

# COMMUNICATIVE ENGLISH - II

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## PREFACE

This textbook on Communicative English envisioned under the leadership of the Hon. Chief Minister of Tamilnadu, **Thiru. Edappadi K. Palaniswami**, by the Honorable Minister for Higher Education **Thiru. K.P. Anbalagan**, and Principal Secretary to Government, Department of Higher Education, **Selvi. Apoorva**, I.A.S., is a pioneering venture and strategic intervention in higher education in Tamil Nadu. It has been prepared with the unstinted support of **Thiru. Vivekanandan**, I.A.S. Member Secretary, TANSCH (Tamil Nadu State Council for Higher Education)

Having achieved the highest GER (Gross Enrolment Ratio), of 50% in higher education in the country, a key indicator of horizontal growth/access to higher education, Tamil Nadu endeavours to fortify this achievement with vertical growth, i.e. by focusing on quality/excellence in higher education. Given the fact that language proficiency is integral to the learning process, the Communicative English courses for Semester 1 and II have been designed to address the competencies that every student needs to acquire in the first year of the undergraduate programme itself.

**Communicative English (Semester II)** has built on the competencies developed in Semester 1 and has much to offer the progressive student and the committed teacher.

# COMMUNICATIVE ENGLISH II

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- b. Listening to problems and offering solutions (informal)

#### 2. Reading and writing

- a. Reading aloud (brief motivational anecdotes)
- b. Writing a paragraph on a proverbial expression/motivational idea.

#### 3. Word Power/Vocabulary

- a. Synonyms & Antonyms

#### 4. Grammar in Context

- Adverbs
- Prepositions



## **UNIT - II**

**2.1 – 2.97**

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- b. Making short speeches- Formal: welcome speech and vote of thanks. Informal occasions- Farewell party, graduation speech

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- a. Writing opinion pieces (could be on travel, food, film / book reviews or on any contemporary topic)
- b. Reading poetry
  - b.i. Reading aloud: (Intonation and Voice Modulation)
  - b.ii. Identifying and using figures of speech - simile, metaphor, personification etc.

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- c. Dramatizing everyday situations/social issues through skits. (writing scripts and performing)

### **3. Word Power**

- a. Collocation

### **4. Grammar in Context: Working with Clauses**

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# 1

## LISTENING AND SPEAKING

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### LISTENING AND SPEAKING

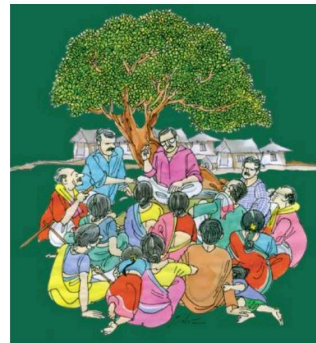
In the Listening and Speaking section of this unit the focus is on listening to “complaints” (in a formal context) and listening to “problems and offering solutions” (informal). “Complaints” call for “action” to be taken after the facts have been ascertained. With regard to listening to “problems”, the listener has to practice active listening and “offer solutions” or “suggest ways” by which the problem can be solved. The onus to solve the problem is not on the listener. Decision-making rests with the one who shares the problem and seeks solutions.

#### Listening and responding to complaints (formal situation)

Complaints could be made in a forum or individually

#### Making Complaints in a Forum

The healthy practice of listening and responding to complaints is deeply ingrained in the administrative system of our country. The village panchayat is a forum where complaints are received and issues resolved.



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# A HANDBOOK ON LITERARY FORMS

Anupama Jose, currently working as Assistant Professor in the Department of English at Nanjil Catholic College, Kaliyakkavilai. She had did her UG and PG under MS university. She had cleared KTET, KSET, and TNSET.

This is a Guide to help the literature students to get the basic ideas regarding different genres in literature in an easy and understandable way. This book covers the history and characteristics of most of the genres in a short and crispy manner. This book will help the students in preparing for their university exam as well as competitive exams. This will also be quite useful for TET, SET, TRB, and UGC NET English aspirants. This book mainly focusses on 1st UG students of MS University.



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**Anupama Jose**



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Prescribed Text: A Background to the Study of English Literature (Revised Edition). B. Prasad, Macmillan

# Section I – Poetry

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# UNIT-I

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## The lyric

### Introduction

- Lyric means Song
- Originated in Greek
- Greek song is divided into two types
  - Melic/ Lyric song – Sung by a single voice with the accompaniment of a lyre
  - Choric song – Intended for collective singing with the accompaniment of instrumental music along with dance.
- Characteristics of lyric – 2
  - a) It is an expression of a single emotion
  - b) It is a musical composition

### The Music in the Lyric

- In ancient times
  - Music provided by the minstrel's harp or lyre formed an external accompaniment to lyric.
  - The language is unpolished in lyric, but the voice of the singer keeping tune with the sound of the instrument gives musical effect for it.
- The more importance was given to the voice of the singer which gives the right emotional effect than the subject matter of lyric.
- Elizabethans
  - Masters in the art of inventing words with the highest musical quality
  - Their lyrics are matchless for their words-music or verbal melody.

- Vowels and consonants are so artistically arranged as to compose a music of their own
- Thus lyric has become independent of the aid of a musical instrument.
- Lyric has been developed as an art by the poets such as Keats, Shelley, Tennyson and Swinburne.
- Tennyson has been universally praised for his word of music.  
*O hark, o hear! How thin and clear,  
And thinner, cleaner, farther going!  
O sweet and far from cliff and scar  
The horns of Elfland faintly blowing*

Note the alliteration and the artistic arrangement of the consonants r, n, s, f and i. There is sufficient music in the words themselves. The lyric has become independent of the lyre.

### **The Subject-Matter of the Lyric**

- Lyric appeals to the heart than to the intellect.
- As a rule it is brief as a song
- The poet wishes to convey his impression swiftly, memorable and musically through his lyric.
- Edger Allan Poe declared that a long lyric was not possible, as “that degree of excitement which would entitle a poem to be so called at all, cannot be sustained through a composition of any great length”
- Lyric is a subjective poem, as it expresses the poet’s emotions

### **The structure of the lyric**

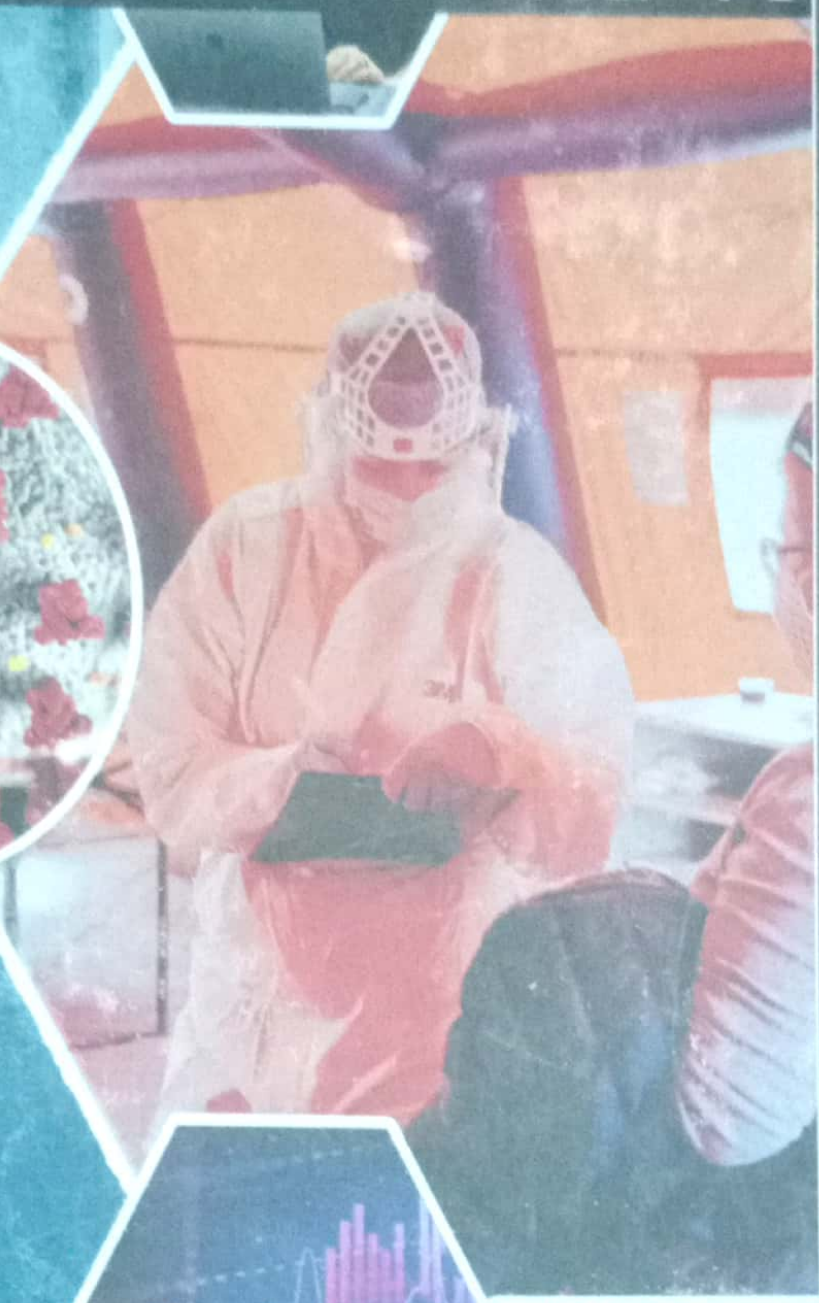
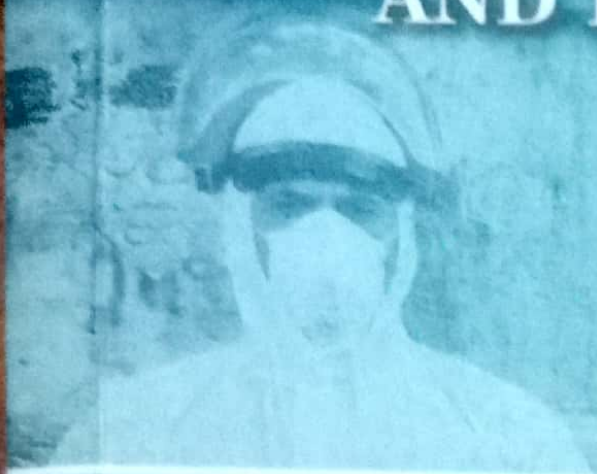
- Lyric, divided into three parts.
- Based on the three moods through which the poet passes
  - 1<sup>st</sup> part
    - First few lines of the lyric
    - States the emotion or the subject which has set the poet’s imagination work
    - N. Hepple calls it as “Motive”
  - 2<sup>nd</sup> part



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**ETHNIC TRAUMA: A STUDY ON TRANSFUSION  
IN NADINE GORDIMER'S *THE PICKUP*  
AND *JULY'S PEOPLE***

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**Abstract:**

South African literature, a branch of African literature, which spread aroma of South African social, economic and political history to the world. Nadine Gordimer is one of the most powerful writers of South Africa, expressed the first hand realistic experience of the oppression of the natives widen the scope of writing in all fields of literature. The paper 'Ethnic Trauma: A Study on Transfusion in Nadine Gordimer's *The Pickup* and *July's People*' focuses on the ethnic flavours spreads in the novel *The Pickup* and *July's people*. It also discusses the issues of hybrid, identity, nationality and migration.

**Key words: Exile, Black consciousness, Language barrier, Migration.**

South African literature is an outcome of hardship and oppression of the land. It is internally fractured due to the black and white writers' contribution from different background. It consists of colonial liberal and radical writings by the white writers' hands whereas the racialism, Africanism and black consciousness by the other. The experiences of oppression provoked the Blacks to contribute the literature. Nadine Gordimer's *The Pickup* and *July's people* have a scrupulous study of life in exile. It also focuses on the idea of immigration and identity in exile.



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## Total Onto Minus Domination Number of Graphs

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### Abstract

A total onto minus dominating function of the graph  $G$  is the total minus dominating function in which the range set is the entire co-domain. The total onto minus domination number of the graph  $G$  is the minimum weight of the set of total onto minus dominating functions of the graph  $G$ . In this paper we have to find out the total onto minus domination number of some graphs.

**Keywords:** Total onto minus dominating function; Total onto minus domination number; Petersen graph; Theta graph; Complete Bi-partite graph.

### 1. Introduction

The total minus dominating function of the graph  $G$  and total minus domination number of  $G$  is defined in [6]. A total onto minus dominating function of the graph  $G$  is the total minus dominating function in which the range set is the entire co-domain. The total onto minus domination number of the graph  $G$ , denoted by  $\gamma_{to}^-(G)$  is defined as the minimum weight among all the total onto minus dominating functions on  $G$ . By the definition  $\{f|f \text{ is a total onto minus dominating function on } G\}$  is a subset of  $\{f|f \text{ is a total minus dominating function on } G\}$ . From this we have  $\min\{f(V)|f \text{ is a total onto minus dominating function of } G\} \geq \min\{f(V)|f \text{ is a minus dominating function of } G\}$ , that is  $\gamma_t^-(G) \leq \gamma_{to}^-(G)$ . Thus if there exists a total onto minus dominating function of weight  $\gamma_t^-(G)$  then  $\gamma_{to}^-(G) = \gamma_t^-(G)$ . If such kind of functions do not exist for the graph  $G$  then we define  $\gamma_{to}^-(G) = \infty$ .

