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NEW HORIZONS IN HUMANITIES AND BASIC SCIENCES

FOR SUSTAINABLE DEVELOPMENT

Volume-II



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PREFACE
ART'S, COMMERCE AND SCIENCE COLLEGE, ONDE

We are very happy to give this edited book entitled **"New Horizons in Humanities and Basic Sciences for Sustainable Development"** at the hands of readers. The present era is the era of interdisciplinary studies. Many trends and perspectives have emerged and are emerging in various disciplines in the present era at the global level. And India is not an exception to this also. It has also been observed and experienced that the higher education is no longer confined to boundaries of a specific subject or discipline. And so, a study of all the disciplines from the point of view of interdisciplinary aspects has been part and parcel of higher education today. And it is strongly felt in tune with NEP-2020 also. Keeping in view the significance of interdisciplinary perspectives and studies in various disciplines.

The purpose of this edited book, a good reference with ample stuff of research from the disciplines like humanities, social sciences, sciences, and commerce, is to collect and compile the research papers related to cutting-edge research results over all aspects of recent trends towards sustainable development and to enhance the knowledge about innovative technologies and present new research findings to promote global scientific and community collaborations in synergy with other Professional Associations.

This book is the compilation of esteemed articles of experts in the various fields on diverse aspects of scientific research of advanced and functional materials, tools and methods in Science, new perspectives in Humanities, Social Sciences and Commerce providing a sufficient depth of the subject. This book will play an instrumental role in opening new vistas in the field of interdisciplinary studies intersecting all the disciplines as we have compiled research papers from the eminent scientists, academicians, and research scholars. Going through this book is one of the profoundest intellectual experiences for the scholars. This experience is felt in the writings of academicians. We also hope that the students, teachers, researchers, scientists, and policy makers in India and abroad will find this book much more useful.

In conclusion we would like to take this opportunity to thank the president of the institution Shri. Milind Patil, I/C Principal Dr. Basweshwar Pandagale for kind support and academicians, research scholars for their contribution. We are also thankful to the Jyotikiran Publication, Pune for taking pains in bringing out this book.

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‘Reviving the Earth: Soil Remediation for Sustainable Agriculture’ A Review

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Abstract:
Soil contamination and degradation present substantial obstacles to sustainable agriculture and environmental well-being. Various soil remediation techniques, including bioremediation, phytoremediation, soil washing, and thermal remediation, provide efficient methods for rehabilitating polluted soils. These techniques aid in reducing the presence of harmful substances such as heavy metals, pesticides, and organic chemicals, thereby improving soil quality and making it suitable for farming. Concurrently, agricultural techniques like organic farming, agroforestry, conservation tillage, and precision agriculture are vital in preserving and enhancing soil health, fostering sustainability, and increasing crop productivity. By combining soil remediation techniques with sustainable agricultural practices, we can achieve a harmonious balance that promotes soil fertility, minimizes environmental pollution, and safeguards food security amidst the growing global challenges. This approach highlights the importance of adopting a comprehensive strategy that integrates technology, sustainable practices, and efficient soil management to ensure a thriving and sustainable future for agriculture.

Keywords: Soil remediation, sustainable agricultural, phytoremediation, pollutants etc

I. Introduction:

Soil is a vital natural resource that is crucial for human survival, as it provides important ecosystem services that support agriculture, water filtration, carbon sequestration, and biodiversity. Unfortunately, soil health has been severely compromised by pollution and deterioration resulting from industrial operations, intensive farming practices, and urban expansion. Soil contamination, caused by pollutants like heavy metals, pesticides, and organic chemicals, poses significant risks to agricultural productivity, human health, and the environment. These harmful substances can remain in the soil for extended periods, resulting in decreased soil fertility, diminished biodiversity, and potential risks to food safety. Simultaneously, modern agricultural practices, although essential for feeding the growing global population, often exacerbate soil degradation through practices like monoculture, excessive use of chemical fertilizers and pesticides, and improper irrigation. These practices can result in soil erosion, loss of organic matter, depletion of essential nutrients, and increased salinization, exacerbating the stress on soil health. [1]

To tackle these challenges, soil remediation and sustainable agricultural practices are of utmost importance. Soil remediation involves the process of purifying and rehabilitating polluted

or damaged soils, enabling them to sustain healthy plant growth and ecosystem functions. The main objective of remediation is to decrease or eliminate soil pollutants, improve soil health, and transform contaminated lands into viable areas for farming and other purposes. Various techniques, such as bioremediation, phytoremediation, soil washing, and thermal remediation, are used to address different types of soil contamination, each tailored to specific pollutants and environmental conditions. Conversely, sustainable agriculture aims to maximize farming practices in a manner that preserves or improves soil health while guaranteeing food availability. Sustainable farming practices prioritize minimizing the harmful effects of agriculture on the environment, preserving soil quality, and enhancing adaptability to climate change. Techniques like organic farming, agroforestry, conservation tillage, and precision agriculture not only enhance the productivity of the land but also play a crucial role in soil conservation, biodiversity preservation, and carbon sequestration. [2] By combining soil remediation techniques with sustainable farming methods, it is possible to revitalize polluted soils, increase soil fertility, and boost agricultural output. By employing environmentally friendly methods to restore contaminated land and integrating them with sustainable farming practices, the dual objectives of safeguarding the environment and guaranteeing long-term food production can be accomplished. By integrating these practices, we can combat soil degradation, minimize pollution's impact, optimize resource utilization, boost agricultural productivity, and protect the environment. Therefore, comprehending and implementing both soil remediation techniques and sustainable farming practices will be crucial in addressing the challenges associated with soil contamination and degradation in the 21st century. [3]

This chapter delves into the essential methods for soil remediation and their relevance to agriculture, emphasizing the connection between ecological restoration and sustainable farming methods. The goal is to offer a thorough understanding of how these practices can be integrated to safeguard soil health, increase food production, and promote environmental sustainability.

2. Types of soil Contamination:

Heavy Metals: Soil contamination can happen naturally or as a result of human actions. Some common pollutants found in the soil are heavy metals such as lead (pb), cadmium (cd), arsenic (as), and mercury (hg), which can be harmful to both plants and animals.

Organic pollutants: pesticides, herbicides, and industrial solvents can remain in the soil, causing ecological imbalance.

Salinity: when there is too much irrigation or if the drainage is not done properly, salts can build up in the soil, making it harder for plants to absorb water.

Imbalances in nutrients: excessive use of chemical fertilizers can result in nutrient imbalances, especially nitrogen, phosphorous, and potassium, causing soil acidification and a decline in biodiversity. [4]

3. Soil Remediation Techniques:

Various soil remediation techniques are utilized to tackle contamination, and these can be categorized into physical, chemical, and biological methods. Soil washing is one of the most frequently used physical methods in

3.1 Soil washing. It employs water or chemical solutions to eliminate pollutants from the soil. This process entails: mechanical agitation of the soil, combined with the addition of water or washing agents. Sieving or centrifuging is used to separate the clean soil from the contaminated particles. Various pollutants, including heavy metals, oils, and organic substances, are extracted from the soil and can be treated individually. Applications of soil washing are suitable for eliminating contaminants that are attached to particles (e.g., heavy metals, oils, and specific organic pollutants).

3.1.1 Excavation and off-site disposal: It is a direct method where contaminated soil is physically removed and transported to a treatment facility or a landfill for disposal. This method is frequently employed when contamination levels are elevated or when alternative approaches would be too time-consuming or inefficient. Thermal treatment or land filling can be used together to treat or

dispose of the contaminated soil. This method is applicable ideally for sites where contamination is severe, highly concentrated, or challenging to treat on-site.

3.1.2 Soil Vapor Extraction: It is a technique employed to eliminate volatile organic compounds from the soil. The process entails using a vacuum to extract air from the soil, which helps remove contaminants from the affected area. The vaporized pollutants are subsequently removed and processed at the surface. The contaminated soil was cleaned by using a vacuum on a network of wells that were drilled into it. VOCs are removed from the ground and processed, usually through carbon adsorption or thermal destruction. Soil Vapor extraction is effective for treating volatile, petroleum-based, and organic compounds.

3.1.3 Air Sparging: is a technique that involves injecting air into the groundwater or soil to enhance the release of contaminants into the air. The air forces the contaminants (often volatile organic compounds) into the vapor phase, making them simpler to extract using soil vapor extraction. Injecting air into the ground below the water table or contaminated soil. Contaminants can ascend as vapors and can be addressed at the surface level. It is suitable for use in assessing the presence of volatile organic pollutants in groundwater and soil. [5]

3.1.4 Electro kinetic Remediation: employs an electric field to transport charged contaminants, such as heavy metals and inorganic pollutants, through the soil towards electrodes where they can be either removed or treated. Electrodes are placed in the ground, and electric current is passed through them. Contaminants with a charge (e.g., heavy metals) are directed towards the electrodes for the purpose of removal or neutralization. This method is particularly effective for heavy metals like lead, arsenic, and cadmium, especially in fine-grained soils like clay.

3.1.5 Thermal Treatment: It is also known as soil heating or thermal desorption, entails subjecting the soil to high temperatures to vaporize contaminants, which are subsequently removed or eliminated. This technique is commonly employed for organic pollutants that are sensitive to heat. Thermal desorption entails subjecting the soil to high temperatures (typically between 200–800°c), resulting in the release of contaminants into the air. The extracted and treated contaminant vapors are typically accomplished through carbon adsorption or combustion. It is suitable for treating hydrocarbons, pesticides, and other organic compounds.

3.1.6 Granular Activated Carbon (GAC): This is employed to adsorb contaminants from soil vapor or groundwater. The soil is treated by removing contaminants into the gas phase, where GAC is employed to capture the pollutants. Carbon filters are employed to eliminate volatile organic compounds (VOCs) and other organic substances from vaporized contaminants. As gases flow through the carbon filters, they get trapped, effectively removing the pollutants. It is beneficial for removing volatile and semi-volatile organic compounds from various substances. [6]

3.1.7 Physical Stabilization Techniques: for soil contamination involve the use of physical barriers or materials to prevent the movement of contaminants in the soil. This could involve: covering or sealing the contaminated soil with materials like clay or synthetic liners. In situ solidification involves mixing soil with stabilizing agents like cement or polymers to prevent the spread of contaminants. This method is frequently employed when removal or active treatment is not feasible, particularly for extensive areas or sites with minimal levels of contamination.

3.1.8 Containment and Barrier technologies: utilize physical barriers or containment systems to separate contaminated soil from its surroundings, with a primary focus on preventing the migration of contaminants into groundwater. These obstacles might include impermeable barriers or slurry walls (usually constructed using concrete or bentonite clay) to prevent the migration of contaminants into groundwater. Geosynthetic liners are used to cover contaminated sites and prevent water from seeping through the ground. It is employed for extensive remediation projects where complete removal is impractical or where contamination has infiltrated the groundwater. One of the benefits of physical methods is their speed, as they are generally faster than biological treatments, which can take a significant amount of time, ranging from months to even years. In many instances, physical methods require minimal or no chemicals, making them more

environmentally friendly compared to other approaches. Effectiveness for specific contaminants: particularly suitable for challenging pollutants (e.g., heavy metals, volatile organic compounds, oils) that are hard to treat using biological methods. [7]

3.2 Chemical Methods

3.2.1 Phytoremediation: It is the utilization of plants to absorb or break down contaminants in the soil is a promising sustainable solution. Certain plants, such as sunflowers, Indian mustard, and willows, have demonstrated their ability to remove heavy metals, organic compounds, and even radioactive substances. Phytoremediation is an eco-friendly and economical method of cleaning up polluted soil and water, employing plants to eliminate, break down, or contain harmful substances in contaminated areas. It capitalizes on the inherent capability of specific plants to absorb, accumulate, or alter harmful substances such as heavy metals, organic pollutants, and radioactive elements. This process can happen either on-site (where the contamination is present) or off-site (where the contamination is removed), making it a flexible method for dealing with different contamination situations. There are several key mechanisms by which plants contribute to phytoremediation.

3.2.2 Phytoextraction: Plants absorb pollutants, such as heavy metals, through their roots, translocating them to their stems or leaves, where they accumulate. Once the plants have reached maturity, they can be collected and disposed of, effectively eliminating the contaminants from the environment.

3.2.3 Phytodegradation: specific plants and the microorganisms they host have the ability to transform organic pollutants into less harmful substances through metabolic processes. This mechanism is particularly efficient for pollutants such as petroleum hydrocarbons, pesticides, and solvents.

3.2.4 Phytostabilization: is a process where plants play a crucial role in immobilizing pollutants in the soil, effectively preventing their dispersion into the surrounding environment. This is especially beneficial for minimizing the harmful effects of heavy metals or radionuclides, making them less accessible to organisms and reducing their ecological impact.

3.2.5 Rhizodegradation: the roots of plants can encourage microbial activity in the soil, resulting in the breakdown of organic pollutants. The organic compounds secreted by plants, known as root exudates, stimulate the growth of microorganisms that aid in the breakdown of contaminants. [8]

Table 1: Types of Chemical Methods for soil remediation [8]

Phytoremediation Mechanism	Description	Pollutants Targeted	Process
Phytoextraction	Plants absorb contaminants from the soil and accumulate them in their tissues (roots, stems, or leaves).	Heavy metals (e.g., lead, cadmium, arsenic, mercury), radionuclides	Contaminants are absorbed by plant roots, translocated through the plant, and concentrated in aerial parts. Plants are later harvested to remove the pollutants.
Phytodegradation	Plants and their associated microorganisms degrade organic pollutants into less toxic forms.	Organic contaminants (e.g., petroleum hydrocarbons, pesticides, solvents)	Plants or microbes break down pollutants through metabolic processes, converting them into non-toxic by-products.
Phytostabilization	Plants reduce the mobility of pollutants in	Immobilization of contaminants in the	Heavy metals, organic contaminants,

	the soil, preventing them from spreading or entering the food chain.	root zone, preventing leaching into groundwater or air.	radionuclides
Phytovolatilization	Plants absorb contaminant sand release them as volatile substances into the air.	Contaminants are taken up by the plant, and then volatilized into the atmosphere, often through transpiration.	Volatile organic compounds (VOCs), some heavy metals (e.g., mercury)
Rhizodegradation	Microorganisms in the rhizosphere (root zone) degrade contaminants, often enhanced by plant root exudates.	Plants release organic compounds from roots that stimulate microbial activity to degrade contaminants	Organic pollutants, hydrocarbons (petroleum)

3.3 Bioremediation Methods: It is a biological method that employs microorganisms, such as bacteria and fungi, or plants to break down or change harmful substances. Microbial populations can be boosted by biostimulation (adding nutrients) or bioaugmentation (introducing new strains). Bioremediation involves utilizing living organisms, such as microorganisms, fungi, or plants, to break down, alter, or eliminate pollutants in the environment, thereby minimizing contamination. It is a sustainable, affordable, and environmentally friendly method for removing pollutants.

