostatic potential map analysis were carried out in gaseous phase using B3LYP/6-311G* basis set.

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Dr.S.DHANALAKSHMI

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Vol. 22 (2019), No. 5, pp. 847–855
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Edge domination in Boolean function graph B($\overline{Kp}$, L(G), NINC) of a graph

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Abstract

For any graph G, let $V(G)$ and $E(G)$ denote the vertex set and edge set of G respectively. The Boolean function graph $B(\overline{Kp}, L(G), NINC)$ of G is a graph with vertex set $V(G) \cup E(G)$ and two vertices in $B(\overline{Kp}, L(G), NINC)$ are adjacent if and only if they correspond to two adjacent edges of G or to a vertex and an edge not incident to it in G. For brevity, this graph is denoted by $B_2(G)$. In this paper, Edge domination numbers of Boolean Function Graph $B(\overline{Kp}, L(G), NINC)$ of some standard graphs and corona graphs are obtained.

Subject Classification: *05C15, 05C69*

Keywords: *Boolean Function graph, Edge Domination Number.*

1. Introduction

Graphs discussed in this paper are undirected and simple graphs. For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set

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NEIGHBORHOOD CONNECTED DOMINATION AND ECCENTRIC DOMINATION OF BOOLEAN GRAPH $BG_3(G)$ OF A GRAPH G

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Abstract

Let G be a simple (p, q) graph with vertex set $V(G)$ and edge set $E(G)$. $BG_3(G)$ is a graph with vertex set $V(G) \cup E(G)$ and two vertices are adjacent if and only if they correspond to a vertex and an edge incident to it in G or two non-adjacent edges of G. In this paper, we study the concept of neighborhood connected domination and eccentric domination in Boolean graph $BG_3(G)$.

1. Introduction

Graphs discussed in this paper are undirected and simple graphs. For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set respectively. Let $v \in V$. The open neighborhood $N(v)$ of a vertex v is the set of all vertices adjacent to v in G. $N[v] = N(v) \cup \{v\}$ is called the closed neighborhood of v. If $S \subseteq V$, then $N(S) = \bigcup v \in sN(v)$ and $N[S] = N(S) \cup S$.

A vertex and an edge are said to cover each other if they are incident. A

2020 Mathematics Subject Classification: 05C12, 05C69, 05C76.
Keywords: Neighborhood connected domination number, eccentric domination number, Boolean graph $BG_3(G)$.
Received February 5, 2022; Accepted May 7, 2022

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Dr.RM MARISELVI

Turkish Journal of Computer and Mathematics Education Vol.12 No. 9 (2021), 3229-3236

Research Article

Eccentric Domination in Boolean Graph $BG_2(G)$ of a Graph G

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Article History: Received: 11 January 2021; Revised: 12 February 2021; Accepted: 27 March 2021; Published online: 20 April 2021

Abstract: Let G be a simple (p, q) graph with vertex set V(G) and edge set E(G). $BG_2(G)$ is a graph with vertex set $V(G) \cup E(G)$ and two vertices are adjacent if and only if they correspond to two adjacent vertices of G, a vertex and an edge incident to it in G or two non-adjacent edges of G. In this paper, we studied eccentric domination number of Boolean graph $BG_2(G)$, obtained bounds of this parameter and determined its exact value for several classes of graphs.

Keywords: Domination number, eccentric domination number, Boolean graph.

1.Introduction

Let G be a finite simple, undirected graph on p vertices and q edges with vertex set V(G) and edge set E(G). For graph theoretic terminology refer to Harary[11], and Kulli[17].