**Theorem: 1** In a graph  $G$ , if  $|N(v)| \leq 2$  for every  $v \in V(G)$  then the graph  $G$  has no total onto minus dominating function.

**Proof:** Let  $G$  be a graph with  $|N(v)| \leq 2 \forall v \in V$ . To get an onto function  $f: V \rightarrow \{-1,0,1\}$  we must assign  $-1$  to one of the vertex  $v_i$  in  $G$ . Since  $|N(v_i)| \leq 2$ ,  $v_i$  has at-most two neighbours say  $v_{i-1}$  &  $v_{i+1}$ . Now for the vertex  $v_{i-1}$  one of the neighbour is  $v_i$  and also it has at-most one neighbour that must assign one of the value from the set  $\{-1,0,1\}$ . In either case we have  $f(N(v_{i-1})) \leq 0$ . Hence the function  $f$  is not a total minus dominating function. Hence there does not exist a total onto minus dominating function for the graph  $G$ .  $\square$

Under any total onto minus dominating function we cannot assign  $-1$  to a vertex, which is adjacent to a vertex of degree less than or equal to 2. For, Suppose under a total onto minus dominating function  $f: V \rightarrow \{-1,0,1\}$  if we assign  $-1$  to a vertex  $v \in V$ , which is adjacent to a vertex  $u \in V$  for which  $deg_G u \leq 2$ . This implies  $deg_G u = 1$  or  $2$ . If  $deg_G u = 1$  then  $N(u) = \{v\}$ . Hence  $f(N(u)) = f(v) = -1 < 1$ . Which is not possible. Again if  $deg_G u = 2$  then there



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### 30. Onto Minus Domination Number of Complete Bi-partite Graph

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#### Abstract

Let  $G = (V, E)$  be a graph with  $n$  vertices. An onto minus dominating function and the onto minus domination number of a graph  $G$  is defined in [1]. In this paper we determined the onto minus domination number of a Complete Bipartite graph, Theta graph, Hajo's graph, Pan graph.

**Keywords:** Minus domination number, Onto minus dominating function, Onto minus domination number, Complete bi-partite graph.

**AMS Classification Number:** 05C69.

#### Introduction

Domination theory has large classification of applications in graph theory. In this interesting application oriented area we focus our attention to minus domination theory. For the clarity of closed neighborhood see [3]. The weight of the real valued function  $f$  is defined in [3]. If a graph  $G$  has no onto minus dominating function then we define its onto minus domination number  $\gamma_o^-(G)$  is equal to  $\infty$ . In this paper we determine the onto minus domination number of a complete bipartite graph  $K_{m,n}$ , Theta graph  $T_a$ , Hajo's graph  $H$  and Pan graph. In real life the definition of onto minus domination is explained as follows.

Suppose we want to collect the feedback of something among a certain set of people (vertices) and they are related (edges) in such a way that the set





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## ONTO MINUS DOMINATION NUMBER OF SOME SMALL GRAPHS

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### Abstract

A minus dominating function  $f: V \rightarrow \{-1, 0, 1\}$  is said to be an onto minus dominating function if it is onto. The weight of an onto minus dominating function  $f$  on  $G$  is  $f(V) = \sum f(v)$  where the sum ranges over all vertices of  $G$ . The onto minus domination number of a graph  $G$ , denoted by  $\gamma_o^-(G)$ , equals the minimum weight of a set of all onto minus dominating functions on  $G$ . In this paper we discuss the onto minus domination number of some small graphs.



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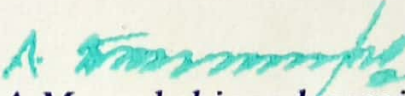
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## Nonsplit Geodetic Number of A Fuzzy Graph

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### Abstract

In this paper, the concept of nonsplit geodetic number  $g_{ns}(G)$ , of a fuzzy graph  $G$  is introduced and its limiting bounds are identified. It is proved that all extreme nodes of  $G$  of the underlying crisp graph  $G^*$  belong to every connected geodetic cover of  $G$ . The nonsplit geodetic number of complete fuzzy graphs and fuzzy cycle graphs are obtained. It is proved that for any pair  $k, n$  of integers with  $3 \leq k \leq n$ , there exists a connected fuzzy graph  $G: (V, \sigma, \mu)$  on  $n$  vertices such that  $g_{ns}(G) = k$ .

**Keywords :** Fuzzy Graph, Geodetic number, Nonsplit Geodetic number.

### 1. Introduction

Fuzzy graphs are introduced by Rosenfeld[1]. Rosenfeld has obtained the fuzzy analogue of several graph theoretic concepts like paths, cycles, trees and connectedness and established some of the properties [1]. Bhattacharyahas introduced fuzzy groups and metric notion in fuzzy graphs. Bhutani and Rosenfeld have introduced the concept of strong arcs [3] and geodetic distance in fuzzy graphs [4]. The definition of a geodetic basis, median are also given by the same author. Several important works on fuzzy graphs can be found in [2]. In this paper, the concept of nonsplit geodetic number,  $g_{ns}(G)$ , of a fuzzy graph  $G$  is introduced and its limiting bounds are identified. It is proved that all extreme vertices of  $G$  of the underlying crisp graph  $G^*$  belong to every connected geodetic cover of  $G$ . The nonsplit geodetic number of complete fuzzy graphs and fuzzy cycle graphs are obtained.

### 2. Preliminaries

Let  $G = (V, E)$  be a graph with vertex set  $V(G)$  and edge set  $E(G)$ . Fuzzy graph theory has several applications in various fields like clustering analysis, database theory, network analysis, information theory etc. In this section, some basic aspects that are necessary for this paper are included.

#### 2.1. Definition

A fuzzy set is characterized by a membership function  $\sigma$  mapping the elements of the domain  $V$  to the unit interval  $[0,1]$ . That is,  $\sigma: V \rightarrow [0,1]$ . Thus a fuzzy set  $\sigma$  in  $V$  may be represented as a set of ordered pairs of a generic element  $u \in V$  and its grade of membership  $\sigma = \{\sigma(u) / u \in V\}$ .





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## 28. Nonsplit Geodetic Parameters of Some Special Graphs

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**Abstract:** Let  $G$  be a graph. If  $u, v \in V(G)$ , a  $u - v$  geodesic of  $G$  is the shortest path between  $u$  and  $v$ . The closed interval  $I[u, v]$  consists of all vertices lying in some  $u - v$  geodesic of  $G$ . For  $S \subseteq V(G)$  the set  $I[S]$  is the union of all sets  $I[u, v]$  for  $u, v \in S$ . A set  $S$  is a geodetic set of  $G$  if  $I(S) = V(G)$ . The cardinality of a minimum geodetic set of  $G$  is the geodetic number of  $G$ , denoted by  $g(G)$ . In this paper, we study the nonsplit geodetic number  $g_{ns}(G)$  of some graphs. The set  $S \subseteq V(G)$  is a nonsplit geodetic set in  $G$  if  $S$  is a geodetic set and  $\langle V(G) - S \rangle$  is connected, nonsplit geodetic number  $g_{ns}(G)$  of  $G$  is the minimum cardinality of a nonsplit geodetic set of  $G$ . In this paper, we computed nonsplit geodetic number of Helm graph, Friendship graph, Ladder graph, Circular Ladder graph, Barbell graph, Gear





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# Non Split Geodetic Sets and Non Split Geodetic Polynomial of Spider Graph

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## Abstract

Let  $G$  be a graph. The set  $S \subseteq V(G)$  is a nonsplit geodetic set in  $G$  if  $S$  is a geodetic set and  $\langle V(G) - S \rangle$  is connected. Let  $\mathcal{N}_s(S_p, i)$  be the family of all non split geodetic set of a spider  $S_p$  with cardinality  $i$ , and let  $n_s(S_p, i) = |\mathcal{N}_s(S_p, i)|$ . In this article we construct  $\mathcal{N}_s(S_p, i)$  and obtain a recursive formula for  $n_s(S_p, i)$ . With the recursive formula, we investigate the nonsplit geodetic polynomial of spider  $N_s(S_p, x) = \sum_{i=g_{ns}(G)}^{n-1} n_s(S_p, i)x^i$  and obtain some properties.

**Keywords:** Non split geodetic set, non split geodetic number, non split geodetic polynomial.



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## THE TOTAL GEODETIC DOMINATION NUMBER OF A GRAPH

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### ABSTRACT

In this chapter the concept of the total geodetic domination number of a graph is introduced. Also, total geodetic domination number of some special graphs like friendship graph and windmill graph are studied. Also, in this paper the total geodetic domination number of path on  $n$  vertices and the wheel graph are studied. It is shown that for every three positive integers  $a$ ,  $b$  and  $c$  such that  $2 \leq a \leq b \leq c$ , there exists a connected graph  $G$  of order  $p$  with  $g(G) = a$ ,  $\gamma_g(G) = b$  and  $\gamma_{gt}(G) = c$ . Also it is shown that for any two positive integers  $m, p$  with  $3 \leq m \leq p$  then there is a connected graph of order  $p$  such that  $\gamma_{gt}(G) = m$ .

**Keywords:** Geodetic set, geodetic number, Total geodetic dominating set, Total geodetic domination number.

**AMS subject Classification:** 05C12.

### INTRODUCTION

By a graph  $G = (V, E)$  we consider a finite undirected graph without loops or multiple edges. The order and size of a graph are denoted by  $p$  and  $q$  respectively. For the basic graph theoretic notations and terminology we refer to Buckley and Harary[3]. For vertices  $u$  and  $v$  in a connected graph  $G$ , the distance  $d(u, v)$  is the length of a shortest  $u$ - $v$  path in  $G$ . A  $u$ - $v$  path of length  $d(u, v)$  is called a  $u$ - $v$  geodesic. A geodetic set of  $G$  is a set  $S \subseteq V(G)$  such that every edge of  $G$  is contained in a geodesic joining some pair of vertices in  $S$ . The edge geodetic number  $g_e(G)$  of  $G$  is the minimum order of its edge geodetic sets.

The neighborhood of a vertex  $v$  is the set  $N(v)$  consisting of all vertices which are adjacent with  $v$ . A vertex  $v$  is an extreme vertex if a subgraph induced by its