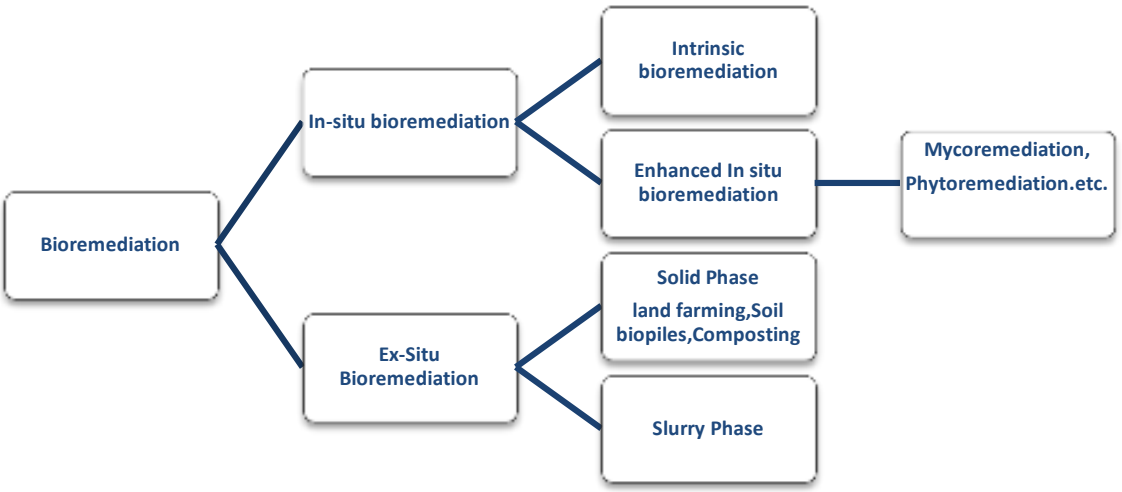


Fig: I Types of Bioremediation [9]

3.3.1 Mycoremediation: It is a specific type of bioremediation that employs fungi to decompose organic pollutants. Fungal species like phanerochaete chrysosporium can degrade lignin, pesticides, and other toxic compounds. Mycoremediation is a form of bioremediation that uses fungi (especially mushrooms) to degrade, absorb, or detoxify pollutants from the environment. Fungi are incredibly effective decomposers in the natural world and have the ability to break down a diverse range of organic and inorganic substances. The method of employing fungi to eliminate, break down, or neutralize toxic substances from the environment, commonly organic pollutants such as petroleum products, pesticides, and heavy metals. Mechanisms: extracellular enzymes: fungi release enzymes like lignin peroxidases, manganese peroxidases, and laccases that can break down complex organic compounds, such as hydrocarbons, plastics, and pesticides. **3.3.2 Vermicomposting:** This is the utilization of earthworms to break down organic waste and pollutants. Earthworms feed on organic material, and their digestive systems aid in breaking down toxic substances. It is a technique that employs living organisms to eliminate or mitigate pollutants in soil, water, and air.

3.3.3 In situ bioremediation: treatment of contaminants at the site of contamination, without moving the polluted material. Ex situ bioremediation: involves removing contaminated material (e.g., soil or water) from the site to treat it elsewhere. Mechanisms: microbial biodegradation: microorganisms (bacteria, fungi) break down contaminants like hydrocarbons, heavy metals, and pesticides.

Phytoremediation: uses plants to remove, stabilize, or degrade contaminants (a specific form of bioremediation). Fungi have the ability to break down organic substances such as petroleum products and pesticides.

Bioaugmentation: introducing particular strains of microorganisms to the polluted area to boost the natural breakdown of contaminants.

Biostimulation: introducing additional nutrients or substances to boost the activity of the microorganisms naturally present in the environment. Microorganisms break down petroleum and its derivatives in oil spills. Microorganisms have the ability to either reduce or stabilize heavy metals such as mercury and lead. They can also break down chemicals like DDT, pesticides, and herbicides. Industrial waste: harmful solvents, paints, and other chemicals found in the effluents of industrial processes. Advantages of this method are more affordable than traditional methods such as incineration or excavation. Environmentally-friendly, producing minimal waste. Eco-friendly and can be implemented on a large scale. Challenges: the effectiveness of the process can be limited by environmental factors, such as temperature, pH levels, and the availability of oxygen. Some contaminants can be so harmful that organisms struggle to break them down efficiently. Bioremediation processes can be time-consuming, necessitating a considerable amount of time to achieve substantial cleanup.

4. Soil Remediation Technologies in Agriculture provide numerous advantages for farming systems: enhancing soil fertility: remediation can replenish vital nutrients in the soil and eliminate harmful substances that impede plant development. This improves agricultural productivity and encourages environmentally friendly farming methods. Techniques such as incorporating organic amendments (compost, biochar) into the soil enhance its structure, which in turn improves water retention and drainage. This is particularly significant in areas impacted by saltiness. Enhancing soil biodiversity: soil remediation can boost microbial diversity and the presence of beneficial organisms like earthworms, which play a crucial role in nutrient cycling and promoting plant growth. Enhancing food safety: by eliminating or neutralizing harmful chemicals, soil remediation minimizes the absorption of toxic substances into crops, ensuring the quality of the food we consume. Despite the benefits of soil remediation, there are still challenges to overcome, such as the high cost of certain techniques and the need for substantial resources. Biological remediation methods, such as phytoremediation and bioremediation, may require several years to demonstrate noticeable improvements. Incomplete removal of contaminants: certain substances, like heavy metals, can be challenging to completely eliminate or neutralize, which may result in the re-contamination of treated soils. Certain remediation methods, particularly those involving chemicals, can inadvertently cause harm to the surrounding environment. [10]

5. Case Studies:

Case study 1: In a research conducted in Poland, scientists investigated the use of plants like mustard and sunflowers to decrease the levels of lead, zinc, and cadmium in agricultural soils. This technique not only eliminated pollutants but also improved soil fertility by facilitating the decomposition of organic matter. [11]

Case study 2: Bioremediation in organic farms: in an organic farming study, soil contaminated with pesticide residues was treated with a blend of bacterial strains known for their ability to break down organophosphates. The application led to a substantial decrease in pesticide levels, revitalizing the soil's health and enabling successful crop cultivation.

6. The future of soil remediation: lies in the advancement of technologies that are not only more efficient and cost-effective but also environmentally friendly. Advancements in nanotechnology, genetic engineering of microbes, and the application of machine learning to anticipate remediation results are demonstrating potential. Furthermore, a comprehensive approach to remediation that integrates various techniques (e.g., bioremediation combined with phytoremediation) could potentially become the new norm. [12]

7. Conclusion: Soil remediation is a crucial aspect of sustainable agriculture, as it helps restore degraded soils and guarantees food security. As contamination levels rise globally, comprehending and implementing efficient remediation techniques becomes crucial for minimizing environmental harm and ensuring a sustainable future for agricultural practices. The ongoing progress in creating cost-effective and environmentally friendly techniques will play a vital role in addressing the obstacles posed by soil contamination.

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A Practical Approach Of Teaching Higher Mathematics

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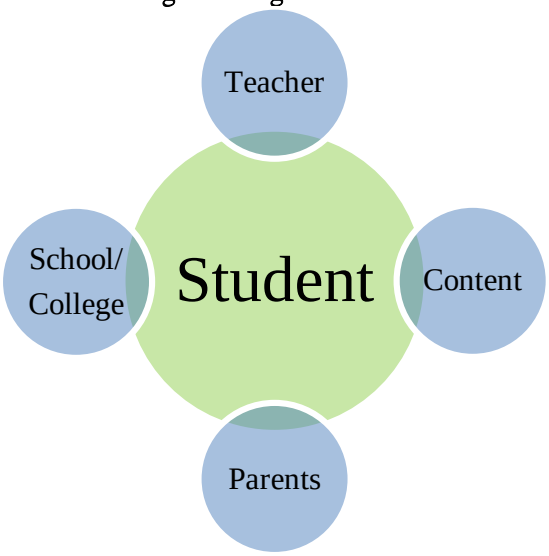
Abstract:

Mathematics has played a vital role in solving problems in real life. It is believed to be a difficult subject. Specially at higher level, student hesitate to opt mathematics because of its abstractness. In this chapter an effort is taken to fascinate higher mathematics. It will not only help learners to develop interest in the subject but also facilitate teachers at higher level to present the subject with a better correlation with real life problems.

Key words: *Higher Mathematics, Abstract concepts, Class Room Teaching, Electrical Circuits, Escape velocity, Statistical Analysis, Machine Learning, Artificial Intelligence*

Introduction:

Important Aspects of Teaching Learning Process



It's been considered from the long past that learning should be always "Student Centric". In ancient days it was considered to be a bipolar process comprising of two poles namely Teacher and student. Next came content into picture making it a tripolar process.

In recent days it is a penta-polar system including students, teacher, content, parents and learning institutes. Each of the poles has equal importance to make the teaching learning a successful and fruitful process.

Readiness:

One of the most important aspects of teaching learning process is readiness. If the students are mentally and physically ready to learn then a teacher's half work is done and to make the student ready to learn it is very important to develop interest among the students towards the subject.

Teaching Higher Mathematics:

Mathematics is considered as a dry and difficult subject at school as well as college level. It's a challenge for a teacher to make it interesting and simple for students. Students face following problems

- Abstract concepts at UG and PG level
- More theorems and proofs
- Applicability of the subject

A teacher should be able to provide convincing answers to solutions to them. Mathematics can be made interesting by correlating it to practical examples.



First inform them about the topics that are actually applicable in real life then explain those with specific examples.

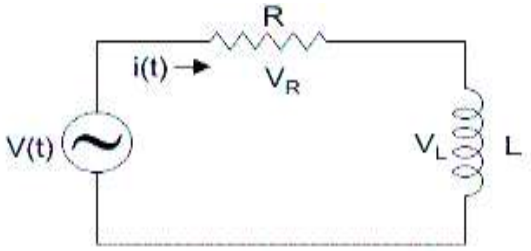
Some areas where mathematics is applied:

- Analysis and Calculus: Derivatives and Integrations play very important role in real-life problems.
- Derivative: rate of change viz; velocity, acceleration, current, tangent, normal etc.
- Integration: length, Area, volume, centre of mass etc.
- Discrete Mathematics: Computer, I T and electronic engineering.
- Differential Equations: Electronic, electrical, mechanical engineering (Fluid Dynamics)
- Statistics and Probability: Statistical Quality Control through Data Analysis and Sampling.
- Integral Transforms: Laplace Transform and Fourier Transform in Signal Analysis.

Few in Details:

1. **Electrical circuits**:

Consider a simple R-L series circuit with voltage supply V. Using Kirchhoff's Law, the Differential Equation governing the flow of current in the circuit can be written as follows.



$$L\frac{di}{dt} + Ri = V$$

$$\frac{di}{dt} + \frac{R}{L}i = \frac{E}{L}$$

Students must be told that the governing equation can be solved only if we know derivatives and integrations.

This is a linear differential equation, its solution is $i = \frac{V}{R} + ce^{-\frac{Rt}{L}}$

Therefore $i(0) = 0 \ \therefore c = \frac{-V}{R}$

$$i(t) = \frac{V}{R} - \frac{V}{R}e^{-\frac{Rt}{L}} = \frac{V}{R}\left(1 - e^{-\frac{Rt}{L}}\right)$$

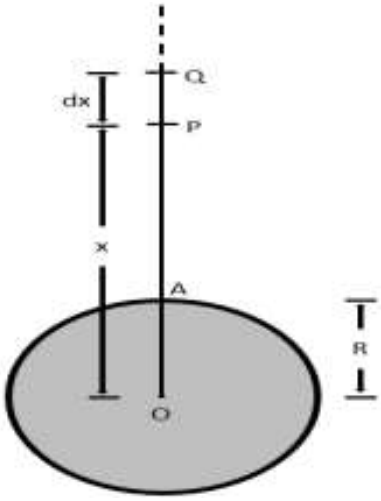
This is a simple example for illustration, upon adding various electrical components in the circuit the governing differential equation becomes richer in the sense that it may include higher order derivatives and even partial derivatives of higher order. The students can be then explained the need

of studying the concepts of derivatives, partial derivatives, integration, multiple integrations, exact and numerical solutions of differential equations so on and so forth.

2. Escape velocity from the Earth's Orbit:

Escape velocity is defined as the minimum initial velocity that will take a body away above the surface of a planet when it's projected vertically upwards.





A body of mass m is projected vertically upward with initial velocity v under gravity of a planet of mass M and spherical in shape with radius R

Kinetic Energy is $K.E = \frac{1}{2}mv^2$ force acting on it at P is $F = \frac{GMm}{x^2}$

Work done to take the mass from P to Q is $dW = Fdx = \frac{GMm}{x^2}dx$

Total work done to escape from the earth's orbit, $W = \int_R^\infty \frac{GMm}{x^2}dx$

Therefore $W = GMm\left[\frac{-1}{x}\right]_R^\infty$ so, we get $W = \frac{GMm}{R}$

For the body to escape from the orbit of planet: $K.E = W$

Therefore $\frac{1}{2}mv^2 = \frac{GMm}{R}, so\ v = \sqrt{\frac{2GM}{R}}$

But for Earth $g = \frac{GM}{R^2}$

So, we get $v = \sqrt{2gR}$

Escape velocity of the earth ,

$v = \sqrt{2 * 9.8 * 6.4 * 10^6} = 11.2 * 10^3 m/s =$ 11.2 km/s

3. Statistical Analysis:

- Mean, Median, Mode are most commonly used measures of central tendency.
- Range, variance, standard deviation and mean deviation are measures of central dispersion.
- Correlation and Regression analysis is done for examining the degree of correlation between given entities(variables)
- Probability distributions like Binomial, Poisson and Normal distributions are used in many real-life situations to find probability or frequency of a random variable (occurrence of some event)
- Testing of Hypothesis is done to check the hypothesis about some parameter of a population or comparison of parameters of two populations



One specific example ...