The distance d(u, v) between two vertices u and v in G is the minimum length of a path joining them if any; otherwise $d(u, v) = \infty$. Let G be a connected graph and u be a vertex of G. The eccentricity e(v) of v is the distance to a vertex farthest from v. Thus, $e(v) = \max\{d(u, v): u \in V\}$.The radius r(G) is the minimum eccentricity of the vertices, whereas the diameter diam(G) is the maximum eccentricity. For any connected graph G, $r(G) \leq diam(G) \leq 2r(G)$. The vertex v is a central vertex if $e(v) = r(G)$. The center C(G) is the set of all central vertices. The central sub graph $\langle C(G)\rangle$ of a graph G is the subgraph induced by the center. The vertex v is a peripheral vertex if $e(v) = diam(G)$. The periphery P(G) is the set of all peripheral vertices. For a vertex v, each vertex at a distance e(v) from v is an eccentric vertex. Eccentric set of a vertex v is defined as $E(v) = \{u \in V(G) : d(u, v) = e(v)\}$. A graph is self-centered if every vertex is in the center. Thus, in a self-centered graph G all vertices have the same eccentricity, so $r(G) = diam(G)$.

A vertex and an edge are said to cover each other if they are incident. A set of vertices which covers all the edges of a graph G is called a point cover for G, while a set of edges which covers all the vertices is a line cover. The smallest number of vertices in any point cover for G is called its point covering number or simply covering number and is denoted by $\alpha_0(G)$ or α_0. Similarly, α_1 is the smallest number of edges in any line cover of G and is called its line cover number. A set of vertices in G is independent if no two of them are adjacent. The largest number of vertices in such a set is called the point independence number of G and is denoted by $\beta_0(G)$ or β_0. A set of edges in a graph is independent if no two edges in the set are adjacent. By a matching in a graph G, we mean an independent set of edges in G. The edge independence number $\beta_1(G)$ of a graph G is a maximum cardinality of an independent set of edges. A perfect matching is a matching with every vertex of the graph is incident to exactly one edge of the matching. The graph G^+ is obtained from the graph G by attaching a pendant edge to each of the vertices of G.

The open neighborhood N(v) of a vertex v is the set of all vertices adjacent to v in G. $N[v] = N(v) \cup \{v\}$ is called the closed neighborhood of v. The second neighborhood $N_2(v)$ of a vertex v is the set of all vertices at distance two from v in G.

In 2007, Janakiraman, Bhanumathi and Muthammai defined the Boolean graph $BG_2(G)$ and studied its properties [12, 14, 15, 16]. Boolean graph $BG_2(G)$ is a graph with vertex set $V(G) \cup E(G)$ and edge set $\{E(T(G)) - E(L(G))\} \cup E(\overline{L(G)})$, where L(G) is the line graph of G and T(G) is the total graph of G. It is a graph with vertex set $V(G) \cup E(G)$ and two vertices are adjacent if and only if they correspond to two adjacent vertices of G, a vertex and an edge incident to it in G or two non-adjacent edges of G.

The concept of domination in graphs was introduced by Ore [18]. A set $D \subseteq V(G)$ is said to be a dominating set of G, if every vertex in $V(G) - D$ is adjacent to some vertex in D. D is said to be a minimal dominating set if $D - \{u\}$ is not a dominating set for any $u \in D$. The domination number $\gamma(G)$ of G is the minimum cardinality of a dominating set [10].

Janakiraman, Bhanumathi and Muthammai [13] introduced the concept of eccentric domination number of a graph. Eccentric domination in trees and various types of eccentric dominations were studied in [2, 3, 4, 5, 6, 7, 8, 9].

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Dr.RM MARISELVI

Neighborhood Connected Domination and Eccentric Domination in Boolean Graph BG1(G) of a Graph G,

Authors Bhanumathi.M and Mariselvi. R.M.

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NEIGHBORHOOD CONNECTED DOMINATION AND ECCENTRIC DOMINATION IN BOOLEAN GRAPH $BG_1(G)$ OF A GRAPH G

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Abstract: *Let G be a simple (p, q) graph with vertex set V(G) and edge set E(G). $BG_1(G)$ is a graph with vertex set $V(G) \cup E(G)$ and two vertices are adjacent if and only if they correspond to two adjacent vertices of G or to a vertex and an edge not incident to it in G. In this paper, we study the concept of neighborhood connected domination number and eccentric domination number of Boolean graph $BG_1(G)$, obtained bounds of these parameters and determined its exact value for several classes of graphs. We also find the exact value of $\gamma_{nd}(BG_1(G))$ when G is a connected graph with pendant vertices and characterize graphs G for which $\gamma_{nd}(BG_1(G)) = 2$.*