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# Programming in C++

**M. Amalanathan**  
**M. Sony Michael Mary**

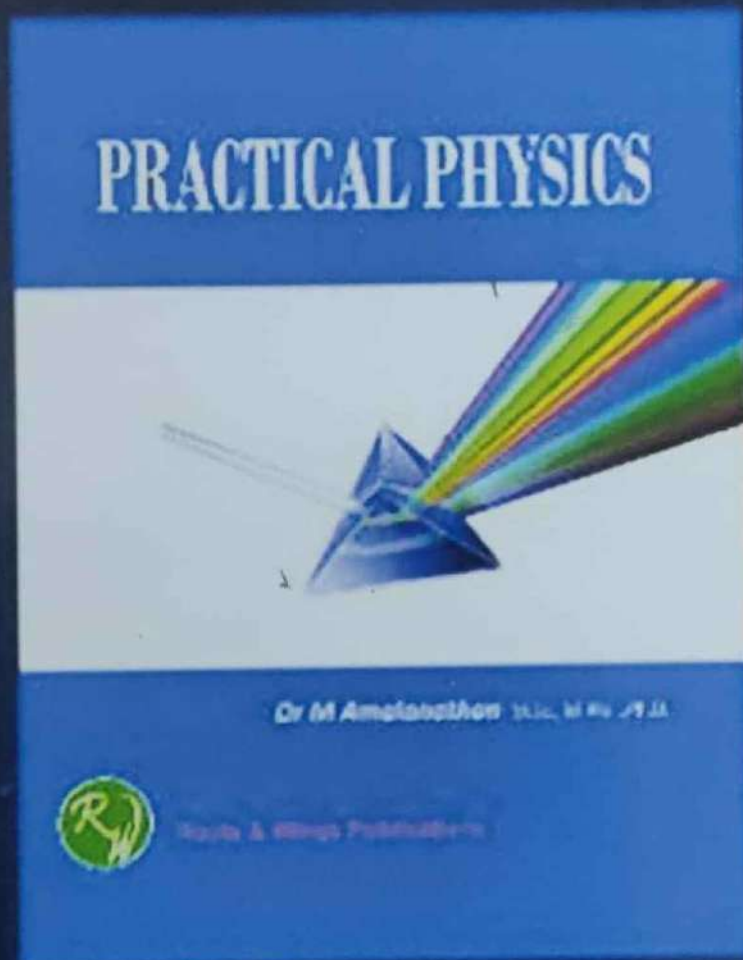


# Programming in C++

BY

M. Amalanathan

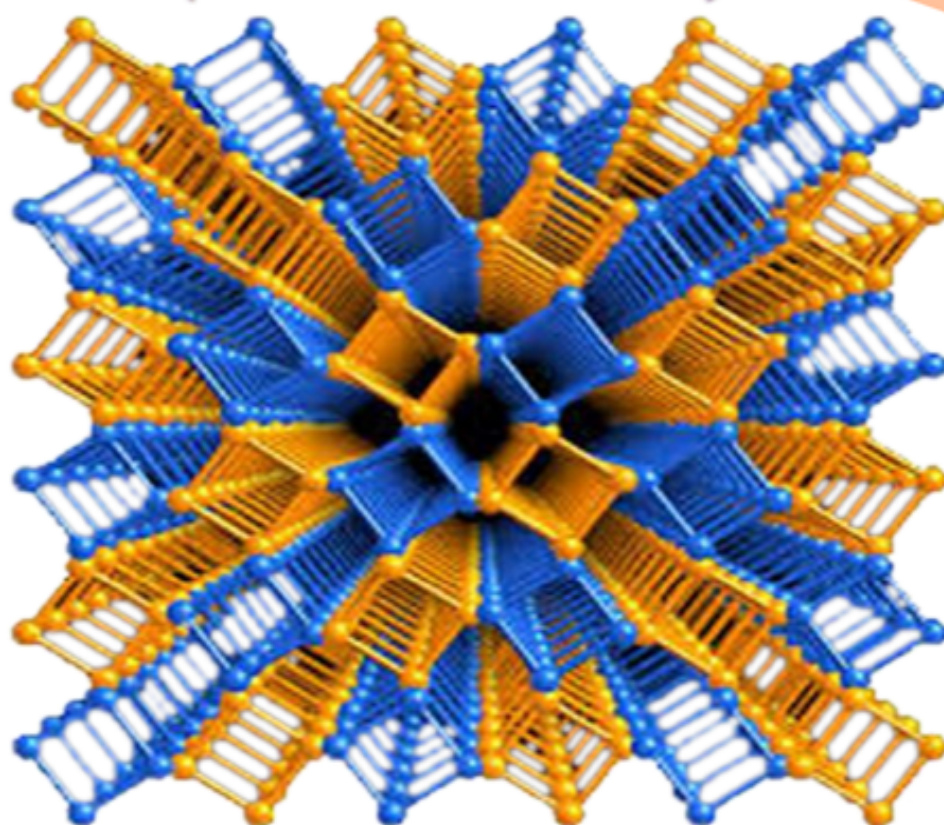
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**Fourth National Conference  
on  
ADVANCED MATERIALS  
(NCAM- 2022 )**



**Conference Proceeding**

**Edited by**

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**CONTRIBUTED PAPERS**

1. Growth and optical analysis of 4-dimethyl amino benzaldehyde-2,4-dinitroaniline single crystals (**S. Abila<sup>a</sup>**, **R.P.Jebin<sup>a\*</sup>**, **T.Suthan<sup>b</sup>**)
2. Studies on optical, thermal and mechanical properties of 2,4-dihydroxyacetophenone single crystal (**P.P. Abirami Priya<sup>a,e\*</sup>**, **T. Suthan<sup>b,e</sup>**, **S. Abraham Thambi Raja<sup>c,e</sup>**, **V. BenaJothy<sup>d,e</sup>**)
3. Variation of solar wind parameters observed during solar cycle 24 (**Abisha S Santham<sup>1\*</sup>** and **A. Iren Sobia<sup>2</sup>**)
4. DFT computations and spectroscopic analysis of a1-(4-CHLOROPHENYL)METHYL]3-PHENYLUREA fungicide (**W.Abisha<sup>1</sup>**, **D.Aruldas<sup>1</sup>**, **I.Hubert Joe<sup>2</sup>**)
5. Periodicities of solar flare activity during solar cycle 23 and 24 (**J.M. Aclin Merisha<sup>1\*</sup>** and **A. Iren Sobia<sup>2</sup>**)
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7. Spectral and structural studies of 3-Bromophenyl Methoxy Methylurea (**P.R.Babila<sup>a</sup>**, **E.S.Ashlin<sup>b</sup>**, **G.Edwin Sheela<sup>c\*</sup>**)
8. Investigation on Antibacterial and Nonlinear Optical properties of hexa aqua copper (II) toluene-4-sulfonate (PTSC) single crystals (**J. Beena<sup>a</sup>**, **A.S.Jebamalar<sup>b\*</sup>**)
9. Green synthesis of MgO and Ag-MgO nanocomposite using Catharanthus Roseus leaf extract for photocatalytic and biomedical application. (**Benisha.R<sup>1</sup>**, **Jeni James.J<sup>2</sup>**, **Amalanathan.M<sup>2</sup>**)
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11. Structural, Effects of hydrogen bonding(C-H...O and C-H...N), FMO, MEP and molecular docking analysis of N-(4-Bromophenyl)-1-(2-nitrophenyl)methanimine (**Bravanjalin Subi E<sup>1,2</sup>**, **D.Aruldas<sup>2</sup>**)
12. Synthesis of silver nanoparticles using Syzygiummalaccense fruit extract and evaluation of their catalytic activity and antibacterial properties (**Herbin Basalius H<sup>a</sup>**, **Amalanathan. M<sup>b\*</sup>**, **Maria Lenin.M<sup>c</sup>**)
13. Structure of sun's magnetic field during polar reversal phase (**Iren Sobia. A<sup>1</sup>** and **Bidhu S S<sup>2</sup>**)

14. Vibrational spectroscopic characterization, DFT studies and structural investigations of N-(2-Hydroxybenzylidene)-2-Iodoaniline (**D.Jayareshmi**<sup>1,\*</sup>, D.Aruldas<sup>2,\*</sup>)
15. Vibrational and Optical Studies of 3,4,5-trimethoxybenzaldehyde single crystals for NLO applications (**R.P. Jebin**<sup>a</sup> and T. Suthan<sup>b</sup>)
16. Vibrational spectral investigation, DFT computational studies and charge transfer interactions analysis of l-lysine monohydrate (**T. Brintha**<sup>1</sup>, J. Jeni James<sup>2</sup>, P.J. Jegan Babu<sup>3</sup>, **M. Amalanathan**<sup>4</sup>)
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23. Crystal growth, XRD and vibrational studies of piperazine p-nitrophenol (ppn) single crystals (**R.Suja**<sup>a</sup>, A.Rathika<sup>\*</sup>)
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27. XRD characterization of zinc oxide (ZnO) nano particles prepared by solution based method (<sup>1</sup>**Abhirami.U.M;** <sup>2,\*</sup>**Murugavel.S**)

28. DFT computational studies on 1 acetyl-2-(4-butoxy-3-methoxyphenyl) cyclopropane (**S. T. Aslin Priya**<sup>1</sup>, J.Jeni James<sup>2</sup>, **M. Amalanathan**<sup>3</sup>)
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32. FTIR characterization of ZnO nano particles prepared by solution based method (**Belbiya.R ; Murugavel.S**)
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36. Coronal holes and coronal mass ejections during three phases of solar cycle 24 (**Dhaiya. M.S**<sup>1\*</sup>, Iren Sobia.A<sup>2</sup>)
37. Molecular Optimization and NCI analysis of Anti-Viral Molecule Diaqua Aspartate Zinc (II) Monohydrate (**X. D. Divya Dexlin**<sup>a</sup>, T. Joselin Beaula<sup>b\*</sup>)
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42. Growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.004 (**B. Jency Paul**<sup>(1)</sup>, **S. Antony Dominic Christopher**<sup>(2)</sup>)
43. Synthesis and structural characterization of Fe doped aluminium oxide nanoparticles (**P. Jeniba**<sup>(1)</sup>, **T.R Jeena**<sup>(2)</sup>)
44. FTIR characterization of TiO<sub>2</sub> nano particles prepared by sol-gel method (**Jenish.J.P,** **Murugavel.S**)
45. Growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.006 (**Jinsha Grace.S.V**<sup>(1)</sup>, **S. Antony Dominic Christopher**<sup>(2)</sup>)
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48. Evaluation of Sodium salt of Orotic acid drug for biological application using DFT studies, HOMO-LUMO and topological analysis (**Malavika.S**<sup>1</sup>, **Amalanathan.M**<sup>2\*</sup>, Benisha R<sup>3</sup>)
49. Studies on the structural, optical, mechanical and non linear optical activity of creatinium hydrogen oxalate monohydrate single crystal (**Monisha S S**<sup>a,b</sup>, S Jeslin Sunitha bai<sup>b</sup>)
50. Investigations on the structural and optical properties of creatinium-toluene sulphonate (**Nifana N**<sup>a</sup>, Anitha Hudson J<sup>b\*</sup>, Sindhusa S<sup>b</sup>)
51. Growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.002 (**Nivitha N**<sup>(1)</sup>, **S. Antony Dominic Christopher**<sup>(2)</sup>)
52. Synthesis and structural characterization of Fe doped magnesium oxide (**S.R. Regi**<sup>(1)</sup>, **T.R Jeena**<sup>(2)</sup>)
53. XRD Characterization of titaniumdioxide nano particles prepared by sol gel method (**Reshma M.B,** **Murugavel.S**)
54. DFT Studies and topology analysis of 1 acetyl -2(4 benzyl0xy-3 methoxy phenyl cyclopropane) (**S. Shalini**<sup>1</sup>, S.Sijana<sup>2</sup>, M.Amalanathan<sup>3</sup>)
55. Experimental and DFT studies on the molecular structure, spectroscopic properties, and molecular docking of 3-Nitroaniline (**Sherlin.S.S**<sup>1</sup>, Benisha.R<sup>2</sup>, **Amalanathan.M**<sup>3</sup>)

56. Computational Evaluation on Molecular Structure, MEP, HOMO-LUMO analysis of Synthesized Compound p-nitrophenol Sodium-bisulfate (**C.L. Shiny<sup>a</sup>**, R. Suja<sup>b</sup>, A. Rathika<sup>c</sup>, T. Joselin Beaula<sup>d\*</sup>)
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63. Relation between solar wind parameters and solar cycles-recent solar maxima (**Jothika G.R<sup>1</sup>**, **Bidhu S<sup>2</sup>**)
64. Characteristics of speed of solar cme's in 24 solar cycle (**Bramya V M<sup>1</sup>**, **Bidhu S<sup>2</sup>**)
65. Slow solar wind fluctuations observations from ulysses orbit (**Jenisha G<sup>1</sup>**, **Bidhu S<sup>2</sup>**)
66. Studies on organic 4-hydroxy benzophenone single crystals (**M.L.Lima Rose<sup>a,b</sup>**, T.Suthan<sup>c</sup>, Gnanasambandam<sup>a</sup>)
67. Synthesis and Characterisation of Ternary Semiconductor Nanoparticles Blended with Medicinal Leaf Extract (**Cinsy N K<sup>\*</sup>** and Racil Jeya Geetha R<sup>1</sup>)

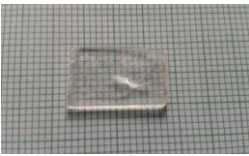
<b>OP-11</b>	<b>Structural, Effects of hydrogen bonding(C-H...O and C-H...N), FMO, MEP and molecular docking analysis of N-(4-Bromophenyl)-1-(2-nitrophenyl)methanimine</b>
<p style="text-align: center;"><b>Bravanjalin Subi E<sup>1,2</sup>, D.Aruldas<sup>2</sup></b></p> <p style="text-align: center;"><sup>1</sup>Register No: 20213112132016, Manonmaniam Sundaranar University, Tirunelveli. <sup>2</sup>Department of Physics &amp; Research Centre, Nesamony Memorial Christian College, Marthandam-629165, TamilNadu, India.</p> <p style="text-align: center;"><b>Abstract</b></p> <p>The present study aims to provide deeper knowledge about the structural, computational, chemical and antimicrobial activity of N-(4-Bromophenyl)-1-(2-nitrophenyl)methanimine. The molecular geometry, hydrogen bonding interaction and vibrational frequencies have been calculated using the density functional method (DFT/B3LYP) with 6-311G (D, P) basis set. The natural bond orbital (NBO), atoms in molecule (AIM), and Hirshfeld surface analysis, and RDG were applied to evaluate the relative strength of hydrogen bond interactions and represent their effect on the stabilities of molecular arrangements. The HOMO and LUMO analysis were used to determine the charge transfer within the molecule. The antimicrobial activity was confirmed on the compounds with molecular docking studies.</p> <p><b>Keywords:</b> NBO; QTAIM; RDG.</p>	