- A certain injection administered to 12 patients resulted in the following changes of Blood Pressure: 5, 2, 8, -1, 3, 0, 6, -2, 1, 5, 0, 4
  Can it be concluded that the injection will be in general accompanied by an increase in Blood Pressure?
- Let x be difference in BP
  x : 5, 2, 8, -1, 3, 0, 6, -2, 1, 5, 0, 4

Sample size: n =12, (small sample)

Sample mean: $\bar{x} = 2.58$

Sample S.D: $s = \frac{1}{n}\sqrt{\sum(x_i - \bar{x})^2} = 8.74$

Null Hypothesis:$\mu = 0$ Alternate Hypothesis: $\mu > 0$

Test Statistic: $t = \frac{\bar{x}-\mu}{s/\sqrt{n-1}} = 2.89$

Level of significance: $\alpha = 0.05$

t-Table value: $t_{\alpha,n-1} = 1.796$

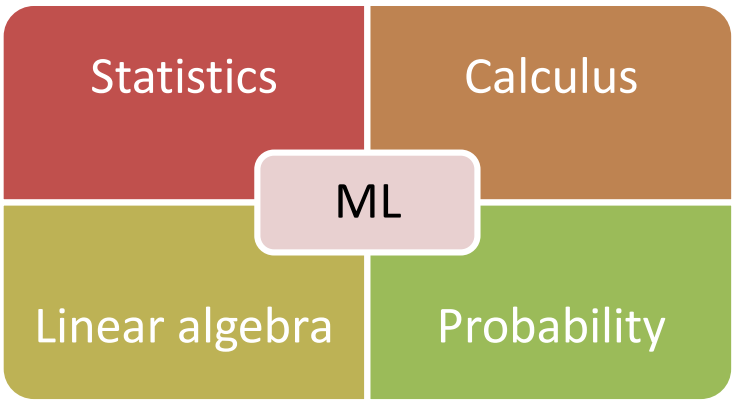
Decision: $t_{\alpha,n-1} > t$

So, reject Null Hypothesis, accept Alternate Hypothesis that change in B.P is Positive i-e the drug in general increases B.P

- This is just one example taken from medical field.
  Statistical Quality Control is done in almost every production company.

4. Role of Mathematics in Machine Learning:

"Machine Learning (ML) proposes different models implementing different algorithms for detection, prediction, and classification. The prediction could be what an object in a picture looks like or what the next price for fuel might be in a certain country or what's the best combination of drugs to cure a certain disease might be. ML is a built-in mathematical prerequisite. It is used to know why something works or why one model is better than another". [3] Following figure shows the components of maths used in ML i-e statistics, calculus, linear algebra, and probability.



5. Role of Mathematics in Artificial Intelligence:

"The role of mathematics in artificial intelligence is critical, as it provides the foundational framework for developing algorithms and models that enable machines to learn, reason, and make decisions. From machine learning to natural language processing and computer vision, Mathematics is essential for building intelligent systems that can adapt and learn from experience."[4]

Calculus plays vital role in artificial intelligence. Calculus is used to optimize machine learning models and algorithms by minimizing errors and maximizing accuracy.

Conclusion (Role of a Mathematics Teacher):

Teachers should include adequate number of examples along with theoretical results. Examples correlating the content with their applicability in Real Life situations. Give the students opportunities to apply learning and use the acquired knowledge for reason beyond passing exam or good grades. Inspire them to Love learning. Remember that

"*Teaching means to make the students Learn*"

and

"*Education is an all-round development of child, so that he/ she can lead a successful life.*"

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For images of illustration

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Review of Crystal Growth Technology with its comparative parameters

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I. Introduction

Crystal growth is in the heart of materials science and technology, it is having so many applications in semiconductor manufacturing to medicinal and pharmaceuticals industries. Crystal growth using Gel is a unique and versatile method because of its ability to provide highly controlled conditions during nucleation and crystallization. The gel method employs a three-dimensional, porous matrix that exhibits both solid and liquid properties it creating a stable and protective medium for crystal growth. This method is used for high purity and allows precise control over the size, shape, and orientation of the growing crystals.

In this article, provided a comprehensive overview of the crystal growth using Gel technique. We will discuss the fundamental principles behind the method, detail the step-by-step process employed during crystal formation in gels, examine the advantages of the gel approach, and explore real-world applications across several industries. This overview is designed to serve as a detailed resource for researchers, engineers, and professionals interested the benefits of gel crystal growth for advanced material synthesis.

2. Fundamentals of Gel Crystal Growth

Gel crystal growth is based on the unique properties of gels substances that exist in a state between a pure liquid and a solid. The gel matrix, typically formed from a gelling agent such as agar's, gelatin, or silica mixed with a solvent typically water or an organic solvent, forms a three-dimensional network with a porous structure. This porous nature not only provides mechanical stability but also regulates the diffusion of solutes within the gel.

2.1 Effect of Gel

The gel matrix acts as a scaffold that serves several essential functions in the crystal growth process:

- **Controlled Diffusion:** The porous structure allows for steady and controlled diffusion of solutes, ensuring that the concentration gradients necessary for nucleation and subsequent crystal growth are maintained.
- **Nucleation Control:** The constrained environment within the gel restricts the uncontrolled aggregation of solute molecules, promoting controlled nucleation sites that lead to the formation of well-defined crystals.
- **Protection from Contaminants:** The matrix provides a protective barrier that minimizes the incorporation of impurities, thereby enhancing the purity and structural integrity of the crystal.
- **Thermal Stability:** The gel environment can moderate temperature fluctuations, offering a more constant thermal environment that is critical for consistent crystal growth.

Gel-Based Crystallization

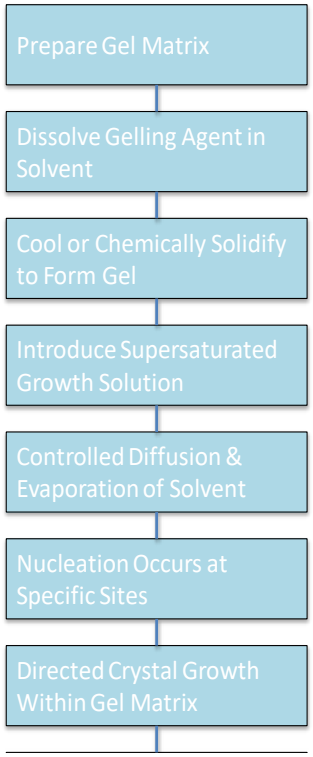
- **Super saturation:** To initiate crystal growth, a supersaturated solution of the desired compound is introduced into the gel. Super saturation is critical for nucleation, as it increases the probability of forming stable nuclei.
- **Nucleation and Growth:** Once nucleation occurs within the porous matrix, crystal growth is dictated by the rate of diffusion of the solute within the gel, the evaporation of the solvent, and the concentration gradients that are established.
- **Diffusion-Controlled Dynamics:** Since the gel slows down the diffusion process compared to a free liquid environment, the growth of crystals tends to be more uniform and ordered.

3. Crystal Growth Gel Method

The methodology for gel crystal growth is a multi-step process that involves careful preparation, controlled nucleation, and sustained crystal growth within the matrix. Below, we detail each of these steps alongside the scientific rationale behind them.

3.1 Process Flow Overview

Below is a flowchart steps that summarizes the key stages in the gel crystal growth process:



3.2.1 Gel Preparation

- **Dissolving the Gelling Agent:**
  The process begins by dissolving a chosen gelling agent (e.g., agarose, gelatin, or silica) in a solvent under controlled heating conditions. The choice of gelling agent and solvent is critical because it determines the pore size and structural stability of the gel.
- **Formation of the Gel Matrix:**

After the gelling agent is fully dissolved, the solution is allowed to cool or chemically react to form a three-dimensional gel. This cooling or solidification phase establishes the porous network, which is crucial for subsequent solute diffusion and crystal growth.

3.2.2 Introduction of the Growth Solution

- **Preparing the Supersaturated Solution:**

A supersaturated solution containing the desired crystal-forming compounds (such as salts or active pharmaceutical ingredients) is prepared separately. The level of super saturation is pivotal because it must be sufficient to trigger nucleation without causing uncontrolled precipitation.

- **Incorporation into the Gel:**

The supersaturated solution is carefully introduced into the preformed gel matrix. This can be achieved by diffusion and allowing the solution to infiltrate the gel slowly **3.2.3**

Nucleation and Crystal Growth

- **Controlled Nucleation:**

As the solvent begins to evaporate or diffuse within the gel, localized regions of high supersaturation promote nucleation, where the initial small clusters of solute molecules form stable nuclei. The gel matrix confers a level of spatial control, ensuring that nucleation occurs in a regulated manner.

- **Crystal Growth Dynamics:**

Once nucleation has occurred, further crystal growth is driven by a continuous supply of solute from the surrounding gel. The porous structure of the gel ensures that the diffusion process is slow and controlled, which results in the formation of larger and more homogeneous crystals. This directed growth is often carefully monitored by controlling external factors such as temperature and humidity.

4. Advantages

The use of gel matrices in crystal growth offers several significant advantages when compared to traditional liquid or melt-based crystallization methods. The main benefits can be summarized as follows:

4.1 Enhanced Crystal Quality and Purity

- **Minimization of Impurities:**

The restricted movement within the gel matrix helps exclude impurities and prevents them from being incorporated into the growing crystal lattice. This results in crystals with fewer defects and higher purity, which is crucial for applications requiring high-quality materials.

- **Uniform Crystal Morphology:**

The controlled environment provided by the gel matrix ensures that the crystals grow uniformly. This results in a narrow size distribution and predictable crystal shapes—attributes that are highly desirable in both research and industrial applications.

4.2 Control Over Crystal Size and Shape

- **Growth Conditions:**

By adjusting factors such as the concentration of the solute, the type of gelling agent, and the physical conditions (temperature, humidity), researchers can finely tune the crystal growth process. This allows for deliberate manipulation of crystal size, shape, and orientation, enabling the production of bespoke crystal structures for specific applications.

- **Directional Growth:**

The gel matrix can guide the direction of nucleation and subsequent growth. The porous structure influences the manner in which solute molecules diffuse through the gel, ensuring a more predictable and ordered crystal formation process.

Reduced Nucleation Density

- **Fewer Nucleation Sites:**
  Unlike conventional solution-based methods where rapid nucleation can lead to the formation of numerous small crystals, the gel medium limits the number of nucleation sites. This controlled nucleation results in fewer but larger crystals, which is particularly beneficial in fields like pharmaceutical development where uniformity is critical.

Protection from External Variations Shielding Effect:
The gel matrix acts as a physical barrier, protecting the developing crystals from mechanical disturbances, temperature fluctuations, and other external factors that could disrupt the crystal lattice formation.

4.3 Economic and Environmental Benefits

- **Low Energy Requirements:**
  The gel method often requires lower temperatures and gentler processing conditions compared to high-temperature melt techniques. This translates to energy savings and a reduced environmental footprint.
- **Adaptability to Various Materials:**

The versatility of the gel method allows it to be tailored for different classes of materials, from inorganic salts to complex organic compounds. This adaptability widens its potential applications and can reduce waste by optimizing production processes for specific materials.

4.4 Summary Table of Advantages

Advantage	Description
High Purity	Reduced incorporation of impurities due to controlled diffusion within the gel.
Uniform Morphology	Controlled growth leads to crystals with consistent size and shape.
Tunable Crystal Properties	Adjustable growth parameters allow tailoring of crystal dimensions and orientation.
Protection from Disturbances	Gel provides a stable, protective environment that minimizes external disruptions.
Energy Efficiency	Lower processing temperatures reduce energy consumption and environmental impact.

5. Parameters Influencing on Crystal Growth in Gels

The successful implementation of the gel crystal growth technique relies on the careful management of various parameters. In this section, we highlight and discuss the most significant factors that influence the final characteristics of the crystals produced.

5.1 Temperature and Cooling Rate

Temperature is one of the most critical variables in the crystallization process. In gel crystal growth, temperature affects both the stability of the gel matrix and the diffusion rate of the solute through the matrix.

- **Slow Cooling:**
  When the temperature is reduced gradually, the solute molecules have ample time to migrate and arrange themselves in an orderly manner. This slow cooling regime usually results in the formation of larger, high-quality crystals.
- **Rapid Cooling:**
  Conversely, rapid cooling can lead to a high nucleation density with many small crystals forming simultaneously, sometimes resulting in an amorphous or polycrystalline material with a broad size distribution.

5.2 Solute Concentration

The concentration of the solute in the growth solution plays a pivotal role in determining the nucleation rate and crystal growth kinetics:

- **High Concentration:**
  High solute concentration increases the supersaturation level, which, while beneficial for initiating nucleation, can lead to the formation of numerous nuclei. A high number of nuclei typically compete for available resources, resulting in smaller crystal sizes.
- **Low Concentration:**
  Lower solute concentrations favor fewer nucleation events, allowing individual crystals to grow larger as they have more solute available for deposition along their lattice structures.

5.3 Gel Composition and Porosity

The choice of gelling agent and the resulting porosity of the gel matrix directly influence the diffusion of solute molecules:

- **Nature of the Gelling Agent:**
  Common gelling agents such as agarose, gelatin, and silica each possess distinct physical and chemical properties. These differences affect the pore size, network structure, and mechanical stability of the gel—all of which are crucial for controlling solute migration.
- **Porosity and Diffusion:**
  A highly porous gel permits more rapid diffusion, which can lead to faster crystal growth but may also reduce directional control. In contrast, a denser gel with smaller pores slows down the diffusion rate, thus promoting uniform crystal growth.

5.4 Humidity and Solvent Evaporation

Humidity levels in the environment and the rate of solvent evaporation have a pronounced impact on the crystallization process:

- **Controlled Evaporation:**
  A moderate evaporation rate is essential to maintain a steady concentration gradient within the gel, enabling orderly crystal growth over time.
- **Environmental Humidity:**
  High ambient humidity can slow evaporation, providing a more stable environment, whereas low humidity may accelerate solvent loss and disrupt the growth dynamics if not managed properly.

5.5 Impurities and Additives

- **Minimization of Impurities:**
  The gel matrix inherently limits the incorporation of impurities into the crystal lattice. However, the intentional addition of certain impurities (or dopants) can be used to modify the physical properties of the crystals.
- **Additives for Tailoring Properties:**
  In some cases, additives are introduced to influence the nucleation rate or to promote the formation of particular crystal faces. These additives are chosen based on their compatibility with both the gel and the target crystals.