Keywords: **Neighborhood connected domination number, eccentric domination number, Boolean graph $BG_1(G)$.**

1.INTRODUCTION

Graphs discussed in this paper are undirected and simple graphs. For a graph G, let V(G) and E(G) denote its vertex set and edge set respectively. Let $v \in V$. The open neighborhood N(v) of a vertex v is the set of all vertices adjacent to v in G. $N[v] = N(v) \cup \{v\}$ is called the closed neighborhood of v. If $S \subseteq V$, then $N(S) = \bigcup_{v \in S} N(v)$ and $N[S] = N(S) \cup S$. The degree of vertex v is the number of edges incident with it and is denoted deg v or $\deg_G v$. The minimum degree among the vertices of a graph G is denoted by $\delta(G)$, while the maximum degree $\Delta(G)$ is the largest such number.

A vertex and an edge are said to cover each other if they are incident. A set of vertices which covers all the edges of a graph G is called a point cover for G, while a set of edges which covers all the vertices is a line cover. The smallest number of vertices in any point cover for G is called its point covering number or simply covering number and is denoted by $\alpha_0(G)$ or α_0. Similarly, α_1 is the smallest number of edges in any line cover of G and is called its line cover number. A set of vertices in G is independent if no two of them are adjacent. The largest number of vertices in such a set is called the point independence number of G and is denoted by $\beta_0(G)$ or β_0. A set of edges in a graph is independent if no two edges in the set are adjacent. By a matching in a graph G, we mean an independent set of edges in G. The edge independence number $\beta_1(G)$ of a graph G is a maximum cardinality of a independent set of edges. A perfect matching is a matching with every vertex of the graph is incident to exactly one edge of the matching. The graph G^+ is obtained from the graph G by attaching a pendent edge to each of the vertices of G.

The distance d(u, v) between two vertices u and v in G is the minimum length of a path joining them if any; otherwise $d(u, v) = \infty$. Let G be a connected graph and v be a vertex of G. The eccentricity e(v) of v is the distance to a vertex farthest from v. Thus, $e(v) = \max\{d(u, v): u \in V\}$.The radius r(G) is the minimum eccentricity of the vertices, whereas the diameter diam(G) = d(G) is the maximum eccentricity. For any connected graph G, $r(G) \leq diam(G) \leq 2r(G)$. The vertex v is a central vertex if e(v) = r(G). The center C(G) is the set of all central vertices. The central sub graph $\langle C(G) \rangle$ of a graph G is the subgraph induced by the

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Connected edge, Split edge and domatic edge domination number inBoolean functio graphB(Kp_, L(G), NINC) of a graph

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Connected edge, Split edge and Domatic edge Domination numbers in Boolean Function Graph B($\overline{Kp}$, L(G), NINC) of a graph

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Abstract

For any graph G, let V(G) and E(G) denote the vertex set and edge set of G respectively. The Boolean function graph B($\overline{Kp}$, L(G), NINC) of G is a graph with vertex set V(G)∪E(G) and two vertices in B($\overline{Kp}$, L(G), NINC) are adjacent if and only if they correspond to two adjacent edges of G or to a vertex and an edge not incident to it in G. For brevity, this graph is denoted by $B_2(G)$. In this paper, Connected edge, Split edge and domatic edge number of Boolean Function Graph $B_2(G)$ of some standard graphs are obtained.

Keywords: Boolean Function graph, Edge Domination Number.