<b>OP-12</b>	<b>Synthesis of silver nanoparticles using Syzygiummalaccense fruit extract and evaluation of their catalytic activity and antibacterial properties</b>
<p style="text-align: center;"><b>Herbin Basalius H<sup>a</sup>, Amalanathan. M<sup>b*</sup>, Maria Lenin.M<sup>c</sup></b></p> <p style="text-align: center;"><sup>a</sup>Reg. No: 18133112131041, Research Scholar, Department of Physics, AnnaiVelankanni College of Arts and Science, Tholayavattam, Tamilnadu, India. <sup>b*</sup>Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Tamilnadu, India. <sup>c</sup>Department of Physics, AnnaiVelankanni College of Arts and Science, Tholayavattam, Tamilnadu, India. <sup>a,b,c</sup>Department of Physics, Manonmaniam Sundaranar University, Tirunelveli, Tamilnadu, India.</p> <p style="text-align: center;"><b>Corresponding Author:</b> <a href="mailto:ria.lenin@gmail.com">ria.lenin@gmail.com</a></p> <p style="text-align: center;"><b>Abstract</b></p> <p>In this study green synthesis of silver nanoparticles, an aqueous <i>Syzygiummalaccense</i> fruit extract was employed as a reducing agent. UV-visible spectroscopy, X-ray diffraction (XRD), UV-visible, Scanning Electron Microscope (SEM), Elemental Dispersive X-ray Analysis (EDX) and Transmission Electron Microscopy (TEM) were used to examine the nanoparticles. The synthesized nanoparticles surface plasmon resonance peak was measured at 438 nm. The absorption spectra of <i>Syzygiummalaccense</i> fruit extract exhibit a blue shift with decreasing particle size as the concentration increases. The silver nanoparticles were uniformly distributed and spherical, with an average particle size of 15 nanometres. Both gram-positive and gram-negative bacteria are inhibited by the silver nanoparticles. The silver nanoparticles that have higher catalytic activity of 94% at the end of 120 mins. This natural silver nanoparticle synthesis technique makes a significant contribution to green synthesis and nanotechnology by eliminating the use of harmful and toxic solvents and trash.</p>	



<b>OP-13</b>	<b>Structure of sun's magnetic field during polar reversal phase</b>
<b>Iren Sobia. A<sup>1</sup> and Bidhu S S<sup>2</sup></b>	
<p><sup>1</sup> Assistant Professor, Department of Physics and Research Centre, Muslim Arts College, Thiruvithancode. <sup>2</sup> Assistant Professor, Department of Physics &amp; Research Centre, Nanjil Catholic College of Arts &amp; Science, Kaliyakkavilai <a href="mailto:irensobia@gmail.com">irensobia@gmail.com</a>, <a href="mailto:bidhuss@gmail.com">bidhuss@gmail.com</a></p>	
<b>Abstract</b>	
<p>Solar wind that is slow, cool and dense wind is related to closed magnetic field lines and the heliospheric current sheet. Ulysses in its first and second orbit observed slow solar wind velocity with high density protons. This observation is quite different from all the earlier observations made on the slow solar wind velocity. This event coincides with a large scale solar phenomena, the solar polar reversal, when the Sun exchanges its solar global magnetic polarity. The polarity reversal mechanism is extremely slow phenomena mainly taking place in the interior of the convective zone, when Sun starts reversing its polarity. During the reversal phase the solar surface is occupied with mixed polarities. The polarities often form closed magnetic loops, found to spread over wide coronal surface, accompanying small coronal holes that forms ambient solar wind from the surface of Sun. The polarity reversal at the poles start after sunspot maximum. The solar wind that emerge during the polarity reversal is found to be having slow solar speed with high concentrations of proton particle.</p>	

<b>OP-14</b>	<b>Vibrational spectroscopic characterization, DFT studies and structural investigations of N-(2-Hydroxybenzylidene)-2-Iodoaniline</b>
<b>D.Jayareshmi<sup>1,*</sup>, D.Aruldas<sup>2,*</sup></b>	
<p><sup>1,*</sup> Assistant Professor, Department of Physics &amp; Research Centre, Women's Christian College, Nagercoil. <sup>2,*</sup> Associate Professor, Department of Physics &amp; Research Centre, Nesamony Memorial Christian College, Marthandam.</p>	
<b>Abstract</b>	
<p>To evaluate the molecular optimized geometry parameter of N-(2-Hydroxybenzylidene)-2-Iodoaniline was performed using gaussian'09 software packages. The observed IR and Raman bands were compared with harmonic vibrational frequencies of the optimized structure of N-(2-Hydroxybenzylidene)-2-Iodoaniline, calculated using the (B3LYP) with 6-31G (d, p) level of theory, and assigned on the base of potential energy distribution (PED). The vibrational frequency assignments were made with a high degree of accuracy with the help of Chemcraft software program. All the calculations were done for the optimized structures in gas phase. GAUSSVIEW program has been considered to get visual animation. The experimental UV-Vis absorption spectrum was recorded and compared with the simulated time-dependent (TD-DFT) approach. HOMO-LOMO energy gap, Charge analysis, Molecular electrostatic potential and Natural Bond Orbital (NBO) analysis were done.</p>	
<p>Keywords: DFT, NBO, Charge Analysis and MESP</p>	

<b>OP-15</b>	<b>Vibrational and Optical Studies of 3,4,5-trimethoxybenzaldehyde single crystals for NLO applications</b>
<p style="text-align: center;"><b>R.P. Jebin<sup>a</sup> and T. Suthan<sup>b</sup></b></p> <p style="text-align: center;"><sup>a</sup><i>Department of Physics and Research Centre, Muslim Arts College, Thiruvithancode – 629174, , India</i> <sup>b</sup><i>Department of Physics, Lekshmipuram College of Arts and Science, Neyyoor-629802, India</i></p> <p style="text-align: center;">corresponding author email id : <a href="mailto:rpjebi@gmail.com">rpjebi@gmail.com</a></p> <p style="text-align: center;"><b>Abstract</b></p> <p>In the recent years, studies of optical nonlinearities in materials have been become more interesting because of their useful application in integrated optics, such as optical modulation, all optical switching and optical information processing. The several NLO behaviors, such as the optical limiting is one of the most promising practical applications, as it may be protect the human eyes and the optical sensors from the damage caused by the intense optical radiations. The researchers are given the appreciable care to develop and improve the quality of the organic single crystals for the technological applications. The organic material 3,4,5-trimethoxybenzaldehyde has been grown by slow evaporation technique using methanol as solvent. The Vibration studies were recorded using FTIR and FT-Raman spectra to identify the functional groups present in the crystal. The optical property of the grown crystal was analyzed by UV-Vis-NIR measurement. The third order nonlinear optical properties of 3,4,5-trimethoxybenzaldehyde was measured by the Z-scan technique using 532 nm diode pumped continuous wave (CW) Nd:YAG laser.</p> <p><b>Keywords:</b> Crystal growth from Solution, FTIR, FT-Raman</p> <p style="text-align: center;"><b>Photograph of 3,4,5-TMOB Single crystals</b></p> <div style="text-align: center;"></div>	

<b>OP-16</b>	<b>Vibrational spectral investigation, DFT computational studies and charge transfer interactions analysis of L-lysine monohydrate</b>
<p style="text-align: center;"><b>T. Brintha<sup>1</sup>, J. Jeni James<sup>2</sup>, P.J. Jegan Babu<sup>3</sup>, M. Amalanathan<sup>4</sup></b></p> <p><sup>1</sup> Research Scholar, (Reg no. 19213112132012, Department of physics, Nesamony Memorial Christian College, Marthandam, Kanyakumari, Tamil Nadu, India. <sup>2</sup> Research Scholar, Department of physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India. <sup>3</sup> Assistant Professor, Department of physics, Nesamony Memorial Christian College, Marthandam, Kanyakumari, Tamil Nadu, India. <sup>4</sup> Assistant Professor, Department of physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India. <sup>1, 2,3,4</sup> Affiliated to Manonmaniam Sundaranar University Tirunelveli, TamilNadu, India.</p> <p style="text-align: center;"><b>Abstract</b></p> <p>In this work, using the Gaussian 09 program, the molecular structure of L-Lysine monohydrate was optimized using the DFT method with B3LYP/6-311++G(d,p) basic sets. The Mulliken atomic charge distribution, vibrational frequencies, frontier molecular orbitals and Topological analysis were calculated. The VEDA 4.0 tool was used to assign the whole theoretically estimated and experimentally observed vibrational frequencies using</p>	

<b>OP-22</b>	<b>Theoretical and spectroscopic studies of orotic acid</b>
<b>S.Sijana<sup>1</sup>, M.Amalanathan<sup>2</sup></b>	
<p><sup>1</sup>Research scholar (Reg.No:21113102132002), Department of physics Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India.</p> <p><sup>2</sup>Assistant Professor, Department of physics Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India.</p> <p><sup>1,2</sup>Affiliated to Manonmanium Sundararnar University Tirunelveli, Tamil Nadu, India.</p> <p>This paper deals with the theoretical and spectroscopic studies of Orotic acid. A comprehensive spectroscopic analysis of Orotic acid's structural behaviour has been undertaken. FT-IR and FT-Raman techniques were used to examine the spectral properties of the Orotic acid molecule in the solid state. The B3LYP/6-311++G (d, p) computations were used to optimize the molecular structure. To provide complete vibrational spectral assignments, normal co-ordinate analysis (NCA) was used. The stability and different types of hydrogen bonds inside the molecule are explained by natural bond orbital analysis (NBO). The topological analysis AIM, ELF, and the reduced gradient of the density are used to examine the intra and intermolecular interactions that exist inside these molecules. These methods make it feasible to investigate the properties of hydrogen bonding in particular. To realize charge, transfer within the molecule, the highest occupied molecular orbital and the lowest unoccupied molecular orbital energy levels are generated, and the matching border energy gaps are computed. The minimal binding energy was obtained using molecular docking studies on the title chemical to examine hydrogen bond interactions.</p> <p>Keywords: Orotic acid; DFT calculation; IR; Raman; NBO; RDG</p>	

<b>OP-23</b>	<b>Crystal growth, xrd and vibrational studies of piperazine p-nitrophenol (ppn) single crystals</b>
<b>R.Suja<sup>a</sup>, A. Rathika*</b>	
<p><sup>a,*</sup> Research Scholar (Reg.No: 21213092132004) Department of Physics and Research Centre, Muslim Arts College, Thiruvithancode, Thuckalay- 629 175, Tamilnadu, India, Affiliated to Manonmaniam Sundaranar University, Tirunelveli - 627 012 *email:rathikarthi87@gmail.com</p> <p style="text-align: center;"><b>Abstract</b></p> <p>Single crystals of piperazine and p-nitrophenol (PPN) crystal was synthesized and yellow coloured good optical quality single crystals were grown methanol as solvent by slow evaporation solution growth technique at room temperature. From the single crystal X-ray diffraction study, the PPN crystal crystallizes in centrosymmetric, monoclinic system with space group P2<sub>1</sub>/c. From the powder XRD data, the appearance of sharp and well defined Bragg's peaks confirmed the crystalline nature of the grown crystal. The peak corresponding to (0 1 7) hkl plane has the maximum intensity of PPN single crystal. The various angles of reflection have been found out. From the vibrational studies, the nitrophenol group C-NO<sub>2</sub> stretching and CH in plane bending occurs at 1160 cm<sup>-1</sup> and 1104 cm<sup>-1</sup> in FT-IR and 1165 cm<sup>-1</sup>, 1105 cm<sup>-1</sup> in Raman spectrum respectively. The peak at 1065 cm<sup>-1</sup> is assigned to wagging CH<sub>2</sub> and NH<sub>2</sub> stretching of piperazine.</p> <p><b>Keywords:</b> Crystal growth from Solution, XRD, Vibrational studies</p>	



<b>OP-24</b>	<b>Structural characterization of Zn and Fe doped aluminium oxide nanoparticles prepared by co-precipitation method</b>
<b>R.Winston <sup>(1)</sup>, T.R Jeena <sup>(2)</sup></b>	
1) M.Phil. Scholar 2) Assistant Professor Department of Physics Nanjil Catholic College of Arts and Science, Kaliyakkavilai.	
<b>Abstract</b>	
<p>A systematic study on the preparation of pure and Zn, Fe doped Aluminum oxide(<math>Al_2O_3</math>) nanoparticles for doping concentration of 2 wt.% has been conducted. Co-Precipitation technique has been used for the preparation of the samples. The structure, crystallite size, lattice parameters and micro strain of the prepared samples and the influence of doping different elements (Zn and Fe) on those parameters were investigated by X-ray diffraction (XRD) analysis. For all three samples XRD patterns revealed rhombohedral structure of <math>Al_2O_3</math>. Also, in the doped samples, the addition of Zn and Fe ions are observed. Also, the precise values of crystallite size and micro strain of the samples were found by constructing W-H plot.</p>	

<b>OP-25</b>	<b>Synthesis and Characterization of Cu-Doped ZnSe Nanoparticles for Photocatalytic Activity</b>
<b>V. Beena <sup>1</sup>, S. L. Rayar <sup>2</sup>, S. Ajitha <sup>1</sup></b>	
<sup>1</sup> Department of Physics, Nanjil Catholic College of Arts and Science, Manonmaniam Sundaranar University, Kanyakumari 629153, India; ajithaphyholy@gmail.com <sup>2</sup> Dept of Physics, St. Judes College, Kanyakumari 629176, India; drslrayar@gmail.com	
<b>Abstract</b>	
<p>Environmental nanotechnology has received much attention due to their removal capacity of toxic elements from the aquatic surface. This work stated that Cu doped ZnSe nanoparticles using the co-precipitation method. The synthesized Cu doped ZnSe nanoparticles were examined by structural, optical and morphological properties with the help of XRD, FTIR, UV-Vis DRS, FESEM and TEM. The synthesized Cu-doped ZnSe nanoparticles revealed the <math>Cu^{2+}</math> presence in the ZnSe lattice.. The synthesized Cu doped ZnSe nanoparticles were examined by photocatalytic activity. The 0.1M copper doped ZnSe nanoparticles exhibited the highest rate of degradation against the methyl orange dye is 87%. The pseudo-first-order kinetics of the Cu doped ZnSe nanoparticles is <math>0.1334 \text{ min}^{-1}</math>. The Cu-doped ZnSe nanoparticles exhibit enhanced photocatalytic activity.</p>	
<b>Keywords:</b> Cu doped ZnSe NP's, MO, Photocatalysis, Visible light	

<b>OP-26</b>	<b>Synthesis and Characterisation of Ternary Semiconductor Nanoparticles Blended with Medicinal Leaf Extract</b>
<b>Cinsy N K* and Racil Jeya Geetha R<sup>1</sup></b>	

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**Abstract**

The characterizations of synthesized CdZnS nanoparticles with Ocimum sanctum leaf extract were done by the chemical precipitation method. The formation of CdZnS nanoparticles with the extract was confirmed using XRD, SEM analysis and EDAX. XRD revealed the structure and the particle size. SEM analysis of CdZnS NPs confirmed shape and size.