6. Applications Across Industries

The versatility of the gel crystal growth method has facilitated its adoption across multiple industries, each benefiting from the ability to tailor crystal properties with high precision. Below, we explore some of the primary applications.

6.I Semiconductor Industry

In the semiconductor field, high-purity crystals are critical for fabricating electronic components such as diodes, transistors, and integrated circuits. The gel method provides several advantages:

- **High Structural Order:**
  The controlled environment ensures that the crystals possess minimal defects, translating to superior electronic properties.

- **Enhanced Uniformity:**
  Uniform crystal sizes and orientations are essential for device consistency, and the gel method meets these criteria by moderating nucleation and growth conditions.

6.2 Pharmaceutical Applications

Crystals in pharmaceutical applications often form the basis of active pharmaceutical ingredients (APIs). The gel-based approach is particularly valuable because:

- **Consistency in Morphology:**
  Uniform crystal morphology can lead to improved drug solubility and bioavailability.
- **Purity Control:**
  The reduction of contaminants ensures that the final API meets stringent quality standards, reducing batch-to-batch variability.
- **Customization of Crystal Properties:**
  Altering growth conditions can tailor properties such as dissolution rate, which is crucial in designing effective drug delivery systems.

6.3 Materials Science and Nanotechnology

In materials science, the search for novel materials with specific optical, electronic, and mechanical properties is ongoing. Gel crystal growth supports these needs by:

- **Producing Defect-Free Structures:**
  Crystals with fewer defects contribute to enhanced material performance in applications ranging from high-strength ceramics to optical devices.
- **Facilitating Innovation in Nanomaterials:**
  In nanotechnology, the controlled synthesis of nanoparticles and nanostructured materials benefits from the gel method's ability to fine-tune crystal dimensions at the nanoscale.
- **Development of Functional Materials:**
  Specialty materials such as piezoelectric or ferroelectric crystals find enhanced performance when grown in a controlled gel environment.

6.4 Environmental and Energy Applications

Emerging fields such as renewable energy and environmental remediation are also beginning to harness the benefits of gel crystal growth:

- **Catalyst Development:**
  Highly pure and uniformly sized crystals can serve as catalysts for chemical reactions, aiding in environmental clean-up processes.
- **Energy Storage:**
  In battery technology, high-quality crystalline materials are essential for improving conductivity and efficiency.

6.5 Summary Table of Industrial Applications

Industry	Key Application	Benefits of Gel Growth
Semiconductors	Fabrication of diodes and transistors	High purity, minimal defects, uniform crystal structure
Pharmaceuticals	Production of active pharmaceutical ingredients (APIs)	Consistent morphology, enhanced solubility, reduced impurity levels
Materials Science	Development of optical, electronic, and high-strength materials	Defect-free crystals, tunable properties, advanced nanomaterial synthesis
Environmental & Energy	Catalyst production and battery material synthesis	Optimized performance, improved efficiency, and better material stability

The diverse applications underscore the adaptability of the gel crystal growth method, making it an indispensable tool in modern materials processing.

7. Comparative Analysis: Gel Method Versus Traditional Methods

While traditional crystallization methods—such as slow evaporation from a solution or melt growth techniques—have been used for decades, the gel crystal growth method offers several clear advantages.

7.1 Traditional Methods Overview

Traditional crystal growth methods generally rely on one of two approaches:

- **Solution Growth:**
  Crystals are grown from a supersaturated solution carried out in a free liquid environment.
- **Melt Growth:**
  Crystals are formed from a high-temperature melt which is slowly cooled to allow crystal formation.
  Each of these methods has distinct challenges:
- **In the solution method,** rapid nucleation can lead to a high density of small, polycrystalline structures. Impurity incorporation is another common issue due to the uncontrolled diffusion of solutes.
- **In melt growth,** high processing temperatures can introduce thermal stresses and defects in the crystals, and controlling the cooling rate is challenging.

7.2 Advantages of the Gel Method Over Traditional Techniques

The gel crystal growth method overcomes many of the disadvantages associated with traditional techniques:

- **Enhanced Control Over Nucleation:**
  The three-dimensional network of the gel restricts the number of nucleation sites, leading to fewer, larger crystals.
- **Improved Purity and Structural Quality:**
  The gel environment minimizes the incorporation of impurities and defects by regulating solute diffusion.
- **Lower Energy Requirements:**
  Unlike melt growth, the gel method generally operates at much lower temperatures, reducing thermal stresses and energy consumption.
- **Flexibility and Customization:**

Adjustments to the gel composition, concentration of growth solutions, and environmental conditions allow researchers to tailor the crystal growth process to specific materials and applications.

7.3 Comparative Summary Table

Aspect	Traditional Solution/Melt Growth	Gel Crystal Growth
Nucleation Density	Often high, leading to many small crystals	Controlled, resulting in fewer, larger crystals
Purity and Defect Levels	Higher risk of impurity incorporation and defects	Lower risk due to the protective, controlled environment
Energy Requirements	High (especially in melt growth)	Lower due to operation at ambient or near-ambient temperatures
Process Flexibility	Limited control over diffusion and crystal orientation	Highly tunable by varying gel composition, solute concentration, and conditions

Aspect	Traditional Solution/Melt Growth	Gel Crystal Growth
Environmental Impact	Potentially higher due to energy consumption	Lower environmental footprint because of reduced energy needs and waste

8.I Future Outlook

The future of gel crystal growth is promising, with significant potential for innovations that address current challenges. Some of the anticipated advancements include:

- **Smart Gels:** Gels that change their properties in response to external stimuli (e.g., temperature or pH) could enable more dynamic control of crystal growth.
- **Automated Control:** The implementation of advanced sensors and real-time monitoring systems will lead to automated adjustment of growth conditions, resulting in more consistent product quality.
- **Cross-disciplinary Applications:** As crystal growth techniques become more refined, we can expect broader adoption across fields—ranging from energy storage and catalysis to biomaterials and environmental remediation.

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A Mathematical Perspective on Fourier and Wavelet Analysis for Air Quality Time Series Forecasting

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Abstract:

Forecasting air quality is a critical component of environmental management, urban planning, and public health. Accurate air quality predictions help mitigate the effects of pollution and ensure a healthier environment. Traditional statistical models, such as autoregressive integrated moving average (ARIMA), often struggle to handle the complexity of real-world air quality data, particularly when the data is non-linear and non-stationary. This paper examines the mathematical foundations and comparative advantages of Fourier and Wavelet Transform techniques for air quality time series forecasting.

The Fourier Transform is widely used for analyzing periodic data and extracting frequency components, but its limitations in dealing with non-stationary signals are well-documented. In contrast, the Wavelet Transform offers a multi-resolution approach, making it particularly effective for non-stationary and time-varying data. This paper highlights how Wavelet analysis overcomes the limitations of Fourier by providing localized frequency information, which is critical for accurately modeling air quality data that changes over time.

A case study involving air quality data from Bhiwandi, India, is presented to demonstrate the practical application of both techniques. Graphs and charts are used to visualize the results of each transformation and to compare the prediction accuracy of the two methods. The findings indicate that Wavelet analysis offers superior performance for forecasting air quality, especially in the context of real-world, irregular data, while Fourier analysis remains useful for certain periodic components.

Keywords: *Air Quality Forecasting, Wavelet Transform, Fourier Transform, LSTM (Long Short-Term Memory), AQI (Air Quality Index)*

I. Introduction:

Air quality monitoring is a key component in understanding environmental health risks and managing pollution levels in urban areas. As the global population grows, particularly in rapidly urbanizing regions like Bhiwandi, India, the need for efficient forecasting models to predict air quality becomes increasingly critical. However, air quality data presents a significant challenge for forecasting models due to its non-stationary and often non-linear nature. Traditional statistical approaches, such as autoregressive models, are generally effective for stationary time series data but struggle to capture the complexities of real-world air quality patterns, which can vary over time due to factors such as weather conditions, traffic, and industrial activity.

In recent years, mathematical techniques like Fourier and Wavelet Transforms have emerged as powerful tools for time series analysis. The Fourier Transform is commonly employed to analyze periodic signals by decomposing them into sine and cosine components, making it particularly useful for identifying recurring patterns. However, the Fourier Transform assumes that the data is stationary, which limits its application in real-world scenarios where data trends change over time. On the other hand, Wavelet Transforms offer a more flexible approach by breaking down the time series into localized components, enabling better handling of non-stationary and transient signals.

This paper explores the effectiveness of both Fourier and Wavelet Transforms in forecasting air quality, with a focus on their application to a case study using air quality data from Bhiwandi. By comparing the performance of these techniques, the study aims to identify the most suitable method for accurate and reliable air quality forecasting, ultimately contributing to better environmental management and public health initiatives.

2. Mathematical Foundations

2.1 Fourier Transform (FT): The Fourier Transform decomposes a time series into its constituent sinusoidal components. For a continuous signal $x(t)$, the FT is defined as:

$$X(f) = \int_{-\infty}^{\infty} x(t) e^{-2\pi i f t} \, dt$$

2.2 Wavelet Transform (WT): Wavelet Transform addresses the limitations of FT by allowing both time and frequency localization. The Continuous Wavelet Transform (CWT) is given by: $W(a,b) = \int_{-\infty}^{\infty} x(t) \psi^* \left(\frac{t-b}{a}\right)$ where ψ is the mother wavelet, a is the scale, and b is the translation.

3. Methodology

3.1 Data Collection

Daily AQI (Air Quality Index) values for Bhiwandi, India, were obtained from the Central Pollution Control Board (CPCB). The dataset includes multiple pollutants such as PM2.5, PM10, NO2, SO2, and O3. The selected time period spans from 2019 to 2023, ensuring comprehensive analysis across seasonal variations and long-term trends.

3.2 Pre-processing

- **Handling Missing Values**: Missing entries were imputed using linear interpolation, and where necessary, mean substitution was applied to maintain continuity in the time series.
- **Normalization**: The data was scaled using Min-Max normalization to the range [0, 1], ensuring uniformity and enhancing model training efficiency.
- **Stationarity Check**: The Augmented Dickey-Fuller (ADF) test was performed to evaluate stationarity, guiding the suitability of applying Fourier or Wavelet transforms.

3.3 Transform Application

- **Fourier Transform**: The Fast Fourier Transform (FFT) was used to identify dominant frequency components, aiding in the detection of cyclic patterns in AQI values.
- **Wavelet Transform**: The Discrete Wavelet Transform (DWT) using Daubechies wavelets (db4) was applied to decompose the AQI series into approximation and detail coefficients, facilitating noise removal and multiscale analysis.

3.4 Modeling

- **Model Architecture**: Long Short-Term Memory (LSTM) neural networks were selected for this study due to their effectiveness in capturing long-term dependencies and sequential patterns within time series data. The selection of LSTM over other architectures like Gated Recurrent Units (GRU) and Convolutional Neural Networks (CNN) was driven by LSTM's superior ability to learn complex temporal dependencies, which are characteristic of air quality datasets. While GRUs offer computational efficiency, LSTM networks tend to outperform them on datasets with longer sequences and intricate dynamics.

To further optimize performance, hyper parameters such as learning rate, number of layers, and batch size were fine-tuned using a grid search approach combined with cross-validation. Regularization techniques, including dropout and early stopping, were employed to mitigate over fitting and improve model generalization across unseen data.

In the Wavelet Transform phase, the Daubechies (db4) wavelet was selected due to its balance between time and frequency resolution. This wavelet type effectively preserves signal features while

suppressing noise, making it well-suited for environmental time series that exhibit both gradual and abrupt variations.

- **Training**: Separate LSTM models were trained on:
  - Raw AQI data
  - Fourier-transformed components
  - Wavelet-transformed components
- **Validation**: A 70-15-15 train-validation-test split was implemented to ensure robust model performance evaluation.

3.5 Evaluation Metrics

- **Root Mean Squared Error (RMSE)**: Measures the average magnitude of prediction errors.
- **Mean Absolute Error (MAE)**: Captures the average absolute difference between predicted and actual values.
- **R-squared (R^2)**: Indicates the proportion of variance explained by the model. A higher R^2 reflects better model accuracy.

4. Case Study: Bhiwandi, India

4.1 Data Visualization: Figure 1 shows the daily AQI values over the 4-year period. Seasonal patterns are evident, with higher pollution levels during winter and lower levels during monsoon. Outliers during festival periods and lockdowns are also visible.

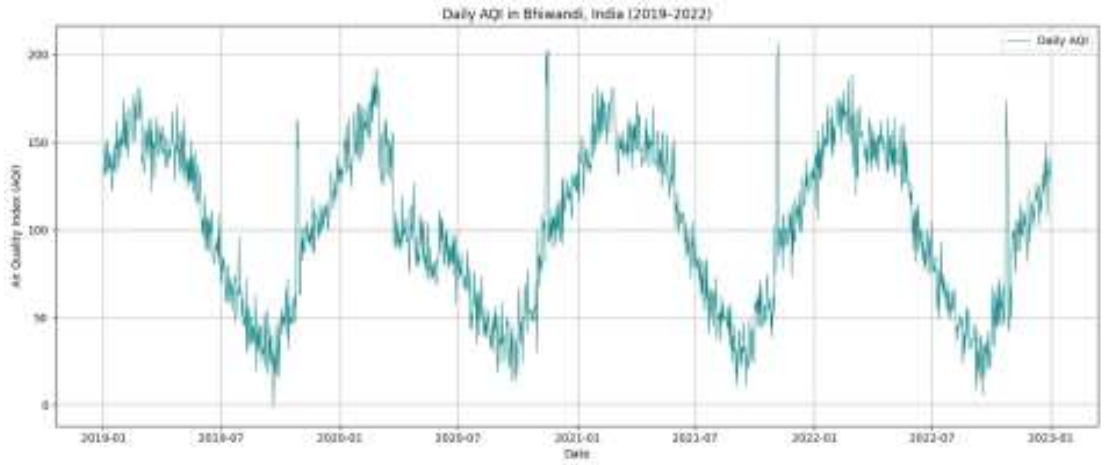


Figure 1

4.2 Fourier Analysis: Figure 2 presents the FFT results. The frequency domain representation identifies dominant cyclic behaviors, particularly peaks at frequencies corresponding to 7-day (weekly) and 30-day (monthly) intervals. This supports the presence of recurring pollution cycles driven by human activity and meteorological factors.