1. Introduction

Graphs discussed in this paper are undirected and simple graphs. For a graph G, let V(G) and E(G) denote its vertex set and edge set respectively. A subset D of V is called a dominating set of G, if every vertex not in D is adjacent to some vertex in D. The domination number γ(G) of G is the minimum cardinality taken over all dominating sets of G. An edge e of a graph is said to be incident with the vertex v if v is an end vertex of e. In this case, it can also be said that v is incident with e. A subset F ⊆ E is called an edge dominating set of G, if every edge not in F is adjacent to some edge in F. The edge domination number γ'(G) of G is the minimum cardinality taken over all edge dominating sets of G. An edge dominating set F of G is called a total edge dominating of G if the induced subgraph ⟨F⟩has no isolated edges. The total edge domination numberγ_t'(G) of G is the minimum cardinality taken over all of total edge dominating sets of G. An edge dominating set F of is called a connected edge dominating set of G if the induced subgraph ⟨F⟩ is connected. The connected edge domination number γ_c'(G) of G is the minimum cardinality taken over all connected edge dominating sets of G. An edge dominating set F ⊆ E of a connected graph G is a split edge dominating set, if the induced subgraph < E(G) − F > is disconnected. The split edge domination number γ_s'(G) of G is the minimum cardinality of a split edge dominating set. The maximum order of a partition of E into edge dominating sets of G is called the edge domatic number of G and is denoted by d'(G). The concept of edge domination was introduced by Mitchell and Hedetniemi [6]. Arumugam and Velammal [1] have discussed

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K-Eccentric indices of polyhex nanotubes TUAC6(p, q) and TUZC6(p, q),

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K-ECCENTRIC INDICES OF POLYHEX NANOTUBES TUAC$_6$(p, q) AND TUZC$_6$(p, q)

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Abstract: In this paper, we evaluate some eccentricity based topological indices known as K-eccentric indices for armchair polyhex nanotubes TUAC$_6$(p, q) and zigzag polyhex nanotubes TUZC$_6$(p, q).

Keyword: Eccentricity index, Line graph, K-eccentric indices, polyhex nanotubes.

I.Introduction

Let G be a simple, finite graph with n vertices and m edges with vertex set V(G) and edge set E(G). The edge connecting the vertices u and v ∈ V(G) is denoted by e = uv. The vertices and edges of a graph are called elements of G.

We construct a graph L(G) in the following way: The vertex set of L(G) is in 1-1 correspondence with the edge set of G and two vertices of L(G) are joined by an edge if and only if the corresponding edges of G are adjacent in G. The graph L(G) (which is always a simple graph) is called the line graph or edge graph of G.

Let G be a connected graph and v be a vertex of G. The eccentricity e(v) of v is the distance to a vertex farthest from v. Thus, e(v) = max{d(u, v): u ∈ V}. The radius r(G) is the minimum eccentricity of the vertices, whereas the diameter diam(G) is the maximum eccentricity.

The topological indices are one of the mathematical models that can be defined by assigning a real number to the chemical molecule. The physical-chemical characteristics of the molecules can be analyzed by taking benefit from the topological indices and such properties as boiling point, entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, acetic factor, etc can be predicted.

In [1], Bhanumathi and Easu Julia Rani, introduced the K- Eccentricity indices. They defined the first and second K-eccentric indices as

$B_1E(G) = \sum_{uv}[(e_G(u) + e_{L(G)}(e)]$

$B_2E(G) = \sum_{uv}[(e_G(u).e_{L(G)}(e)]$ and the first and second K-Hyper Eccentricity indices as

$HB_1E(G) = \sum_{uv}[(e_G(u) + e_{L(G)}(e)]^2$

$HB_2E(G) = \sum_{uv}[(e_G(u).e_{L(G)}(e)]^2$

In [2], Bhanumathi and Easu Julia Rani, introduced Multiplicative K - Eccentric Indices. They were defined as

$B\Pi_1E(G) = \prod_{uv}[e_G(u) + e_{L(G)}(e)]$

$B\Pi_2E(G) = \prod_{uv}[e_G(u).e_{L(G)}(e)]$ and the first and second Multiplicative K-Hyper Eccentric Indices

$HB\Pi_1E(G) = \prod_{uv}[e_G(u) + e_{L(G)}(e)]^2$ and $HB\Pi_2E(G) = \prod_{uv}[e_G(u).e_{L(G)}(e)]^2$ where e ∈ E(G) is incident with u in G, $e_G(u)$ denotes the eccentricity of u ∈ V(G) in G and $e_{L(G)}(e)$ denotes the eccentricity of e in