Key words:

Chemical precipitation, hydrodynamic radius, dynamic light scattering

<b>PP-1</b>	<b>Synthesis and structural characterization of zinc doped magnesium oxide</b>
<p><b>B.C. Abhinisha</b> <sup>(1)</sup>, <b>T.R Jeena</b> <sup>(2)</sup></p> <p>1) M.Sc. Student 2) Assistant Professor, Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai.</p> <p><b>Abstract</b></p> <p>Pure and 2 wt.% Zn doped magnesium oxide nano particles were synthesized via co-precipitation method using chemical route. The synthesized nanoparticles are analysed using X-ray diffraction technique. The structure, crystalline size, lattice parameter and micro strain of pure and zinc doped magnesium oxide nanoparticles were found from the diffraction pattern. For both the samples XRD patterns revealed cubic structure of magnesium oxide. Also in the doped samples, the addition of zinc ions are observed.</p>	

<b>PP-2</b>	<b>XRD characterization of zinc oxide (ZnO) nano particles prepared by solution based method</b>
<p><sup>1</sup><b>Abhirami.U.M;</b> <sup>2,*</sup><b>Murugavel.S</b></p> <p>Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai</p>	

**Abstract**

In the present study Zinc oxide (ZnO) nano particles were prepared by simple solution based method using Zinc Chloride (ZnCl<sub>2</sub>). The prepared sample was characterized by X-Ray Diffraction Technique. XRD study confirmed that synthesised samples are Zinc Oxide (ZnO) nano particles.

**KEYWORDS**

Zinc Oxide, Nano particle, X-Ray Diffraction (XRD), Characterization.

<b>PP-3</b>	<b>DFT computational studies on 1 acetyl-2-(4-butoxy-3-methoxyphenyl) cyclopropane</b>
<p style="text-align: center;"><b>S. T. Aslin Priya<sup>1</sup>, J. Jeni James<sup>2</sup>, M. Amalanathan<sup>3</sup></b></p> <p><sup>1</sup> M.Sc, Department of physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India. <sup>2</sup> Research Scholar, Department of physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India. <sup>3</sup> Assistant Professor, Department of physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India. <sup>1, 2, 3</sup> Affiliated to Manonmaniam Sundaranar University Tirunelveli, TamilNadu, India.</p> <p style="text-align: center;"><b>Abstract</b></p> <p>In the present work the optimized molecular geometry of 1 acetyl -2-(4-butoxy-3-methoxyphenyl) cyclopropane calculated by DFT/B3LYP method with 6-31 G (d, p) basis set using Gaussian 09 software has been investigated. Mulliken atomic charges are calculated and interpreted. Charge transfer within the molecule is indicated by HOMO and LUMO. The energy gap between the ground state HOMO and first excited state LUMO energies were determined and the band gap energy of the title molecule is found to be 3.8115. The electron distribution and reactive site on the surface of the molecule are analyzed using ELF and LOL analysis. The noncovalent interaction (NCI) analysis provides the most important interaction informations such as Vander Waals interactions, hydrogen bonds and steric interactions present in the molecule.</p> <p>Keywords: NCI, Mulliken, ELF, LOL, DFT.</p>	

<b>PP-4</b>	<b>Theoretical computation of 2-chloro-3-nitro toluene using turbomole software</b>
<p style="text-align: center;"><b>J. S. Aswin* and Dr. T. Asenath Benitta</b></p> <p style="text-align: center;">Department of Physics, Nesamony Memorial Christian College, Marthandam.</p> <p style="text-align: center;"><b>Abstract</b></p> <p>The optimized geometry and simulated IR and Raman spectrum of 2-chloro-3-nitro toluene have been obtained by using the Turbomole software. Experimental FT-IR and FT-Raman spectra of 2-chloro-3-nitro toluene were collected from literature and was compared with theoretical vibrational spectra. The normal modes of vibration</p>	

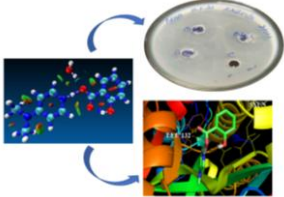


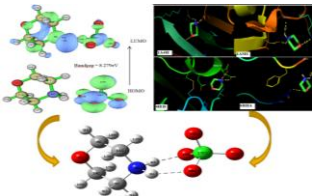
of the title compound were compared with that obtained with Turbomole software. The comparison shows that theoretical values are approximately equal to the theoretical values already available in literature. Thermodynamic properties such as entropy, enthalpy, chemical potential, zero-point energy of 2-chloro-3-nitro toluene were obtained using Turbomole software.

<b>PP-5</b>	<b>Synthesis and structural characterization of magnesium doped aluminium oxide nanoparticle</b>
<p><b>S. Babisha<sup>(1)</sup>, T.R Jeena<sup>(2)</sup></b></p> <p>1) M.Sc. Student 2) Assistant Professor, Department of Physics Nanjil Catholic College of Arts and Science, Kaliyakkavilai.</p> <p><b>Abstract</b></p> <p>Pure and Mg doped Aluminium oxide nanoparticles for a doping concentration of 2 wt. % has been synthesized using co-precipitation technique. Prepared samples were characterized using X-ray diffraction (XRD) analysis to analyse the structure, crystalline size, lattice parameters and microstrain of the prepared samples. In addition, the influence of doping Mg on these parameters were also investigated. For both the samples XRD patterns revealed rhombohedral structure.</p>	

<b>PP-6</b>	<b>Impact of Charge Interaction, H-Bonding Elucidations by Structural and Biological Activity of Diammonium Hydrogen Orthophosphate</b>
<p><b>G.Bagavathi Sankar<sup>1</sup>, D.Usha<sup>2</sup></b></p> <p><sup>1</sup>Reg.No18223282131003, Department of Physics, St.Johns College of Arts and Science Ammandivilai <sup>2</sup>Associate Professor, Department of Physics, Womens Christian College, Nagercoil-629001 <sup>1,2</sup>Affiliated to Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli-627 012, Tamilnadu, India</p> <p><b>Abstract</b></p> <p>The structure-activity of diammonium hydrogen orthophosphate optimized using the density functional theory method using B3PW91/6-31++G (d, p) set. Hydrogen bonding interactions confirmed by Natural Bonding orbitals (NBO) Analysis. The frontier molecular orbital analysis provided a electron transport in the molecule. The most reactive site of the molecules was predicted by the molecular electrostatic potential map and also natural charge analysis. Vibrational spectral assignments predicted the aid of Normal Coordinate Analysis. Antimicrobial activity performed for biological activity screening of the molecules along with drug likeness confirmed its antibacterial activity.</p>	

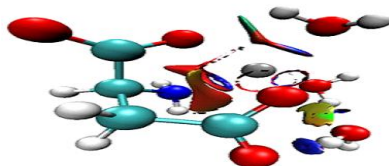
<b>PP-7</b>	<b>FTIR characterization of ZnO nano particles prepared by solution based method</b>
<p style="text-align: center;"><b>Belbiya.R ; Murugavel.S</b></p> <p style="text-align: center;">Department of Physics, Nanjil Catholic College Of Arts And Science, Kaliyakkavilai.</p> <p style="text-align: center;"><i>Abstract</i></p> <p>In the present study ZnO nano particles were prepared by simple solution based method using Zinc chloride. The prepared sample was characterized by Fourier Transform Infrared (FTIR) spectroscopy techniques. The characteristic peak confirmed that synthesized samples are Zinc oxide particles.</p> <p><b>KEY WORDS : Zinc Oxide, Nano particles, FTIR , Characterization .</b></p>	

<b>PP-8</b>	<b>Exploring the Covalent, Non-Covalent interactions and Pharmacokinetics properties of the Antibacterial compound 4-Dimethylaminopyridinium Salicylate Monohydrate</b>
<p style="text-align: center;"><b>J. D. Deephlin Tarika<sup>a</sup>, R.S. Bemina<sup>b</sup>, T. Joselin Beaula<sup>c*</sup></b></p> <p><sup>a,b,c</sup>Department of Physics and Research Centre, Malankara Catholic College, Mariagiri-629153, Tamilnadu, India. <sup>a,b,c</sup>Affiliated to Manonmaniam Sundaranar University, Abishekapatti-627012, Tirunelveli, Tamilnadu, India <a href="mailto:*joselinbeaula@gmail.com">*joselinbeaula@gmail.com</a></p> <p>Antibacterial resistance is regarded as one of the most serious public health issues, since it has a large economic impact over the world. Pyridine moieties play an imperative role in medicinal chemistry ascribed to their anti-microbial, anti-viral, anti-diabetic, anti-cancer, anti-oxidant, anti-malaric, anti-inflammatory and anti-bacterial properties. RDG analysis reveals the weak hydrogen bonding interactions, steric effect and strong hydrogen bonding interactions, whereas DORI analysis reveals information about the non-Covalent interactions as well as the Covalent interactions. Antibacterial testing of DPSM using agar well diffusion method reveals that DPSM inhibits the <i>Klebsiella pneumoniae</i> more and the second pathogen that was inhibited more was the <i>Streptococcus pneumoniae</i>. Both these bacteria are the main source for the pneumococcal infections and as DPSM inhibits these bacteria it is clear that DPSM can be used to treat the infections caused by these bacteria. Molecular Docking also confirms that DPSM has high binding affinity with the <i>Klebsiella pneumoniae</i> protein with a binding energy of -5.84 kcal/mol. Moreover, Drug likeness and ADMET analysis also validates that DPSM can be used as an oral drug to treat the antibacterial infections. DPSM is efficiently absorbed by the small intestine and is distributed evenly throughout the blood and plasma. As DPSM is not mutagenic and does not disrupt the liver, it is feasible that it may be deployed as a medication.</p> <div style="text-align: center;"></div>	

PP-9	<b>Structural, Electronic properties and Docking Analysis of Antifungal Molecule MorpholiniumPerchlorate -A DFT Approach</b>
<p style="text-align: center;"><b>C. DaboraVincy<sup>a</sup>, T. JoselinBeaula<sup>b*</sup></b></p> <p><sup>a</sup>Reg.No: 19113092132004, Research Scholar, Department of Physics and Research Centre, Malankara Catholic College, Kaliyakkavilai-629153, TamilNadu, India.</p> <p><sup>b</sup>Department of Physics and Research Centre, Malankara Catholic College, Kaliyakkavilai-629153, TamilNadu, India.</p> <p>Affiliated to ManonmaniamSundaranar University, Abishekapatti-627012, Tirunelveli, Tamilnadu, India <a href="mailto:*joselinbeaula@gmail.com">*joselinbeaula@gmail.com</a></p> <p style="text-align: center;"><b>Abstract</b></p> <p>Morpholine is a heterocyclic featured in numerous approved and experimental drugs as well as antifungal and antibacterial active molecules. Morpholine and its derivatives are extensively used in many chemical reactions with a lot of important pharmacological properties. Structural and electronic properties of Morpholinium perchlorate was studied by molecular optimised, HOMO-LUMO, electrostatic potential and docking studies. Electronegative groups such as Cl atoms in an anion can show higher antimicrobial activity. Theoretical computations of morpholinium perchlorate have been accomplished using density functional theory with B3PW91/6-31G (d, p) basis set using the Gaussian'09 software package. Optimized geometric bond lengths, bond angles and dihedral angles of the molecule were calculated and analyzed. Molecular electrostatic potential (MEP) surface analysis of the molecule was performed in order to predict the reactive site of the molecule. Charge transfer in a molecule has been illustrated using the frontier molecular orbitals. Molecular docking studies were performed to identify the antifungal activity of the title compound.</p> <div style="text-align: center;"></div>	

PP-10	<b>Growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.008</b>
<p style="text-align: center;"><b>K. Athira<sup>(1)</sup>, S. Antony Dominic Christopher<sup>(2)</sup></b></p> <p><sup>(1)</sup>M.Sc Student, Nanjil Catholic College of Arts and Science Kaliyakkavilai.</p> <p><sup>(2)</sup>Assistant Professor, Nanjil Catholic College of Arts and Science Kaliyakkavilai.</p> <p style="text-align: center;"><b>Abstract</b></p> <p>L-threonine is an optically active form of threonine having L-configuration. They show high non-linearity and low refractive indices. The crystals were grown by slow evaporation technique. Methyl violet (C<sub>24</sub>H<sub>28</sub>N<sub>3</sub>Cl) is used as the dye dopant in the ratio 0.008. The grown crystal was characterised by X-ray diffraction analysis. It confirms the grown crystals belong to orthorhombic system.</p>	





PP-13

**Experimental and Theoretical Investigation on L-Phenylalanine L-phenylalaninium malonate**

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<sup>b</sup> Department of Physics & Research Center, Nesamony Memorial Christian College, Marthandam - 629165, Tamilnadu, India.