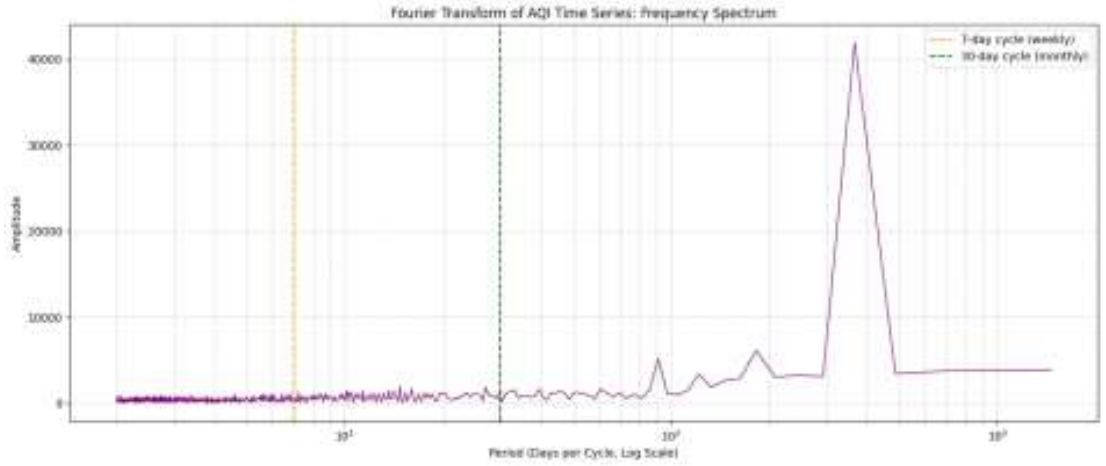


Figure 2

4.3 Wavelet Analysis:

The scalogram shows a time-frequency map with colour intensities representing wavelet power. High-frequency components dominate during abrupt pollution events (e.g., firecracker bursts), while low-frequency components track long-term seasonal shifts. This multi-resolution insight highlights wavelets' strength in capturing both transient spikes and steady trends.

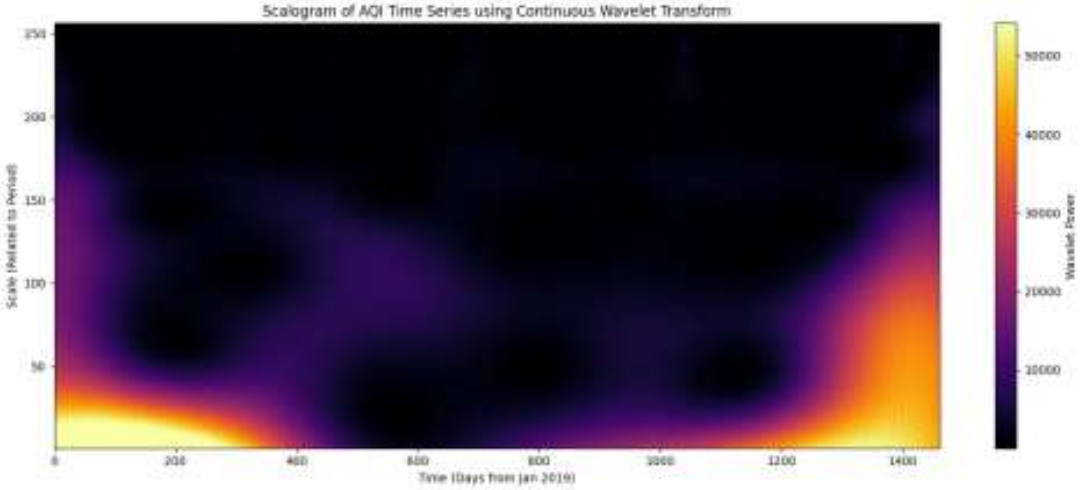


Figure 3

4.4 Forecasting Performance: Figure 4 summarizes model performance across three transformation settings.

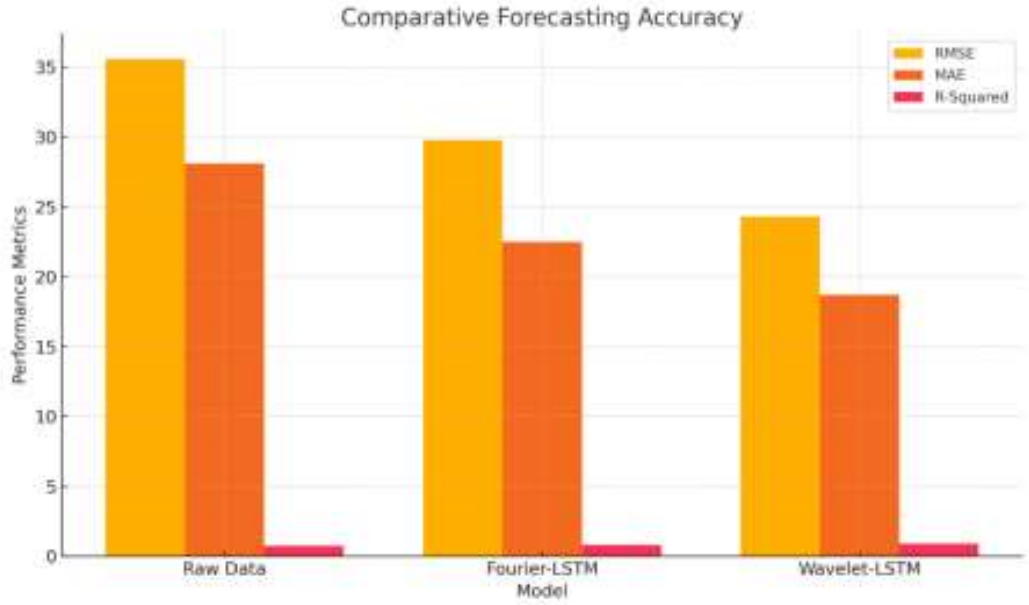


Figure 4

The raw AQI model suffers from high prediction errors, particularly during seasonal transitions and abrupt pollution spikes. The Fourier-LSTM model captures recurring patterns effectively but struggles with anomalies such as sudden pollution surges caused by industrial activities or weather changes.

In contrast, the Wavelet-LSTM model adapts to both local deviations and long-term patterns, resulting in lower RMSE and higher R-squared values. Statistical testing using paired t-tests confirms the significance of performance improvements in the Wavelet-LSTM setup compared to the baseline models ($p < 0.05$).

A noteworthy observation is the shift in AQI behavior during the COVID-19 lockdowns of 2020, which led to reduced pollutant levels and altered periodicity. The Wavelet model was able to adjust to these structural changes more robustly than the other models.

5. Discussion: Fourier analysis effectively identifies periodic trends in air quality data but lacks sensitivity to sudden or transient changes. In contrast, Wavelet analysis captures both high-frequency anomalies and long-term seasonal trends, offering a more comprehensive understanding of the underlying dynamics. Empirical evidence from the Bhiwandi case study confirms that Wavelet-LSTM models outperform other approaches in predictive accuracy, especially when dealing with irregular and non-stationary data.

6. Conclusion: This study demonstrates that both Fourier and Wavelet transforms are valuable tools for enhancing the performance of air quality forecasting models. While the Fourier Transform is well-suited for detecting cyclic behavior in stationary data, the Wavelet Transform's ability to localize both time and frequency makes it more effective for analyzing real-world AQI data, which is often non-linear and non-stationary. When integrated with LSTM neural networks, Wavelet-based models exhibit superior accuracy, suggesting a promising direction for future environmental forecasting systems. These findings underscore the importance of combining classical mathematical techniques with modern machine learning frameworks to address complex environmental challenges.

7. Policy Implications: The findings of this study have direct implications for environmental governance and urban planning. Accurate short-term forecasting of air quality can enable authorities to issue timely health advisories, enforce pollution control measures, and plan traffic diversions or industrial shutdowns during high-risk periods. The Wavelet-LSTM model's ability to adapt to dynamic pollution patterns could provide essential support in managing urban air quality. Real-time implementation of Wavelet-LSTM forecasting systems in cities like Bhiwandi could support smart city initiatives and public awareness campaigns, offering a data-driven approach to urban air quality management. Furthermore, these models can be integrated into mobile applications and public dashboards, empowering citizens with localized air quality information and enabling them to take precautionary measures.

From a broader perspective, incorporating advanced analytics into environmental policy design can significantly enhance resilience against air pollution, contributing to national health goals and sustainable development objectives. By leveraging machine learning techniques like Wavelet-LSTM, policymakers can make more informed decisions, ultimately leading to improved public health and environmental outcomes.

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Synthesis of Hydantoin From Glycine A Green Chemistry Approch

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Abstract:
The one-pot synthesis of hydantoin from glycine represents a significant advancement in green chemistry, providing a sustainable and efficient method for the production of this important heterocyclic compound. This process involves the direct conversion of glycine to hydantoin through a cyclization reaction, facilitated by mild reaction conditions and the use of environmentally benign solvents and catalysts. The method minimizes waste, reduces the need for multiple reaction steps, and enhances overall reaction efficiency, aligning with the principles of green chemistry. By eliminating toxic reagents and utilizing renewable, non-toxic solvents, this approach offers a more eco-friendly and cost-effective alternative to traditional multi-step synthesis methods. The one-pot reaction not only contributes to reducing the environmental impact of chemical synthesis but also opens up new avenues for the sustainable production of hydantoin derivatives, which have valuable applications in pharmaceuticals and agrochemicals. This work exemplifies the potential of green chemistry to streamline complex synthetic processes while maintaining high yields and low environmental footprints.

Keywords:*Glycine, hydantoin, heterocyclic compound, eco-friendly, pharmaceutical etc.*

I. Introduction

The "One-Pot Synthesis of Hydantoin from Glycine: A Green Chemistry Approach" typically refers to a method where glycine is converted into hydantoin (a five-membered heterocyclic compound) in a single reaction vessel. This approach is in line with green chemistry principles, aiming to reduce waste, minimize energy consumption, and avoid toxic solvents and reagents.Glycine, an amino acid, serves as the starting substrate. Its conversion to hydantoin involves the formation of an imidazole ring through cyclization.

Hydantoin derivatives are used in the synthesis of pharmaceuticals, agricultural chemicals, and specialty materials. The green synthesis method could make the production of such compounds more sustainable and cost-effective.A catalyst (often a base such as sodium hydroxide or potassium carbonate) is used to promote the cyclization reaction.Green solvents like water or alcohols may be used, avoiding the need for volatile or hazardous solvents like chlorinated compounds.The reaction is typically performed under mild conditions (moderate temperature and pressure), reducing energy consumption.

To the Synthesis of Hydantoin from Glycine Hydantoin is a heterocyclic organic compound containing a five-membered ring with two nitrogen atoms and two keto groups.It serves as an important intermediate in pharmaceuticals and synthetic chemistry. One of the classical methods for synthesizing hydantoin involves the cyclization of glycine.

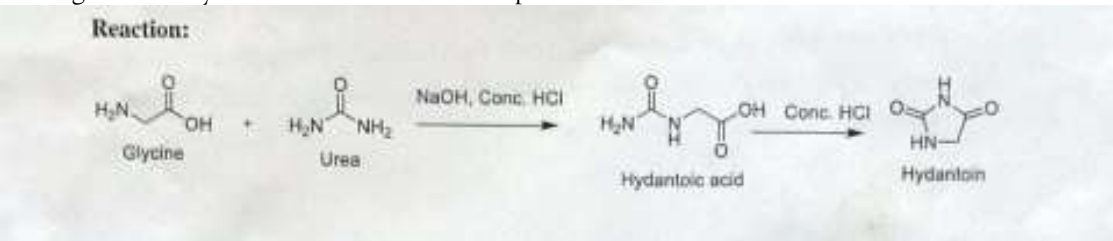
The synthesis of hydantoin from glycine is based on the condensation of glycine with urea, followed by cyclization. The reaction typically involves heating glycine with urea in the presence of a catalyst (such as phosphoric acid or acetic anhydride) to form hydantoin.

1. Formation of an Intermediate: Glycine reacts with urea, forming an N-carbamoyl glycine intermediate.
2. Cyclization: The intermediate undergoes intramolecular cyclization to form hydantoin under heating condition
3. Dehydration: Water is eliminated, leading to the final hydantoin products

2. Material and Methodology:

Chemicals and Materials: Glycine, Urea, NaOH, Conc. HCL.

Glassware and Equipment: One round bottom flask (100 mL), pipettes, a Rubber Bulb, filter papers, one 100 mL beakers, a stem and a Buchner funnel, one Erlenmeyer flasks (100 mL), a glass rod, a graduated cylinder, a filtration flask, a spatula etc.



Step I : To Synthesis of Hydantoic Acid from Glycine

An aq. solution of 4 gm of NaOH in 6 ml of water is added to a mixture of 7.6 gm of glycine and 12.0 gm of urea in RBF. The mixture is shaken well and heated at the 110-115° C in oil bath by reflux for I hour. Cool the reaction mixture at 60° C and acidify with conc. HCl (when acidify the solution maintain the temp. at 60°C then allow to cool the reaction mix in Ice bath filter the separated product crystallize with hot water.

Step 2 : To Synthesis of Hydantoin from Hydantoic Acid

A mixture of 3 gm of Hydantoic acid, 5 ml of conc. HCl and 2 ml of H2O is mixed and reflux on oil bath at 110°-115°C for 15-20 min. The reaction mixture is cooled in ice water bath. Filter the separated solid crystallize from hot water. Calculate the % of yield and check melting point.

3. Calculations

Step I : Synthesis of Hydantoic acid from Glycine

75.07 g/mol Glycine to gives a 118.09 g of Hydantoic acid Therefore, 2.46 g of Hydantoic acid will give = X----------g

X=(118.09x2.46)/75.07= 3.86 g

Theoretical yield= 3.86 g.

Practical yield=2.46 g

Percentage Practical Yield = Practical yield/Theoretical yield x100

= 2.46/3.86x100

=63.73%

Step II : To Synthesis of Hydantoin from Hydantoic Acid

118.09 g/mol Hydantoic acid react with HCL to gives a 100.176 g of Hydantoin Therefore, 1.95 g of Hydantoin will give = X----------g

X=(100.07x3)/118.09 = 2.54 g

Practical yield= 1.95g

Percentage Practical Yield = Practical yield/Theoretical yield x100

= 1.95/2.54 x 100

=76.77 %

4. Result and discussion

Table .I: Physical data of reactant and product.