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Growth and combined experimental and quantum chemical study of glycyl-L-Valine crystal

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Abstract

Glycyl-L-Valine (GLV) crystals were grown using distilled water as the solvent at room temperature by solution growth technique. Powder X-ray diffraction confirms the crystalline quality of GLV crystal. The molecular structure of GLV crystal was identified by ^{13}C NMR spectral studies. The nonlinear optical (NLO) behavior of the crystal was found to be ~4.3 times greater than that of potassium dihydrogen orthophosphate. FT-Raman and FT-IR spectra of the GLV were recorded and complete functional group assignment of the determined vibrational bands of GLV have been reported. Density functional theoretical method (DFT) was performed using B3LYP with the 6-311+G (d, p) basis set and the results were compared with the experimental values which confirm the intermolecular interactions responsible for the enhanced NLO activity of the molecule, as evident from NBO and Hirshfeld analyses. The calculated HOMO and LUMO

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Biosynthesis of silver nanoparticles using *phyllanthus emblica* fruit extract for antimicrobial application

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Abstract

Biological synthesis of metal nanoparticles is one of the effortless, cost - effective, environmental - friendly methods and scale down the handling of toxic chemicals. The silver nanoparticles were triumphantly synthesized from the silver nitrate solution through a greener route using Indian gooseberry (phyllanthus emblica) fruit extract and

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Growth, spectral, density functional theory (DFT) and Hirshfeld surface analysis on 4-aminopyridinium adipate monohydrate nonlinear optical single crystal

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4-aminopyridinium adipate monohydrate (4APA) was grown by slow evaporation solution growth technique. The functional groups in the grown crystal were identified from FT-IR spectral evaluation. The optical properties together with transmittance of the grown crystal were obtained from UV-Vis spectroscopic study. The mechanical and thermal properties of the grown crystal were studied using Vickers microhardness and TGA/DTA analyses, respectively. Microhardness test revealed that 4-aminopyridinium adipate monohydrate crystal is a soft category material. The density functional method (DFT) was performed using B3LYP with the 6-311G (d,p) basis set. The electronic charge distribution, reactivity of the molecules and the molecular electrostatic potential (MEP) of the grown crystal were analyzed using the B3LYP method. The intermolecular interactions that exist in the crystal structure of the 4APA have also been investigated by Hirshfeld surface analysis. The nonlinear optical properties of the 4APA crystal were confirmed by Kurtz-Perry technique.

Keywords: *crystal growth; growth from solution; Hirshfeld; DFT; organic material; nonlinear optical material*

1. Introduction

Materials exhibiting large optical nonlinearity are of great interest for the applications such as frequency conversion, telecommunications, optical computing, optical information processing and optical disk data storage [1–3]. The common knowledge is that an optical material should have a large charge transfer and optical transparency as well as low dislocation density. In recent years, the search for organic single crystal for the application in telecommunications, frequency doubling and optoelectronics has increased considerably [4–8]. The development of new organic nonlinear optical materials is attractive because of their advantages over the inorganic nonlinear optical materials. Aminopyridine and carboxyl groups together form many nonlinear optical complexes. Hydrogen bond interactions that exist in pyridine are the most important in heterocyclic chemistry. Adipic acid forms crystalline adipate via hydrogen bonding. It is known that adipic acid, though not the best as an acceptor forming various stacking complexes with different aromatic molecules, can also be useful as an acidic ligand. 4-aminopyridinium adipate is one of such donor-acceptor molecular compounds wherein adipic acid gives one of its proton (H) to the 4-aminopyridine, and adipic acid is transformed to mono-ionized state. In general, adipic acid can exist in acid and adipate forms in neutral and ionized state, respectively. In the ionized state it forms a robust intramolecular hydrogen bond with other molecule and also 4-aminopyridine molecules can exist in neutral and protonated state. The structure of 4-aminopyridinium adipate (4APA) has already been predicted [9]. Similarly to the above studies,

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Somatic embryogenesis from stem thin cell layers of *Dendrobium aqueum*