**Abstract**

The crystal structure investigations of L-Phenylalanine with Methanedicarboxylic acid, namely L-Phenylalanine L-phenylalaninium malonate have been investigated by means of single crystal X-ray diffraction method. The title compound crystallizes in monoclinic crystal system, and the space group is  $P2_1$  with  $a=14.031(3)\text{\AA}$ ,  $b=5.5082(10)\text{\AA}$ ,  $c=14.601(3)\text{\AA}$  and  $Z=2$ . Its optical behaviour has been examined by UV-vis spectral analysis, which shows the absence of absorbance in the visible region. Nonlinear optical efficiency was confirmed by Kurtz Perry powder technique. The structural study and Hirshfeld surface analysis allowed us to establish the importance of hydrogen bond and intermolecular interaction in the crystal packing and their role in the NLO properties.

Keywords: Crystal growth, Nonlinear optics, hirshfeld.

PP-14

**DFT studies, structural determination, chemical properties and topological analysis of 1 acethyl-2-(4-ethoxy-3-methoxyphenyl)**

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<sup>2</sup> Research Scholar, Department of physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai, Kanyakumari, Tamil Nadu, India.

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<sup>1,2,3</sup> Affiliated to Manonmaniam Sundaranar University Tirunelveli, TamilNadu, India.

**Abstract**

The purpose of our work is to present a theoretical study of 1 acethyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane. Geometry optimization such as bond length, bond angle and dihedral angle has been carried out in the gas phase by B3LYP level of DFT. The Mulliken population analysis on atomic charges has been computed. Global reactivity descriptors (ionization potential, electron affinity, electron negativity, global hardness, softness, electrophilicity index and chemical potential) were predicted with the help of HOMO LUMO values. The energy gap value suggests

<b>PP-16</b>	<b>Spectroscopic and Structural Investigations on Acethyl 2(3-methoxy -4 proporxy pheny)by FTIR, NBO and Topological analysis</b>
<p style="text-align: center;"><b>Jebina Rose.J<sup>1</sup>, Amalanathan.M<sup>2*</sup>, Benisha R<sup>3</sup>.</b></p> <p style="text-align: center;"><sup>1,2*,3</sup> <i>Department of Physics, Nanjil Catholic College of Arts &amp; Science, Kaliyakkavilai, Tamil Nadu, India.</i> <sup>1,2*,3</sup> <i>Affiliated to Manonmaniam Sundaranar university, Abishekapatti, Tirunelveli-627 012</i> <i>Tamil Nadu, India.</i></p> <p style="text-align: center;"><b>Abstract</b></p> <p>FT-IR spectral analysis was used to describe the title compound, Acetyl 2(3-methoxy -4 proporxy pheny). Density functional theory (DFT) B3LYP technique with 6-311++G(d,p) basis set was used to determine the optimized geometry, vibrational wavenumbers, infrared intensities, and Raman scattering activities. The VEDA programme was used to do a detailed interpretation of the vibrational spectra. Charge transmission within the molecule is demonstrated by the computed HOMO and LUMO energies. Natural bond orbital analysis was used to investigate the stability of the molecule as a result of hyperconjugative interactions and charge delocalization (NBO). To quantify non-covalent and covalent bond interactions in the molecule, RDG (Reduced density gradient) is used. The chemical bonding of the chosen molecule is determined using ELF and LOL.</p> <p>Keywords: Topology, Mulliken analysis, RDG, NBO, VEDA.</p>	

<b>PP-17</b>	<b>growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.004</b>
<p style="text-align: center;"><b>B. Jency Paul<sup>(1)</sup> S. Antony Dominic Christopher<sup>(2)</sup></b></p> <p style="text-align: center;"><sup>(1)</sup> M.Sc. Student, Nanjil Catholic College of Arts and Science, Kaliyakkavilai <sup>(2)</sup> Assistant Professor, Nanjil Catholic College of Arts and Science, Kaliyakkavilai</p> <p style="text-align: center;"><b>Abstract</b></p> <p>L-threonine is an extremely interesting optically active amino acid in addition to its biological properties. It acts as a proton donor, proton acceptor and nucleophilic reagent. The crystals were grown by slow evaporation technique. Methyl violet (C<sub>24</sub>H<sub>28</sub>N<sub>3</sub>Cl) is used as the dye dopant in the ratio 0.004. The grown crystal was charecterised by X-ray diffraction analysis. It confirms the grown crystals belong to orthorhombic system.</p>	

<b>PP-18</b>	<b>Synthesis and structural characterization of Fe doped aluminium oxide nanoparticles</b>
<p style="text-align: center;"><b>P. Jeniba<sup>(1)</sup>, T.R Jeena<sup>(2)</sup></b></p> <p style="text-align: center;">1)M.Sc. Student 2)Assistant Professor, Department of Physics Nanjil Catholic College of Arts and Science, Kaliyakkavilai.</p> <p style="text-align: center;"><b>Abstract</b></p> <p>Fe doped (2 wt. %) and pure Aluminium oxide nanoparticles has been synthesized using co-precipitation method of preparing nanoparticles. The structural characteristics of the prepared samples were investigated using X-</p>	

ray diffraction (XRD) technique. The structure, crystalline size, lattice parameters and microstrain of both the prepared samples and the influence of doping Fe on these parameters were investigated using the diffraction pattern. For both the samples XRD patterns revealed rhombohedral structure.

<b>PP-19</b>	<b>FTIR characterization of TiO<sub>2</sub> nano particles prepared by sol-gel method</b>
<b>Jenish.J.P, Murugavel.S</b>	
Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai.	
<b>Abstract</b>	
In the present study TiO <sub>2</sub> nano particles were prepared by SOL-GEL method. The prepared sample was characterized by fouriertransforminfrared spectroscopy techniques.FTIRcharacteristic peak confirmed that synthesized samples are Titaniumdioxide particles.	
<b>Key words</b>	
Titaniumdioxide, Nano particles, FTIR ,Characterization.	

<b>PP-20</b>	<b>Growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.006</b>
<b>Jinsha grace.S.V<sup>(1)</sup>, S.Antony Dominic Christopher<sup>(2)</sup></b>	
<sup>(1)</sup> MSc Student, Nanjil Catholic College of Arts and Science, Kaliyakkavilai.	
<sup>(2)</sup> Assistant professor, Nanjil Catholic College of Arts and Science, Kaliyakkavilai.	
<b>Abstract</b>	
The crystals were grown by slow evaporation technique. The dye used in the study for dopant in the ratio 0.006 is Methyl Violet (C <sub>24</sub> H <sub>28</sub> N <sub>3</sub> Cl). L-threonine is an essential amino acid that helps to maintain the proper protein balance in the body. The grown crystal were characterised X-ray diffraction analysis confirms the grown crystals belong to orthorhombic system.	

<b>PP-21</b>	<b>Synthesis and structural characterization of Zn doped aluminium oxide nanoparticles</b>
<b>S.S. Joji Thomas<sup>(1)</sup>, T.R Jeena<sup>(2)</sup></b>	



1)M.Sc. Student 2) Assistant Professor,  
Department of Physics  
Nanjil Catholic College of Arts and Science, Kaliyakkavilai.

**Abstract**

A systematic study on the preparation of pure and zinc (Zn) doped Aluminium oxide nanoparticles for a doping concentration of 2 wt. % has been conducted. Precipitation technique has been used for the preparation of the samples. Prepared samples were characterized using X-ray diffraction (XRD) technique to find the structure, crystalline size, lattice parameters and microstrain of the samples and to investigate the influence of doping Zn with aluminium oxide on these parameters. XRD patterns revealed Rhombohedral axes structure for both the samples.

**PP-22**

**UV Spectroscopic study of titaniumdioxide nano particles prepared by sol-gel method**

**Josephin darling J, Murugavel S**

Department of Physics,  
Nanjil Catholic College of Arts and Science,  
Kaliyakkavilai.

**Abstract**

In the present study TiO<sub>2</sub> nano particles were prepared by SOL-GEL method. The prepared sample was characterized by UV spectroscopy techniques. UV Spectroscopy study confirmed that synthesized samples are semiconducting nano particles.

**KEY WORDS :**

Titaniumdioxide, Nano particles, UV Spectroscopy, Characterization

**PP-23**

**Evaluation of Sodium salt of Orotic acid drug for biological application using DFT studies, HOMO-LUMO and topological analysis**

**Malavika.S<sup>1</sup>, Amalanathan.M<sup>2\*</sup>, Benisha R<sup>3</sup>.**

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<sup>1,2\*,3</sup> Affiliated to Manonmaniam Sundaranar university, Abishekapatti, Tirunelveli-627 012  
Tamil Nadu, India.

**Abstract**

The title compound, Sodium salt of Orotic acid was synthesized and characterized by FT-IR, and FT-Raman, spectral analysis. The optimized molecular geometry, the vibrational wavenumbers, the infrared intensities and the Raman scattering activities were calculated by using density functional theory(DFT) B3LYP method with 6-311++G(d,p) basis set. The detailed interpretation of the vibrational spectra has been carried out by VEDA program. The calculated HOMO and LUMO energies show that charge transfer within the molecule. Stability of the molecule arising from hyperconjugative interactions, charge delocalization have been analyzed using natural bond orbital

evaporation technique and to analyze its structural , optical and mechanical properties . The Single Crystal X-ray Diffraction analysis (SXRD) is carried out to identify the structural parameters. Hirshfeld surface analysis explains the interactions present in the synthesized material. The optical property has been examined by using UV-visible spectral analysis and the optical constants such as band gap energy, extinction coefficient and refractive index were evaluated. HOMO-LUMO and MESP maps were successfully generated and analysed .Th emission behavior was analysed by fluorescence spectral analysis. Second order optical nonlinearity was confirmed by kurtzperry powder technique. Mechanical property of the material has been analysed by Vicker'smicrohardness analysis .  
Keywords: X-ray Diffraction, Optical property, Emission behaviour, Mechanical property

**PP-26**

**Growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.002**

**Nivitha N<sup>(1)</sup> and S Antony Dominic Christopher<sup>(2)</sup>**

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**Abstract**

The crystals were grown by slow evaporation technique. The dye used in the study for dopant in the ratio 0.002 is methyl violet (C<sub>24</sub>H<sub>28</sub>N<sub>3</sub>Cl).L-threonine provide various health benefits like muscle tightness, liver health and so on. The grown crystal was characterized X-ray diffraction analysis. IT CONFIRMS the grown crystals belong to orthorhombic system.

**PP-27**

**Synthesis and structural characterization of Fe doped magnesium oxide**

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Department of Physics,

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**Abstract**

Pure and 2 wt. % Fe doped magnesium oxide nano particles were synthesized via co-precipitation method using chemical route. The synthesized nanoparticles are analysed using X-ray diffraction technique. The structure, crystalline size, lattice parameter and micro strain of pure and Fe doped magnesium oxide nanoparticles were found from the diffraction pattern. For both the samples XRD patterns revealed cubic structure of magnesium oxide. Also in the doped samples, the additions of ferrous ions are observed.

**PP-28**

**XRD characterization of titaniumdioxide nano particles prepared by sol gel method**

**Reshma M.B, Murugavel.S**

Department of Physics,  
Nanjil Catholic College of Arts and Science,  
Kaliyakkavilai

**Abstract**

In the present study Titanium dioxide nano particles were prepared by sol gel method. The prepared sample was characterized by X-Ray Diffraction technique. XRD study confirmed that synthesized samples are titanium dioxide nano particles.

Keywords: Titanium dioxide, nano particle, XRD Characterization.