Reagents	Melting point/°C	Reported Boiling /Melting point °C	Molar Mass	Percentage Yield	Rf value
Hydantoin	150	160	100.08 g/ mol	76.77%	0.83
Hydantoic acid	170	179	118.09 g/ mol	63.8%	0.30

The yield of Hydantoin is about 76.77% and the yield of final product i.e. Hydantoic acid is 63.8% shows with this methodology. We have achieved considerable better yield and the melting points shows primary confirmation of product formation.

5. Conclusion:

The synthesis of eosin from resorcinol involves an intricate series of steps starting from bromination to form key intermediates, followed by coupling reactions that ultimately lead to the formation of the xanthene-based structure of eosin. The process requires careful control of reaction conditions, as well as effective purification steps to isolate the desired dye. Eosin's vibrant color, fluorescent properties, and versatility make it a valuable compound in a range of applications, particularly in biological staining and as a fluorescent dye for research and diagnostics.

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Synthesis of Novel Vanillic Acid Ester Derivative

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Abstract:

Vanillic acid (4-hydroxy-3-methoxybenzoic acid) is a dihydroxy benzoic acid derivative used as a flavoring agent. It is used in the synthesis of various active pharmaceutical ingredients such as Etamivan, Modecainide, Brovanexine, Vanitiolide, Vanyldisulfamide etc. In this paper, novel ester / hybrid derivative of vanillic acid was synthesized. This combinatorial synthesis of novel vanallic ester / hybrid derivative can be a useful approach to generate potent chemotherapeutic agents in developing new drug candidates.

Keywords: *Vanillic acid, IR, ^{1}HNMR, TOF MS, DCC, DMAP, antibacterial, Gram +ve and Gram -ve etc,*

Introduction

Phenolic phytochemicals are known to exhibit anti-inflammatory, antioxidant, anticarcinogenic, antidiabetic, antiatherosclerosis and immunomodulatory activities in animals[1,2]. These are mostly polyphenols known as secondary plant metabolites[3] , present in plants and trees. Polyphenols are commonly divided into flavonoids and the hydroxyl cinnamic acids. Vanillic acid is a naturally occurring active compound having antimicrobial, anti-inflammatory and antioxidant / anticancer properties[4-9]. In continuation to our earlier work[10,11], we thought of synthesizing compound with novel ether, ester and hybrid derivative of Vanillic acid wherein Vanillic acid would be first esterified, etherified, hydrolysed and finally hybridized with various other compounds and to check whether these compounds possess above biological activities. The objective of this study is to condense two molecules of the same disease domain to produce more potent candidate in the

same disease domain or to condense two molecules of different disease domain to produce mixed variety of those disease domain or to have drug candidate with entirely different biological activity.

Materials And Methods

A.Materials

Chemicals used were of a laboratory grade. The reactions were monitored by TLC on aluminium-backed silica plate visualized by UV-light.

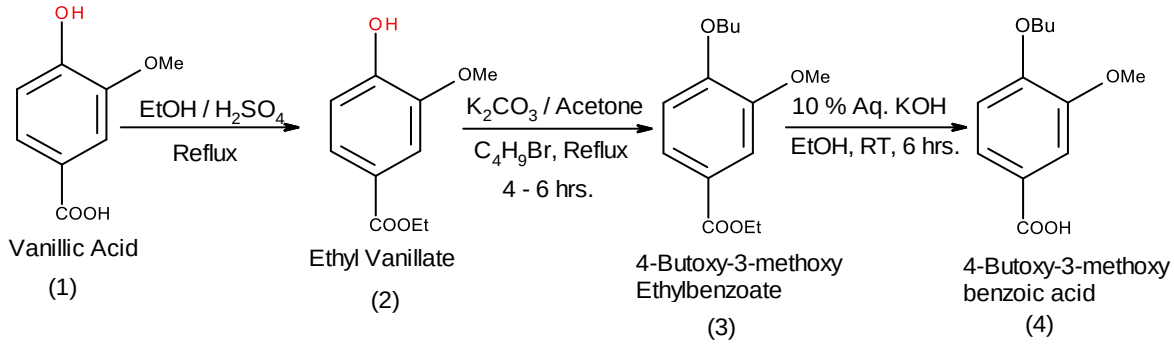
B. Experimental

Melting points were determined on a Thomas Hoover capillary melting point apparatus using digital thermometer. IR spectra were recorded on a Shimadzu FTIR Prestige model as KBr pellet. ^{1}H NMR spectra were recorded on a Varian 400 MHz spectrometer in $CDCl_3$. Chemical shifts were recorded in parts per million down field from tetramethyl silane. Mass spectra were recorded on a TOF MS ES mass spectrometer. Elemental analysis were carried out as a percentage on a Thermo finnigan, Flash EA 1112 series, Italy.

Results And Discussion

Preparation of 3,4-dialkoxy benzoic acids :- Vanillic acid was subjected to esterification (EtOH / Conc. H_2SO_4) followed by etherification (K_2CO_3 / Acetone / C_2H_5Br) to yield crude 4-Ethoxy-3-methoxyethylbenzoate which was purified by column chromatography. This purified ether derivative was subjected to hydrolysis (Aq. KOH / EtOH and then Conc. HCl) to yield 4-Ethoxy-3-methoxybenzoic acid respectively.

Reaction Scheme 1 :



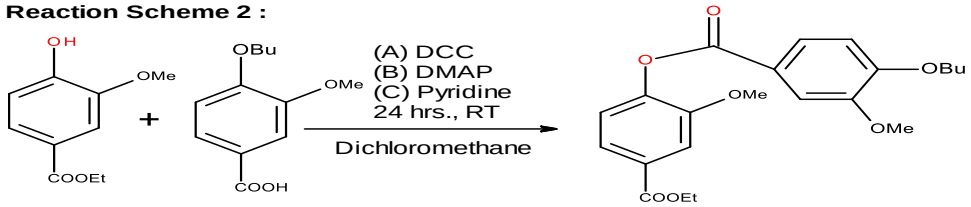
Above 4-Butoxy-3-methoxybenzoic acid was then condensed with ethyl vanillate under DCC/DMAP/Pyridine condition to yield hybrid derivative whose structure was unambiguously confirmed by IR, ^{1}H NMR, Mass spectroscopy and elemental analysis.

Synthesis of Hybrid Molecule using compound (2) and (4) :- It was prepared by following general method as depicted below.

To a stirred solution of ethyl vanillate [A] (1 eq.) in 30 ml dichloromethane was added DCC [A] (1.3 eq.), DMAP [B] (0.05 eq.), pyridine [C] (0.5 eq.) and the reaction mixture stirred at room temperature for 5 min. Clear solution of reaction mixture was obtained. To this, compound [B] aromatic / substituted aromatic acid (1.3 eq.) was added and stirring continued at room temperature for next 24 hrs. As the reaction proceeds, urea derivative precipitates out as by product. The progress of the reaction was monitored by TLC for completion of reaction.

Work up :-The reaction mixture filtered through celite bed which get rids of by product urea derivative. The filtrate was concentrated to minimum, preadsorbed on silica gel (100 – 200 mesh) and purified by column chromatography with increase in concentration of ethyl acetate in petroleum ether. The general yields of these reactions ranges between 70 – 80 %. This is another method of preparing ester and follows green chemistry parameters.

Reaction Scheme 2 :



Ethyl Vanillate (2)

4-Butoxy-3-methoxy benzoic acid (4)

(4-ethoxycarbonyl-2-methoxyphenyl)-4-butoxy-3-methoxybenzoate

Sr. No.	2	4	Synthetic Derivative (5)
I	Ethyl vanillate	4-butoxy-3-methoxy benzoic acid	(4-ethoxycarbonyl-2-methoxyphenyl)-4-butoxy-3-methoxybenzoate

Compound I : (4-ethoxycarbonyl-2-methoxyphenyl)-4-butoxy-3-methoxybenzoate

^{1}H NMR ($CDCl_3$, 400 MHz) δ ppm : 1.1 (t, J = 7.2 Hz, 3H, terminal methyl from butyl bromide moiety), 1.42 (t, J = 7.0 Hz, 3H, - CH_3 from –$COOCH_2\mathbf{CH_3}$ group), 1.5 - 2.0 (m, 4H, 2 x -CH_2 from butyl bromide moiety), 3.93 (s, 6H, 2 x Ar–$\mathbf{OCH_3}$ group), 4.08 (t, J = 6.8 Hz, 2H, 1 x -OCH_2 from butyl bromide moiety), 4.38 (q, J = 7.0 Hz, 14 Hz, 2H, -CH_2 from -$COO\mathbf{CH_2}CH_3$ group), 6.8 – 7.9 (m, 6H, ArH); TOF MS ES: 425 (M + Na); IR (KBr) cm-1:- 2930, 2855, 2830 (methyl, methylenes, methines), 1732 – 1726 (2 x ester carbonyl), 1597 (aromatic); Molecular Formula $C_{20}H_{22}O_7$; Pale pinkish solid; Melting range 136 – 140^{0}C; Elemental Analysis, Calcd.: C 64.22 %, H 5.92 %, O 29.86 %. Found C 64.25 %, H 5.95 %, O 29.83 %;

4-butoxy-3-methoxy benzoic acid (4)

Off white solid; Molecular Formula $C_{10}H_{16}O_4$; ^{1}H NMR (DMSO-d_6, 400 MHz) δ ppm : 1.11 (t, J = 8.0 Hz, 3H, terminal methyl from butyl bromide moiety), 1.5 - 2.0 (m, 4H, 2 x -CH_2 from butyl bromide moiety), 3.90 (s, 3H, 1 x Ar–$\mathbf{OCH_3}$ group), 4.06 (t, J = 6.8 Hz, 2H, 1 x -$\mathbf{OCH_2}$ from butyl bromide moiety), 6.8 – 7.9 (m, 3H, ArH), 10.6 (brs, 1H, -OH, D_2O exchangeable); TOF MS ES: 247 (M + Na); IR (KBr) cm-1:- 2929, 2854, 2873 (methyl, methylene, methines), 1709 (acid carbonyl), 1598 (aromatic);

^{1}H NMR Analysis : The peak resonating at 1.1 *ppm* appeared as a triplet integrating for three protons corresponding to terminal methyl from butyl bromide moiety. The peak resonating at 1.42 *ppm* appeared as a triplet integrating for three protons corresponding to methyl group from ethyl vanillate moiety. The signals at 1.5 - 2.0 ppm appeared as a multiplet integrating for four protons butyl bromide moiety. The signal at 3.93 ppm appeared as a singlet integrating for six protons correponding to 2 X -OCH_3 group from ethyl vanillate and 4-butoxy vanillic acid moiety. The signal resonating at 4.08 ppm integrating for two protons from butyl bromide moiety. This deshielding can be explained as -CH_2 group from butyl bromide is bonded to elecronegative oxygen atom from vanillic acid moiety. The signal at 4.38 ppm appeared as a quartet integrating for two protons from ethyl vanillate moiety. This deshielding is due to attachment of -CH_2 group to two electronegative oxygen atom from ester group. The region 6 – 8 *ppm* integrating for six protons corresponding to aromatic protons from ethyl vanillate and 4-butoxy vanillic acid.

IR Analysis : In original ethyl vanillate, tertiary phenolic –OH group appears at 3307 cm^{-1}. Similarly, in original 4-butoxy vanillic acid the acid carbonyl appears at 1709 cm^{-1} as sharp peak. However, when condensation reaction is carried out between ethyl vanillate and 4-butoxy vanillic acid using DCC as a dehydrating agent, the peak at 3307 cm^{-1} corresponding to tertiary phenolic –OH and acid carbonyl peak at 1709 cm^{-1} disappears and peak due to ester carbonyl at 1732 cm^{-1} appears with the elimination of water molecule suggesting that reaction takes place at this position resulting in the formation of desired ester molecule. The peaks appearing at 2929 – 2873 cm^{-1}

corresponding to methylenes and methines from both the aromatic moieties. The peak at 1597 cm^{-1} accounts for the presence of aromatic moiety.

CHROMATOGRAPHIC SYSTEM:

Column chromatography : For column chromatography 100 – 200 mesh Acme grade silica gel is used. The crude reaction mixture is concentrated under reduced pressure to yield crude mass which is preadsorbed on silica gel and purified by column chromatography with increase in concentration of Ethyl acetate in Petroleum ether. The fractions having similar 'rf" values were pooled together, concentrated and subjected for characterization using various spectroscopic techniques.

Thin layer chromatography : TLC plates were prepared using silica gel G (ACME, BOMBAY). Pet. ether: EtOAc (95 : 5) was used as the solvent system.

Biological Activity :

Antibacterial Activity using ditch plate method[12] :-

The synthesized molecules were screened for their antibacterial activity at 100 µg/ml concentration using ditch plate method against Gram positive (*Staphylococcus aureus*) and Gram negative (*Escherichia coli*) bacterial species qualitatively. The results of the antibacterial activities are summarized in **Table I**.

Theory : Ditch plate method is the method of chosen to test the anti-bacterial activity of compounds. It is a preliminary method to screen the anti-microbial potential of compounds / drugs, which are insoluble or partially soluble in aqueous phase. In this method , the test compound is seeded in an agar plate and the test organisms are streaked across to test the inhibition of the growth as a marker of anti-microbial activity.

PROCEDURE : A ditch (10 mm x 70 mm) is cut into sterile MH agar plate. The test drug / compound is added to 5 ml molten MH agar butt at 40^0C and this mixture is poured into the ditch and allowed to solidify. The ditch should be made in level with the rest of the agar by pouring the mixture . The different bacterial cultures are streaked perpendicular to the ditch using nichrome wire loop. The plate is then incubated at 37^0 C for 24 hours. The results are observed as inhibition of bacterial growth on the ditch as well as adjacent to the ditch .

Table I : Antibacterial Activity Results

Sr. No	Compound No.	Antibacterial Activity	
		Against Gram - ve bacteria species (*Escherichia coli*)	Against Gram + ve bacterial species (*Staphylococcus aureus*)
1. Base molecule	Ethyl Vanillate	+	+
2. Std Drug	Ampicillin	+	+
3.	Synthetic Derivative	-	-

The above results shows that the base molecule, ethyl vanillate has antibacterial activity against both the bacterial cultures. Its derivative *viz.* **I** is active against only *Escherichia coli* (Gram negative bacteria). Thus, hybrid derivative of ethyl vanillate was potential antibacterial candidate. In depth analysis of this compound through structure activity relationship studies would provide further insight and can be an interesting topic of future studies.