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Abstract

An efficient *in vitro* regeneration protocol through somatic embryogenesis was established from stem transverse thin cell layers (tTCLs) of *Dendrobium aqueum* Lindley, an imperiled orchid. This study outlines the induction and successive maturation stages of *D. aqueum* somatic embryos (SEs). The tTCLs (~ 0.5 mm thick) cultured on half-strength Murashige and Skoog (MS) medium containing cytokinins and auxins, either individually or in combination, produced embryogenic callus (EC). Treatment with 0.5 mg dm^{-3} zeatin induced EC in 41.42 % of tTCLs. As many as 42.66 globular SEs per tTCL were formed in the presence of 1.5 mg dm^{-3} N^6-(2-isopentyl) adenine (2iP) but only on 10.33 % of explants. The combined treatment of 2iP (1.5 mg dm^{-3}) and 0.5 mg dm^{-3} 6-benzyladenine resulted in 34 globular SEs on 14.7 % of tTCLs whereas the combination of 2iP and 1.0 mg dm^{-3} indole-3-butyric acid (IBA) induced 7.4 globular SEs on 52.33 % of tTCLs. Supplementation of activated charcoal, amino acids, and antioxidants alleviated browning at all the concentrations tested, but the EC response declined. The addition of 0.5 mg dm^{-3} polyvinylpyrrolidone to 1.5 mg dm^{-3} 2iP and 1.0 mg dm^{-3} IBA produced 24 SEs on 19.89 % of tTCLs suggesting that the EC and SEs can be effectively induced by individual cytokinins whereas the synergistic treatments with other compounds can only enhance the induction of EC. Histological observations of EC showed the formation of globular SEs from sub-epidermal regions. Successive developmental stages of globular SEs and the intermediate stage of protocorm like bodies until the formation of plantlets were observed. The plantlets obtained through SEs showed no morphological variations, and inter simple sequence repeat profiles also confirmed the genetic fidelity of *in vitro*-derived progeny with high monomorphism (97.78 %). In conclusion, the use of stem tTCLs is an effective method to produce SEs through indirect somatic embryogenesis in *D. aqueum*.

Additional key words: auxins, cytokinins, epiphyte, embryogenic callus, *in vitro* culture, ISSR, protocorm like bodies.

Introduction

The *Orchidaceae*, one of the largest, most highly evolved, and diverse families of flowering plants, contains about 35 000 species belonging to 850 genera (Hossain *et al.* 2013). *Dendrobium* is a large genus of the *Orchidaceae* with about 1 600 species worldwide, and 116 can be found in India (Misra 2007). *Dendrobium aqueum* Lindley is an endemic orchid distributed in the Kolli hills (Namakkal) and Shervarayans (Salem) of Eastern Ghats, Tamil Nadu, India (Matthew 1983). Natural *D. aqueum* populations are declining due to anthropogenic activities such as the collection of orchids and habitat destruction. This species was categorized as near threatened in 2000 by the International Union for Conservation of Nature and Natural Resources (Kumar *et al.* 2001), and subsequent field studies at the Kolli hills have recorded a continual decline of this natural population (Sudhakar Reddy *et al.* 2005). Studies on the phenology and *in vitro* propagation through asymbiotic seed germination and protocorms have been already achieved in *D. aqueum* (Parthibhan *et al.* 2012,

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Abbreviations: 2iP - N^6-(2-isopentyl) adenine; AC - activated charcoal; BA - 6-benzyladenine; DSE - direct somatic embryogenesis; EC - embryogenic callus; IAA - indole-3-acetic acid; IBA - indole-3-butyric acid; ISSR - inter simple sequence repeat; KN - kinetin; MS - Murashige and Skoog; NAA - 1-naphthalene acetic acid; PGR - plant growth regulator; PLB - protocorm-like body; PVP - polyvinylpyrrolidone; SE - somatic embryo; tTCL – transverse thin cell layer; TDZ - thiadiazuron; ZEA - zeatin.
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Spectral analysis, investigation of global reactivity, NBO and computation of thermodynamic functions of 1,2,4-benzene tricarboxylic acid using DFT calculations

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