**PP-29**

**DFT studies and topology analysis of 1 acetyl -2(4 benzyloxy-3 methoxy phenyl cyclopropane)**

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The computational investigation on 1 acetyl-2(4 benzyloxy-3 methoxy phenyl cyclopropane) were done using DFT/B3LYP/6-311g(d,p) to study the molecular structure. The highest occupied molecular orbital and the lowest unoccupied molecular orbital energy levels are calculated and the corresponding frontier energy gaps are determined to realize the charge transfer within the molecule. The intra and intermolecular interaction exist within this compound is analyzed by different methods namely topology analysis ELF, LOL and RDG. The calculation of atomic charge by Mulliken plays a vital role in the application of the molecular system. Charge distributions of Mulliken and NBO are also analysed.

Keywords: DFT calculation, ELF, RDG, Mulliken

**PP-30**

**Experimental and DFT studies on the molecular structure, spectroscopic properties, and molecular docking of 3-Nitroaniline**

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**Abstract**



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**Abstract**

The main aim of this work is to synthesize creatininium 2-chloroacetate (CR2CIA) single crystal by using slow evaporation technique and to analyze its structural, optical and mechanical properties. The Single Crystal X-ray Diffraction analysis (SXRD) is carried out to identify the structural parameters. Hirshfeld surface analysis explains the interactions present in the synthesized material. The optical property has been examined by using UV-visible spectral analysis and the optical constants such as band gap energy, extinction coefficient and refractive index were evaluated. Third order optical non linearity was confirmed by Z scan analysis. Mechanical property of the material has been analysed by Vicker's microhardness analysis.

**Keywords:** X-ray Diffraction, Optical property, Emission behavior, Mechanical property

<b>PP-33</b>	<b>Growth and XRD analysis of pure and dye doped L-threonine single crystal in the ratio 1:0.010</b>
<p><i>N. Subeena<sup>(1)</sup>, S. Antony Dominic Christopher<sup>(2)</sup></i></p> <p><sup>(1)</sup>M.Sc Student, Nanjil Catholic College of Arts and Science Kaliyakkavilai. <sup>(2)</sup>Assistant Professor, Nanjil Catholic College of Arts and Science Kaliyakkavilai.</p> <p>L-threonine is an essential amino acid that is used in the biosynthesis of proteins. The crystals were grown by slow evaporation technique. Methyl violet (C<sub>24</sub>H<sub>28</sub>N<sub>3</sub>Cl) is used as the dye dopant in the ratio 0.010. The grown crystal was characterized by X-ray diffraction analysis. It confirms the grown crystals belong to orthorhombic system.</p>	

<b>PP-34</b>	<b>FT-IR, UV-Vis and NMR Characterization and Investigation of Reactive Properties of 4-Amino-5-(naphth-2-oyl)-2-ethyl/propylaminothiazoles by Molecular Simulations and DFT Calculations</b>
<p><b>K.Thibi Mol<sup>a,b</sup>, T.F.Abbs Fen Reji<sup>b*</sup>, H.Marshan Robert<sup>c</sup></b></p> <p><sup>a</sup><i>Research Scholar (Reg.No:19213112032006); Affiliated at Manonmaniam Sundaranar University, Tirunelveli-627012</i> <sup>b</sup><i>Department of Chemistry, Nesamony Memorial Christian College, Marthandam, kanyakumari District, Tamil Nadu-629165</i> <sup>c</sup><i>Department of Physics &amp; Research Centre, Nanjil Catholic College of Arts and Science, Kaliyakkavilai-629151, Tamil Nadu, India.</i></p>	

Corresponding author: [abbsfen@gmail.com](mailto:abbsfen@gmail.com)

**Abstract**

The compounds 4-amino-5-(naphth-2-oyl)-2-ethyl/propyl aminothiazoles was synthesized and characterized with spectroscopy methods. The molecular framework of the compounds were optimized and the structural features were analyzed by DFT method with 6-311 G(d,p) basis set. FT-IR spectra of synthesized compounds were recorded in the region 4000–400  $\text{cm}^{-1}$ . The computed energies of MOs reveal charges that move inside the molecule. UV-Visible spectra show the various electronic transitions of title compounds. The material steadiness emerging from hyper conjugative connections, charge delocalization was discussed utilizing NBO examination. MEP and Fukui functions were performed to predict reactive site of the present compounds. The RDG examination was used to anticipate the weak interaction of the particle with the assistance of electron thickness. The observed hydrogen ( $^1\text{H}$ )-NMR values agreed computed values. The in vitro antioxidant activity of 4NET and 4NPT compound was evaluated using DPPH radical scavenging assay. The investigated molecule possesses lower activity against *E.coli* with 19 mm at 80 $\mu\text{L}$  and *Candida albicans* with 15 mm at 80 $\mu\text{L}$ . To concentrate on bio-active applications, Docking was performed to recognize the binding energy between ligand and protein through hydrogen bond interaction with various anticancer proteins. A cytotoxic screening reveals title compound shows efficient response against SKMEL cancer cells lines.

**Keyword:** FTIR, UV-Vis,  $^1\text{H}$ -NMR, DFT, TG-DTA, Molecular Docking.

PP-35	<b>Synthesis and structural characterization of aluminium doped magnesium oxide</b>
<b>S.N. Viji<sup>(1)</sup>, T.R Jeena<sup>(2)</sup></b>	
1) M.Sc. Student 2) Assistant Professor, Department of Physics Nanjil Catholic College of Arts and Science, Kaliyakkavilai.	
<b>Abstract</b>	
Pure and 2 wt. % Al doped Magnesium oxide nanoparticles have been synthesized by co-precipitation method. The synthesized nanoparticles were analysed using X-ray diffraction technique. The structure, crystalline size, lattice parameter and micro strain of both pure and aluminium doped magnesium nanoparticles were found from the diffraction pattern. For both the samples XRD patterns revealed cubic structure of magnesium oxide. Also in the doped samples, the addition of aluminium ions are observed.	

PP-36	<b>DFT studies and topology analysis of 1 acetyl – 2 (4 – isopropoxy – 3 - methoxyphenyl) cyclopropane</b>
<b>Jibin D<sup>1</sup>, S. Sijana<sup>2</sup>, M. Amalanathan<sup>3</sup>.</b>	
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<sup>1,2,3</sup>Affiliated to Manonmaniam Sundararar University Tirunelveli, Tamil Nadu, India

The computational investigations on 1 acetyl-2(4-isopropoxy-3-methoxyphenyl) cyclopropane, were done using DFT/B3LYP/6-311G (d, Sp) basic set by Gaussian 09W software. The HOMO and LUMO energies, Ionisation potential (I), Electron affinity (A), Energy gap, chemical hardness ( $\eta$ ), chemical potential ( $\mu$ ), Electrophilicity Index ( $\omega$ ), Nucleophilicity Index (N), Global Softness (S), Additional Electronic Charges ( $\Delta N$ ) and Optical Softness ( $\sigma_o$ ) were calculated. The intra and intermolecular interaction exist within this compound is analyzed by different methods namely topology analysis ELF, LOL and RDG.

Keywords: DFT calculation, ELF, RDG.

<b>PP-37</b>	<b>Fluctuating radial solar wind</b>
<p style="text-align: center;"><b>Rini Reshma Crass T<sup>1</sup>, Bidhu S<sup>2</sup></b></p> <p style="text-align: center;">Department of Physics</p> <ol style="list-style-type: none"><li>1. PG student, Nanjil Catholic college of arts and science, Kaliyakkavilai</li><li>2. Assistant Professor, Nanjil Catholic college of arts and science, Kaliyakkavilai</li></ol> <p style="text-align: center;"><b>Abstract</b></p> <p>Radial variations of solar wind during 1990-2009 are analysed. Using the data of Voyager 2 and Ulysses spacecrafts the studies extensively mentioned long and short term parameters respectively. Analysed the solar wind parameters, temperature, proton density and solar wind speed. Voyager 2 continues to explore the outer heliosphere as Ulysses studies the latitudinal dependence of the solar wind.</p> <p>Keywords: Solar wind, long and short term , solar parameter.</p>	

<b>PP-38</b>	<b>Relation between solar wind parameters and solar cycles-recent solar maxima</b>
<p style="text-align: center;"><b>Jothika G.R<sup>1</sup>, Bidhu S<sup>2</sup></b></p> <p style="text-align: center;">Department of Physics</p> <ol style="list-style-type: none"><li>1. PG student, Nanjil Catholic college of arts and science, Kaliyakkavilai</li><li>2. Assistant Professor, Nanjil Catholic college of arts and science, Kaliyakkavilai</li></ol> <p style="text-align: center;"><b>Abstract</b></p> <p>Solar wind parameters are used to study the solar activity in different solar cycles. Solar wind parameters have strong connection with solar cycles. This is investigated for solar cycle 23 and 24. ACE and WIND spacecrafts data are used to determine the connection between solar wind plasma parameters and solar cycle. The solar wind parameters like solar wind velocity, density, temperature and magnetic field during 23 and 24 solar maximum activity phase are analyzed. In solar cycle 24, solar wind velocity and temperature have strong relation with solar cycle. But In solar cycle 23, solar wind density and magnetic field have good relation with solar cycle.</p> <p>Key words: solar wind parameters- velocity, density, temperature and magnetic field.</p>	

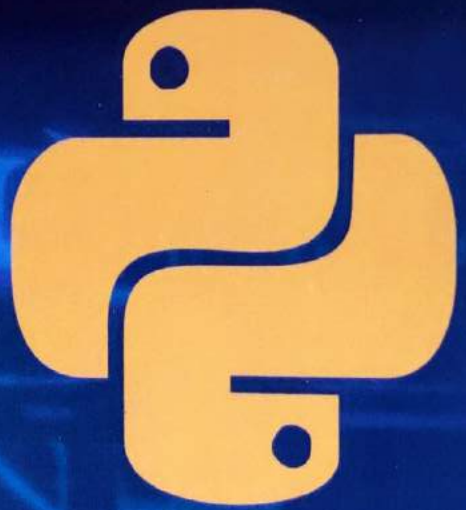


<b>PP-39</b>	<b>Characteristics of speed of solar cme's in 24 solar cycle</b>
<p style="text-align: center;"><b>Bramya V M<sup>1</sup>, Bidhu S<sup>2</sup></b></p> <p style="text-align: center;">Department of Physics</p> <ol style="list-style-type: none"><li>1. PG student, Nanjil Catholic college of arts and science, Kaliyakkavilai</li><li>2. Assistant Professor, Nanjil Catholic college of arts and science, Kaliyakkavilai</li></ol> <p style="text-align: center;"><b>Abstract</b></p> <p>The properties and recent results on coronal mass ejections(CMEs), obtained from the Solar and Heliospheric Observatory (SOHO) during 2008–2015 are investigated. In Cycle-24, due to the reduced ambient pressure, CMEs expand anomalously. SOHO/LASCO CMEs, were obtained from the LASCO catalogue. The type of CMEs are determined using solar wind linear speed. We report on a comparison between space weather events that occurred around the two peaks in the sunspot number (SSN) during solar cycle 24. The two SSN peaks occurred in the years 2012 and 2014. Even though SSN was larger during the second peak, we find that there were more space weather events during the first peak.</p> <p>Keywords: coronal mass ejections, sunspot number, solar cycle</p>	

<b>PP-40</b>	<b>Slow solar wind fluctuations observations from ulysses orbit</b>
<p style="text-align: center;"><b>Jenisha<sup>1</sup> G, Bidhu S<sup>2</sup></b></p> <p style="text-align: center;">Department of Physics</p> <ol style="list-style-type: none"><li>1. PG student, Nanjil Catholic college of arts and science, Kaliyakkavilai</li><li>2. Assistant Professor, Nanjil Catholic college of arts and science, Kaliyakkavilai</li></ol> <p style="text-align: center;"><b>Abstract</b></p> <p>During rising phase, maximum activity phase and declining phases of solar cycle 22 and 23, Ulysses' spotted slow solar wind. The spacecraft observed the slow solar wind in first orbit; during the decline phase of solar cycle 22, in second orbit; in polar region during the maximum phase of solar cycle 23 and in ecliptic region during the decline phase of solar cycle 23. When the polarity reversal takes place ie; during maximum phase of solar cycle 23, slow wind was found in polar region. The multi-polarities have key-role for the formation of slow solar wind. The solar wind that emerges during the polarity reversal detected slow solar wind due to the high concentration of proton particle.</p> <p>Key words: Solar cycle, slow wind, multi-polarities.</p>	

<b>PP-41</b>	<b>Studies on organic 4-hydroxy benzophenone single crystals</b>
<p style="text-align: center;"><b>M.L.Lima Rose<sup>a,b</sup>, T.Suthan<sup>c</sup>, Gnanasambandam<sup>a</sup></b></p> <p><sup>a</sup>ResearchScholar( Reg.No18133152132034),Department of Physics, S.T. Hindu College, Nagercoil – 629002, India <sup>b</sup>AssistantProfessor,Department of Physics, Malankara Catholic College, Mariagiri – 629153, India <sup>c</sup>AssistantProfessor, Department of Physics, Lekshmipuram College of Arts and Science, Neyyoor – 629802, India <sup>a</sup>Associate Professor, Department of Physics, S.T.Hindu College, Nagercoil - 629002, India</p>	

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## Factors Influencing Consumers' Buying Behaviour of Honda Motors with Special Reference to Kanyakumari District

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### Abstract

Consumers buying behaviour is a process by which consumers identify their needs, collect information, evaluate alternatives, and make the purchase decision. It is a series of choices made by a consumer prior to making a buying that begins once the consumer has established a willingness to buy. The consumer must then decide where making the purchase, when making the buying, how much to spend and what method of payment will be used. The marketer attempts to influence each of these decisions by supplying information that may shape the consumers evolution. The six stages of the consumers buying behaviour process are Problem Recognition, Information search, Evaluation of alternatives, Purchase Decisions, Purchase, Post- Purchase evaluation. This project focuses on finding the various determinants of consumer buying behaviour and to construct model for consumer buying behaviour related to purchase of two wheelers. A descriptive research is carried out with a specific objective and it results in definite conclusions. The survey conducted from 120 respondents and used convenience sampling method. The tools used for data analysis are percentage analysis, ranking method, cluster analysis and ANOVA. By analysis it is found that most of the consumers strongly agree with brand loyalty as the consumer buying behaviour and the decision factors also plays a major role in consumer buying behaviour. This enriches the showroom in achieving the goals and objectives.