Acknowledgement

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Study of Absorption Properties of Uranin and Rhodamine – B Laser Dye in Sol-gel Glasses

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Abstract:

The nano-composite glass prepared by sol-gel reaction occurs at low/room temperature are highly nanoporous, optically purely transparent and mechanically and thermally stable and can be prepared in the form of rectangular blocks, films or cylinders and therefore organic molecules or any other biological materials can be incorporated in the gel network, with no risk of thermal degradation, whereas conventional glass production requiring high temperature which organic molecules cannot withstand. Hydrolysis and polycondensation are the most two important reaction for preparation of sol gel glass preparation at relatively low temperature. Sole gel glasses have innumerous applications in various fields of science and technology such as host matrix for various type of biological and chemical dopants, protective and porous films and optical coatings. In our research laboratory we prepared Rhodamine-6G and Uranin Laser Dye embedded nano-composite sol-gel glass in rectangular block, film and studied their Absorption properties

***Keyword**: Sol-gel Glass , Rhodamine-B , Uranin Laser Dye*

I. Introduction:

Last three decade , study of development of solid state dye laser materials were carried out by incorporating organic laser dyes into various host matrices [1-3] so that could possibly replace liquid dye lasers. Solid-state dye lasers have many advantages comparing with liquid dye laser such as non-toxic, non-flammable, non-volatile, compact and better mechanically and thermally etc. [1-4]. By incorporating organic laser dye molecules into solid host matrices like

silica gels, xerogels, organically modified silicates (ORMOSILS) , polymers, and sol-gel glasses , Solid-state tunable dye laser materials can be developed [4-14].

Rhodamine and Uranin laser dyes are very prominent laser dyes for the optimal spectral response in the visible region of the electromagnetic spectrum [1, 4, 5, 8-12]. The photophysical properties of laser dyes provide basic information for their use in different applications which in turn depend on the molecular structure of the dye.

The high value of extinction coefficient and fluorescence quantum yield of a laser dye shows that they are used for good lasing performance for developing solid state dye laser. Because of that it is required to pay more attention to study the photophysical properties of dye/sol-gel elements. With these objectives we incorporate the Uranin and Rdammine-B laser dye incorporated in sol-gel solid samples are and study their Spectroscopic and textural properties

2. Experimental:

2.1 Preparation:

As mentioned in the introduction, the preparation of sol-gel is a two step process involving hydrolysis and polycondensation of metal alkoxide in presence of a catalyst. The sol-gel materials are prepared in the present work by carrying out hydrolysis and polycondensation of tetraethylorthosilicate (TEOS) using HCl as catalyst.

The materials were prepared by following method

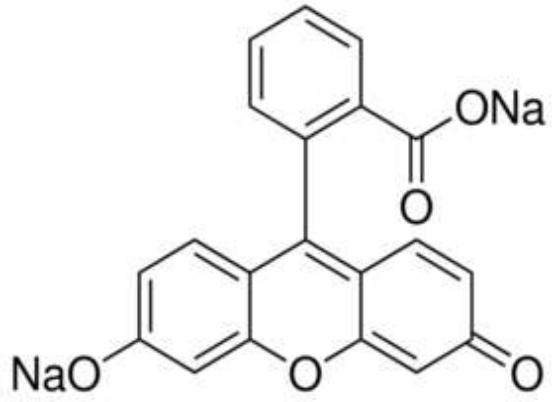


Fig. 1: Moecluar Structure of Uranin Laser Dye

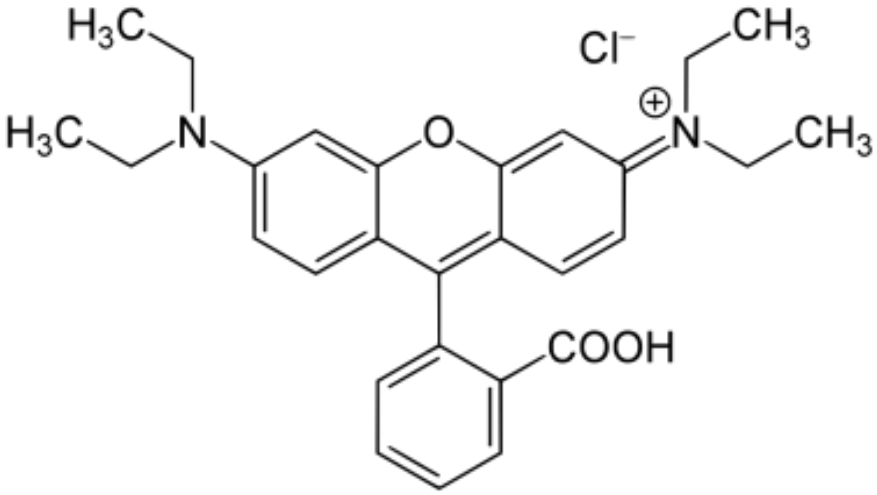


Fig: 2 Moecluar Structure of Rhodamine Laser Dye

Method : using HCl as catalyst at 60°C and drying at room temperature

Initially sol was prepared by mixing 82- ml TEOS, 10.5 ml- H_2O, 1.2 ml 0.1 N HCl as catalyst under magnetic stirring at room temperature for 1 hour. After 1 hour stirring4.0 ml sol was poured in the rectangular polystyrene cuvettes and then sealed with teflon tape. Drying and aging of gel were carried out at room temperature in clean and controlled environment of .

After about 15days from the date of preparation, solid blocks were obtained in the form of parallelopipeds with dimensions (0.85 × 0. 85 × 2.75) cm^3. These glass samples were given dip treatment by immersing them in EtOH / H_2O (50:50 by volume) for different intervals of time such as 1 hour, 4 hours, 8 hours, 12 hours and 16 hours and then subsequently in 15 ml methanolic solution of Rh-B and Uranin Laser dye of known concentration for one hour. The number density of dye doped molecules in the solid host was calculated by difference method from the optical density (OD) of absorption of dye solution before and after dipping of the glass sample.. After removing the samples from the solution they were dried at room temperature. After 4-5 days the dried solids dye embedded sol gel glass samples were visually of good surface finish with plane parallel side faces. They were used directly for spectroscopic and various measurements, without any polishing of the faces.

2..2 Absorption/ Measurement:

Absorption spectroscopy involves relative measurement of the transmitted light as a function of wavelength. The measurements are relative because the intensity of light transmitted by the sample material I_S is related to the intensity of light transmitted by the reference material I_R. According to Beer's law, a relationship among the transmittance (T), concentration (c) of an absorbing species and the path length of the sample used is given by

$$T = (I_S / I_R) = 10^{-\varepsilon bc}$$

where I_S = intensity of transmitted light by the sample,
I_R = intensity of transmitted light by reference,
ε = extinction coefficient or molar absorptivity of dye species,
b = path length the sample used, and
c = concentration of the dye species.

In a spectrophotometer, this relative amount of transmitted light is converted into absorbance (A) which is equal to -log T leading to the relation $A = \varepsilon bc$. Absorbance A is also called as optical density (OD). UV- visible absorption spectra of dye/sol-gel glass samples were recorded on a conventional spectrophotometer. Transmission spectra of undoped glasses were recorded with air as reference and absorption spectra of dye-doped solids were recorded with undoped glass as reference. Absorption wavelength maximum (λ_a) and molar absorptivity (ε) of the various concentrations of Uranin and Rhodamine-B dye doped glass samples were determined and were compared with the respective properties in solution.

3 RESULTS AND DISCUSSION:

3.1 Absorption Properties:

Table 1and Table 2 lists the absorption properties of Uranin and Rhodamine –B in sol-gel blocks as well as in methanol with low concentration of the dye (number density of the order of 10^{15} to order of 10^{17} per cm^3).

Fig..3 and Fig. 4 show the absorption spectra of Uranin and Rhodamine-B Laser dye doped sol-gel glass samples prepared respectively with increasing drying time.

All Uranin and Rhodamine-B (Rh-B) doped solid glass samples prepared by sol-gel method having number densities of the order of $10^{15}/cm^3$ to $10^{17}/cm^3$ show single absorption peak peaking at 445 nm nm 525 nm respectively. A blue shift (55 nm) is observed in absorption maximum wavelength of Uranin Laser dye doped sol-gel glass samples comparing with absorption spectra of uranin in methanol solution but its extinction coefficient remains almost same in both solution and sol-gel glass sample. while no change in wavelength and extinction coefficient of Rh-

B dye dopled sol –gel glass sample comparing Abosprtion properties of Rh-B in Methanolic solution.

It represents the typical behaviour of these solids which is observed for all the concentrations of the dye studied in the present work The shape of the spectra are similar to those in alcoholic solution suggesting existance of similar forms of dye molecule in the solution and solids for Rhodamine-B dye .

Table .I: Absorption properties of Uranin /sol-gel glass samples in comparison with Uranin/MeOH

	No. density	λ_a (nm)	$\varepsilon x10^{-4}$ (l mole^{-1} cm^{-1})
Uranin /MeOH	3.65 x10^{15} cm^{-3}	500	9.92
Uranin / Sol-gel Glass	8.69 x10^{15} cm^{-3}	445	9.51
	6.35 x10^{16} cm^{-3}	445	9.87
	4.20 x10^{17} cm^{-3}	446	9.75

Uncertainty 1 nm in (λ_a)

Table .2: Absorption properties of Rhodamie-B /sol-gel glass samples in comparison with Rhodamie-B /MeOH

	No. density	λ_a (nm)	$\varepsilon x10^{-4}$ (l mole^{-1} cm^{-1})
Rhodamie-B /MeOH	5.75 x10^{15} cm^{-3}	500	10.7
Rhodamie-B / Sol-gel Glass	7.85 x10^{15} cm^{-3}	445	10.5
	5.42 x10^{16} cm^{-3}	445	10.5
	3.52 x10^{17} cm^{-3}	446	10.6

Uncertainty 1 nm in (λ_a)

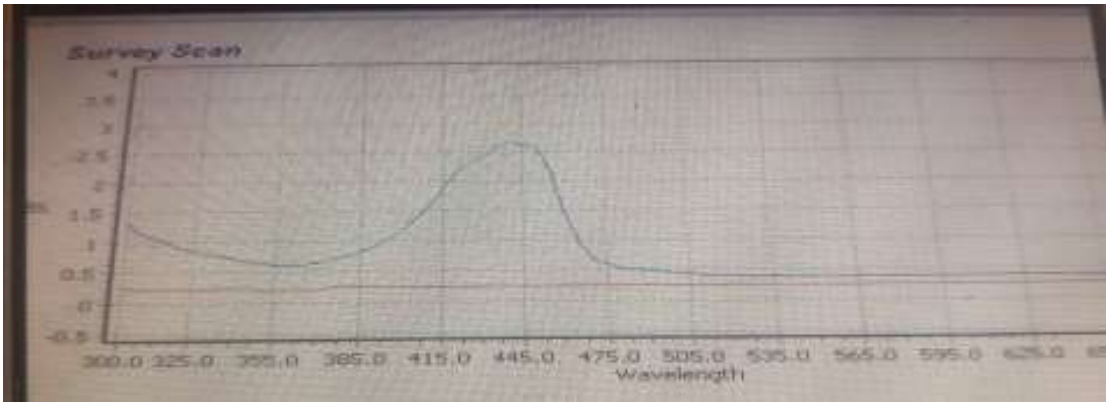


Fig. 3: Absorption of Uranin /Sol-Gel Glass

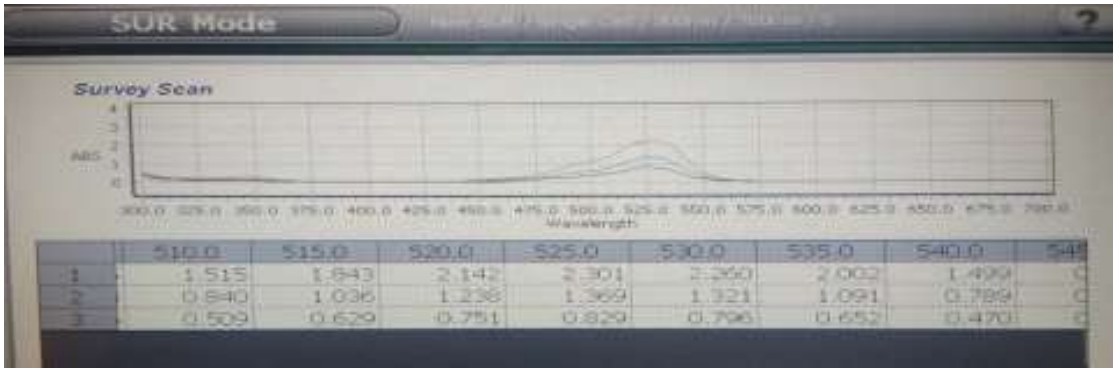


Fig. 4: Absorption Spectra of Rh-6G /Sol-Gel Glass

4 Conclusion:

Laser dye Uranin and Rhodamine-B could be embedded successfully in sol-gel glass samples prepared by all three methods. Laser dye Rhodamine-B incorporated in sol-gel glass samples showed extinction coefficient and aborption peak wavelength comparable to that in methanolic solution. The absorption wavelengths of Uranin Laser dye showed blue shift in case of dye doped solids as compared to that in the solution. This can be combined effect of higher refractive index of solids and environment surrounding the dye molecule.

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Revealing the Chemistry of Mindfulness and Impact of Yoga on Brain Chemistry

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Abstract:

This study reflect a scientific approach of understanding that yoga practices affect biochemical processes in the body, contributing to physical and mental well-being and also emphasizes the scientific exploration of yoga and mindfulness practices that affect brain neurochemistry, highlighting their impact on mental well-being and cognitive processes.

Keywords: *Yoga, Mindfulness, Chemistry, Well-being*

Introduction:

The Indian knowledge tradition encompasses a vast and ancient body of knowledge that has evolved over several millennia. Central to this tradition is yoga, which is both a spiritual and physical discipline aimed at achieving harmony between the mind and body.

Yoga include asanas, pranayama and meditation. The goal of yoga is to attain a state of mental and physical well-being, as well as spiritual enlightenment.

Indian knowledge tradition includes rich philosophical systems such as Vedanta, Samkhya, Nyaya, and others. These philosophies explore fundamental questions about existence, consciousness, morality, and the nature of reality.

Central texts like the Vedas, Upanishads, Bhagavad Gita, and Yoga Sutras of Patanjali provide insights into spiritual practices, metaphysics, and ethical teachings. They are foundational to understanding both yoga and broader Indian philosophical thought.