**Keyword:** Buying behaviour, Determinants of buying behaviour.





## **Efficiency Enrichment of Faculties in Self Financing Arts and Science Colleges in Kanyakumari District**

**G. Rajesh Babu<sup>1\*</sup> and G. Jenit Hanson<sup>2</sup>**

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### **Abstract**

Every education institution, higher management consistently looks for different ways of evaluation and development of their faculty members. Today, a faculty involved in many activities such as planning and updating the curriculum, developing learning environment, facilitating discussion, creating interactive environment, preparing tests, setting assignment, providing feedback and proper counseling of students. This study focuses on efficiency enrichment in self financing arts and science colleges in Kanyakumari District.

The objectives are to identify the specific factors which play a major role and challenges of efficiency enrichment of faculty members. This study adopted descriptive research design. The survey was conducted in 83 faculty members of 16 self financing arts and science colleges and used stratified random sampling method. The primary source comprised of information gathered from the respondent through questionnaires. Chi square test is used in tools for analysis. The major findings are, the self financing faculties are not participating in the efficiency enrichment programs they would not have any direct impact on their API score. They also felt the financial burden and struggling to pay the registration fees.

Many self financing colleges did not grant leaves for faculties to participate in such efficiency enrichment programs. The major suggestions are self financing colleges could work out a competitive salary structure, which is flexible, experience and knowledge gained prior to joining the present institution. Managements unintentionally try to sustain the existing culture due to a lack of vision of how to successfully bring about change. Faculties should build competencies of learners through best pedagogic practices and also contribute to research. Policy makers in education have an important responsibility of creating policy framework for effective functioning of the institutions. If all these steps are followed in the true spirit then the envisioned higher education institute will turn into a reality.

**Key words:** Efficiency enrichment, evaluation, implementation.



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## CONCURRENT SESSION B

Time : 10.30 a.m. to 12.30 p.m

Parallel Session V : Professional Social Work Practice in the Crisis Situation  
(Natural Disasters / Pandemics / Financial Uncertainties)  
Link : <https://zoom.us/j/6371860819?pwd=Zi9iT2k0aGMzcDFoZzROZEFWVC9Cdz0>  
Meeting ID : 637 186 0819  
Passcode : Power

**Session Coordinator** : **Dr. SAM DEVA ASIR R. M**, Assistant Professor

**Chair Person** : **Dr. J.M ARUL KAMARAJ**

Assistant Professor of Social Work  
Loyola College, Chennai

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## THE IMPORTANCE OF MENTAL HEALTH AMONG SOCIAL WORKERS WORKING DURING THIS PANDEMIC CRISIS AT CHENNAI.

Martina Tigga<sup>1</sup> and Francis Divakar JP<sup>2</sup>

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### Abstract

Mental health is one of the most important factors in an individual's life. It is interlinked with all other aspects such as an individual's physical and emotional health, work life, relationships etc. Any disruptions in one of these aspects can affect all the other factors. It refers to the condition of being mentally and emotionally sound that is characterized by the absence of any mental illness and by adequate adjustment especially as reflected in feeling comfortable about oneself, positive feelings about others, and the ability to meet the demands of daily life (Merriam-Webster 1828). With the present situation of Covid-19 it has taken a toll on most of our mental health. In the context of the present situation with shortage of adequate medical utilities, massive spike in Covid-19 cases around the country, as well as the mismanagement of the government regarding this situation, social work professionals along with other professionals have been working continuously to help the people who are in desperate need of help. The amount of work and commitment that this period demands especially in the part of a social work profession can affect their mental health to a great extent. Therefore this study aims to examine the importance of mental health among Social Workers working during this pandemic crisis. For this study, the researcher used descriptive and quantitative research method. 30 samples for the study were collected through convenient sampling method. This Study will help us to understand mental health aspect of social workers which in turn help us to know more about the difficulties faced by people who are helping and supporting others.

**Keywords:** *Mental Health, Social worker, Pandemic*

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## DIGITAL GAMING BEHAVIOR AND ITS ASSOCIATIONS WITH COVID 19 PANDEMIC

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### Abstract

The novel Coronavirus 2019 (COVID 19) pandemic has changed the daily routine life all over the world. India is devastating the second Wave of COVID 19. To combat, the government of India followed many public health measures such as quarantine, lockdown protocols, social distancing, promoting healthy lifestyles and self-isolation policies etc. As a consequence, the measures have led to occupational and educational disruption and psychological distress among the youth. bring the lockdown pandemic situation and also explore the association of components such as hours of gaming per day, changing daily routine, psychological problems with the lockdown period of COVID 19. Conclusion: Even though students may think digital gaming can be healthy way to relieve from stress and changing mood especially during lockdown but excessive engagement in digital gaming leads to developing unhealthy daily routine.

**Keywords:** *COVID 19, Gaming behavior, Digital Gaming, Daily routine, Psychological Problems.*

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# **Bohal Shodh Manjusha**

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## कृष्ण बलदेव वैद के नाटकों में चित्रित वृद्ध समस्या

-डॉ. कार्तिका.एस.के

असिस्टन्ट प्रोफेसर, नॉनजिल कॉटोलिक कॉलेज आफ आर्ट्स आण्ड साइन्स  
वी.आर.भवन निरप्पुकोणम्, उरुदुम्बलम, तिरुवनन्तपुरम, केरला-695507

बहुमुखी प्रतिभावाले कृष्ण बलदेव वैद जी हिंदी साहित्य का सशक्त हस्ताक्षर हैं। उनका रचना-संसार बहुत विस्तृत है। उपन्यास, कहानी, नाटक, समीक्षा, अनुवाद, आलोचना, साक्षात्कार आदि अनेक विधाओं में उनकी गति रही है। वैद जी का व्यक्तित्व अपने आंच में तपे व्यक्तित्व है। वैद जी ने कुल आठ नाटक लिखे- भूख आग है (1998), हमारी बुढ़िया (2000), सवाल और स्वप्न (2001), परिवार अखाड़ा (2002), मोना लिज़ा की मुस्कान (2003), कहते हैं जिसको प्यार (2004), अन्त का उजाला (2012), पार्क के पीर (2015)।

वैद जी अपने नाटकों के द्वारा मानवजीवन की विसंगतियों को प्रस्तुत करने का सफल प्रयास किया है। प्रतिदिन बढ़ती हुई व्यक्ति की निराशा, संवेदन शून्यता आदि को वैदजी ने अपनी रचना का विषय बनाया। मानव अपने जीवन में अकेलापन, निराशा, कुंठा आदि से त्रस्त होकर जीते हैं। उनको कहीं से सहारा नहीं मिलेगा तो जिंदगी अस्तव्यस्त हो जाएगी। यही वैदजी अपने नाटकों के द्वारा समाज को दिखाना चाहते हैं।

एक मनुष्य अकेलापन, निराशा, कुंठा आदि से ग्रस्त होकर जीनेवाला समय वृद्धावस्था ही है। वैद जी के नाटकों में हमारी बुढ़िया, अन्त का उजाला आदि में वृद्ध जीवन में गुज़रनेवालों की कई समस्याएँ प्रस्तुत किया है।

### ‘हमारी बुढ़िया’ में प्रस्तुत वृद्ध जीवन की समस्याएँ :-

हमारी बुढ़िया में गठरी लेकर बैठी हुई एक बुढ़िया का चित्रण है। गोद में अपनी गठरी लेकर एक खंडहर के चबूतरे पर पड़े पलंग पर बैठती है। वह गांव में रहती थी लेकिन अपने बच्चे जो शहर में आ गये थे उनकी खोज में वह इस अनजान शहर में फटक रही है। माता-पिता छोटी आयु में हमें पाल पोसकर बड़े बनाते हैं। अपनी गलतियों को समझाते हैं। लेकिन बच्चे बड़े हो गया तो मां-बाप की गलतियों को क्षमा करना नहीं जानते। वह किसी भी तरह उन्हें अपनों से दूर कराते हैं। उस बूढ़ी माँ के प्रति कई तरह की सवाल जवाब उडता है। पहला सवाल यह था कि यह कौन है? उसका वहाँ बैठने के कारण का वे लोग अनुमान करते हैं। कुछ लोग कहते हैं कि उस बुढ़िया का सारा सामान इस गठरी में ही होगी। उस गठरी क्या है इसका भी कई अनुमान होता है।

इसी तरह की वार्तालाप के बीच वे यह भी सोचते हैं अगर वह हमारी माँ है? सच में वे लोग यह भी नहीं जानता है कि अपनी माँ घर पर है या नहीं। यही आज की स्थिति है। हमारे अपनों के बीच में क्या हो रहा है यह भी हम नहीं जानते हैं। हम सब भागते हैं पैसे के पीछे। वैद जी ने हमारे अस्त-व्यस्त शहरी सडक के किनारे



खंडहर में पडी पलंग पर एक गठरी लेकर बैठती बुढ़िया के माध्यम से आधुनिक सामाजिक समस्याओं का प्रस्तुतीकरण किया है। वृद्धावस्था सबके पास आनेवाली अवस्था है यही सोचकर हम सतर्क रहना चाहिए।

### ‘अन्त का उजाला’ में प्रस्तुत वृद्ध जीवन की समस्याएँ :-

अन्त का उजाला 2012 में वैद जी द्वारा लिखित नाटक है। प्रस्तुत नाटक में बूढ़ापे में ठहरे पति-पत्नी की मनोदशा को एक अनौपचारिक भाषिक उपक्रम में व्यक्त करता है। बच्चे अपने-अपने कार्यों में व्यस्त हो जाते हैं तब बूढ़े माँ-बाप की याद भी न करते। प्रस्तुत नाटक में पत्नी हमेशा अपने बच्चों का फोन या ईमेल करने के लिए वृद्ध पति को मजदूर करती है। लेकिन वह कहता है :-

“मेरा मन न करता।

जब मेरा मन कहेगा तब करूँगा।”

नाटक में मियाँ-बीवी द्वारा बूढ़े माँ-बाप का चित्रण है। बूढ़ापे में अपने बच्चों का प्रेमपूर्ण व्यवहार उनके लिए अंधेरे की रोशनी ही है। लेकिन बच्चे कभी न समझ पाता है। मियाँ और बीवी अपने अंत की प्रतीक्षा कर रहे हैं। मियाँ कहता है :-

“अब हो ही क्या सकता है

अंत के अलावा।”

दोनों अपने जीवन आगे बढ़ाने के लिए कहानियाँ कहते हैं। हर समय एक ऐसी कहानी मियाँ बीवी को सुनाती है उसमें कुछ न कुछ जोड़ता रहता है। उसमें ज़िंदगी आगे बढ़ाने की क्षमता भी है। आजकल दवाओं के कारण आगे बढ़ने वाली ज़िंदगी का इशारा भी है। वह कहती है :-

“बूढ़ापे लम्बे होते जा रहे हैं

नई-नई दवाओं के कारण ...।”

अंत तक वे किसी की प्रतीक्षा करती रहती है। अंत में स्वयं अपने को समझने के लिए मियाँ कहता है-

“तो हम मान लेंगे वे हम से ऊब गये।

और अब हम दोनों को उनके बगैर जीना मरना है।”

इसी तरह वास्तविकता को स्वीकार करने के लिए वे लोग तैयार हो जाते हैं।

वृद्धावस्था ऐसी एक दशा है उसी अवसर में हम सबको अपने ही पास चाहते हैं। लेकिन हमें अपने बच्चों के पीछे जाना पड़ेगा। ऐसे जाने वाले लोगों की दशा ही वैद जी हमारी बुढ़िया की बुढ़िया के द्वारा दिखाता है। अपने बच्चों की राह देखकर चुपचाप अखिरी साँस की इंतज़ार में रहने वाले अनेकों के प्रतीक के रूप में अन्त का उजाला के दम्पतियों को चित्रित किया है। हम आगे की पीढ़ी ऐसा न होना चाहिए। हमें संभालने वाले माँ-बाप को संभालने की क्षमता हमेशा हमें होना चाहिए।

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