Yoga is not just a physical exercise routine but a holistic approach to health, encompassing mental, emotional, and spiritual well-being. Practices like meditation and mindfulness, rooted in yoga, are increasingly recognized worldwide for their health benefits.

In recent decades, yoga has become immensely popular worldwide, adapted and integrated into various cultures and lifestyles. This global acceptance underscores its universal appeal and effectiveness in promoting physical health and mental tranquillity.

Yoga is deeply rooted in the broader Indian knowledge tradition, offering insights into philosophy, spirituality, and holistic well-being.

Yoga contributes to both physical and mental health, highlighting its holistic benefits and therapeutic effects on the human body and mind.

The fundamental human capacity to be totally present, aware of our surroundings and our actions, and to avoid becoming too reactive or overwhelmed by them is known as mindfulness.

In meditation, the current moment is explored rather than erased. When we meditate, we explore our mental processes, including our feelings, thoughts, and sensations.

By putting aside our judgement of the mind's processes and embracing our innate curiosity in what is going on in the moment, mindfulness meditation invites us to be present in each moment with warmth and kindness, both towards ourselves and towards others.

Furthermore, despite the fact that others may find this absurd or even silly, study indicates that cultivating this innate ability to observe ourselves and our surroundings non-judgmentally and with consideration has profound and beneficial effects on our well-being that undulate out into our everyday lives and societies.

Science involved in mindfulness:

Meditation may help alleviate stress-related health issues like depression and anxiety. The detrimental aspects of psychological stress can be effectively reduced by participating in mindfulness meditation programmes, such as Mindfulness-Based Stress Reduction, Mindfulness-Based Cognitive Therapy, and other mindfulness meditations. The results are similar to those that would be anticipated from the use of an antidepressant.

A randomised controlled study by Richard A. Davidson and Jon Kabat-Zinn published in Psychosomatic Medicine found that after receiving a flu vaccine, meditators who completed an eight-week mindfulness training programme had significantly more flu antibodies (Improved immune function) than their non-meditating peers. Positive sentiments and antibody responses to immune system challenges were shown to rise in both meditators' and non-meditators' brain activity, according to measurements. The increase in healing observed in psoriasis therapy studies with thoughtful reflection during treatment may be explained by improved immune system activity.

Mindfulness-based programmes may help aspects of cognition, according to a recent meta-analysis of 18 studies comparing eight weeks of Mindfulness-Based Stress Reduction (MBSR) and Mindfulness-Based Cognitive Therapy (MBCT). These include autobiographical and short-term memory, cognitive flexibility, and meta-awareness (self-awareness, for example), which are essential skill sets that enable people to become aware of harmful thought patterns so they can adopt different perspectives and reactions to situations. Additional studies (by Alan Wallace, Richie Davidson, and Amishii Jha) have discovered notable improvements in the regulation of attention in people who have received mindfulness meditation training.

When we are not focused on a particular activity, the brain's default mode network (DMN), which is linked to mind-wandering and self-referential thinking, becomes quite active. The DMN of experienced meditators was found to be less active. Research suggests that meditation training can indeed have positive effects on human heart health. Meditation, particularly mindfulness meditation, has been shown to reduce the body's response to stress. Chronic stress can contribute to high blood pressure, inflammation, and heart disease. By lowering stress levels, meditation may help mitigate these risk factors. Studies have indicated that regular meditation practice can lead to reductions in blood pressure. High blood pressure (hypertension) is a major risk factor for heart disease, stroke, and other cardiovascular problems. Meditation techniques such as deep breathing and focused attention can help relax the body and lower blood pressure over time. Time variation between heart beats is known as Heart rate variability (HRV). Better cardiovascular health and increased resilience to stress are linked with Higher HRV. Meditation has been shown to improve HRV, indicating a more balanced autonomic nervous system and potentially better heart health. Chronic inflammation is linked to atherosclerosis (hardening of the arteries) and other cardiovascular conditions. Meditation practices have been found to reduce inflammatory markers in the body, such as C-reactive protein (CRP), which can contribute to improved heart health.

Meditation can promote emotional resilience, reduce anxiety, and improve mood. Emotional factors play a significant role in heart health, as chronic negative emotions like anxiety and depression are associated with increased risk of heart disease. By fostering a positive emotional state, meditation may indirectly support heart health.

Cardiovascular problems are arises due to poor sleep also. Meditation practices, especially those focused on relaxation and mindfulness, can improve sleep quality by reducing insomnia symptoms and promoting deeper, more restorative sleep.

Regular meditation practice is often associated with healthier lifestyle choices, such as improved diet, increased physical activity, and reduced substance use. These behaviours contribute to overall cardiovascular health.

Overall, while meditation alone may not replace traditional medical interventions for heart disease, it can serve as a valuable adjunct therapy by promoting relaxation, reducing stress, improving emotional well-being, and potentially mitigating risk factors associated with cardiovascular disease.

Meditation training offers a valuable adjunct to conventional mental health treatments, providing individuals with practical tools to manage symptoms, enhance emotional well-being, and promote overall mental resilience. Integrating meditation into treatment plans can empower individuals to actively participate in their healing process and cultivate long-term mental health benefits.

Reduction in cellular aging with meditation training, the accumulating evidence suggests that regular practice of mindfulness and related techniques may support cellular health and longevity. Integrating mindfulness into lifestyle and health practices could potentially offer benefits beyond mental well-being, extending to physical health and aging processes.

Self-confidence and leadership may improve after meditation training by fostering self-awareness, emotional regulation, resilience, and authentic communication, meditation training can significantly enhance self-confidence and leadership capabilities. These qualities contribute to effective decision-making, team engagement, and overall organizational success. Integrating meditation into leadership development programs can help cultivate these skills and empower individuals to lead with clarity, compassion, and confidence.

Methodology: Based on the Yoga and its beneficial effects mentioned in introduction part of this paper, the chemical science and its relation with Yoga are mentioned in Result and discussion part of this paper.

Result and Discussion:

Biochemistry of Yoga: Yoga practices such as Asanas (postures), pranayama (breathing exercises), and meditation can have profound effects on the biochemistry of the body. For example, deep breathing techniques in yoga can influence the balance of oxygen and carbon dioxide in the blood, affecting pH levels and thereby influencing biochemical reactions.

Neurochemistry and Yoga: Yoga has been shown to influence neurotransmitters such as serotonin, dopamine, and GABA, which are involved in mood regulation, stress response, and overall mental health. Regular yoga practice can potentially alter these neurotransmitter levels, promoting relaxation and reducing stress.

Yogic Diet and Chemistry: Some forms of yoga emphasize a sattvic diet, which is believed to promote clarity and equanimity. This diet typically includes fresh fruits, vegetables, nuts, seeds, and dairy products, while avoiding stimulants like caffeine and heavily processed foods. The chemical composition of foods in a sattvic diet can have implications for health and well-being.

Chemistry of Yoga Materials: In a more literal sense, the materials used in yoga practice, such as yoga mats and clothing, involve which have distinct chemical properties affecting durability, grip, and environmental impact. For instance, yoga mats are often made from materials like PVC or natural rubber.

Psychological and Emotional Chemistry: The psychological benefits of yoga, such as improved mood, reduced anxiety, and enhanced self-awareness, are closely tied to changes in brain chemistry and hormone levels. Practices like mindfulness meditation can influence the release of neurotransmitters and hormones that impact mood and emotional regulation.

Mindfulness, as a practice rooted in ancient contemplative traditions and now widely studied in modern psychology and neuroscience, has intriguing connections to chemistry, particularly in how it affects the brain and body. Mindfulness practices, such as meditation and focused breathing, have been shown to influence neurotransmitter levels in the brain. For example:

Serotonin: Mindfulness meditation may increase serotonin production or receptor sensitivity. Serotonin is crucial for mood regulation, sleep, and appetite.

Mindfulness practices can lead to increased dopamine release. Dopamine is involved in reward-motivated behavior, pleasure, and focus. Mindfulness has been associated with higher levels of gamma-aminobutyric acid (GABA), which is a neurotransmitter that helps regulate anxiety. Mindfulness practices can also influence hormone levels in the body. Mindfulness meditation has been shown to reduce cortisol levels, which are elevated during times of stress. Lower cortisol levels contribute to a calmer state of mind. Endorphins are natural mood enhancers and pain relievers that can be released through mindfulness exercises.

Studies using neuroimaging techniques like MRI have demonstrated that mindfulness practice can lead to structural changes in the brain.

Mindfulness is associated with increased activity and cortical thickness in the prefrontal cortex, which is responsible for higher-order cognitive functions such as decision-making and emotional regulation.

Mindfulness has been linked to increased grey matter density in the hippocampus, which is involved in memory formation and emotional regulation.

Chronic stress and inflammation are closely related, and mindfulness practices have been shown to reduce markers of inflammation in the body, such as C-reactive protein (CRP). This anti-inflammatory effect can have far-reaching implications for overall health.

Recent research suggests that mindfulness practices may influence gene expression through epigenetic mechanisms. This means that mindfulness could potentially turn certain genes on or off, affecting health outcomes and resilience to stress.

Conclusion:

Impact of Yoga on brain chemistry is comprehensive and beneficial. By influencing neurotransmitter activity, hormone levels, brain structure, and inflammatory processes, yoga contributes to improved mental health, emotional resilience, cognitive function, and overall physiological well-being. These effects underscore role of yoga as a holistic practice that enhances both mind and body health through its various techniques and disciplines.

Understanding the chemistry of mindfulness provides insights into how these practices promote mental and physical well-being. By influencing neurotransmitters, hormones, brain structure, and even gene expression, mindfulness offers a holistic approach to enhancing resilience, reducing stress, and fostering emotional balance. Ongoing research continues to uncover the intricate ways in which mindfulness impacts our biological systems, underscoring its potential as a powerful tool for health and wellness.

While chemistry and yoga may appear disparate, they intersect in numerous ways that contribute to understanding the holistic effects of yoga on the body, mind, and environment. Exploring these intersections can provide insights into both fields and potentially lead to innovations in health, wellness, and materials science.

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A Brief Review on the Synthesis of Thiazole Derivatives and its Biological Activities

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Abstract

Thiazole, a five-membered heterocyclic compound featuring sulfur at position 1 and nitrogen at position 3, has garnered significant attention in medicinal chemistry due to its wide range of biological activities. These include antibacterial, antifungal, antiviral, anthelmintic, antitumor, and anti-inflammatory effects. The structural versatility of thiazole allows for the modification of its substituents to create novel derivatives with enhanced therapeutic potential. Through the development of various synthetic pathways, thiazole derivatives have been explored extensively in drug research, leading to the creation of combinatorial libraries aimed at discovering new, biologically active compounds. This review highlights the chemistry, synthesis, and biological significance of thiazole and its derivatives, emphasizing their role in the discovery of new therapeutic agents.

Keywords: *Thiazole; synthetic pathway; substituent modification; biological activities; Combinatorial libraries.*

1) Introduction:

Thiazole (C_3H_3NS) is a five-membered heterocyclic compound containing nitrogen and sulfur. It has a light-yellow liquid appearance and a pyridine-like odor. The molecule exhibits resonance, where electrons are delocalized over the ring, enhancing its stability and reactivity.

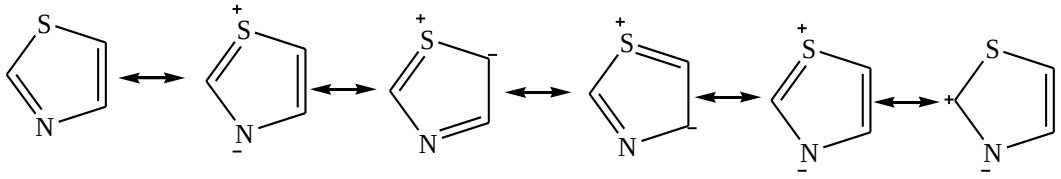


Figure 1. Resonating structures of thiazole.

Thiazoles are heterocyclic compounds featuring nitrogen and sulfur, known for their catalytic and biological significance. They are used as catalysts in reactions like the Stetter and benzoin condensation, facilitating important chemical transformations [1,2]. First studied for their biological activity in 1887 [3], thiazoles exhibit a range of medicinal properties, including antimicrobial and anticancer effects. Their molecular structure, with nitrogen being the most electronegative atom, contributes to their reactivity and similarities to other heterocycles like pyridine and thiophene [4]

2) Properties of Thiazole:

2.1 Physical Properties of Thiazole:

Thiazole is a five-membered heterocyclic compound containing both sulfur and nitrogen atoms, which gives it distinctive chemical properties. This compound is often used in organic synthesis due to its ability to serve as a versatile building block in the creation of biologically active molecules. Thiazole derivatives have found applications in medicinal chemistry, with many showing significant antimicrobial, antifungal, and anticancer activities. Its solubility in organic solvents makes it easy to work with in laboratory settings, and its structural properties contribute to its

importance in drug design and development.

- Thiazole are pale-yellow flammable liquid.
- Thiazole has pyridine like odour.
- It is sparingly soluble in water and fairly soluble in ether and alcohol.
- Boiling point of Thiazole is 116-118°c and pka of 2.5 (conjugated acid).
- Density is 1.2 gm/cm^3 and its ionization potential is 9.50 Ev.
- Dipole moment of 1.61D

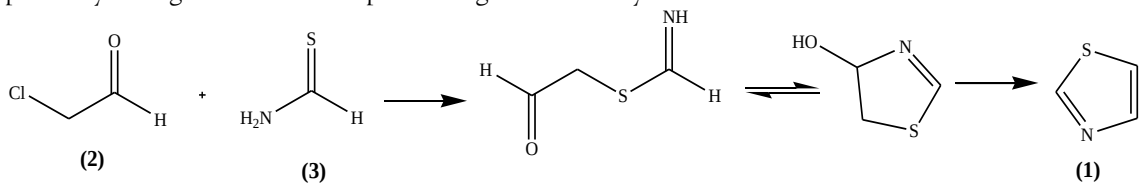
Thiazoles are an important class of heterocyclic compounds that have gained significant attention in cancer research due to their potential therapeutic properties. These compounds are known to interact with various biological targets, offering promising anticancer activity. Aromatic thiazoles, in particular, possess the ability to inhibit cancer cell proliferation, induce apoptosis, and disrupt key signaling pathways involved in tumor growth. As a result, thiazole-based drugs are being explored for their potential use in cancer therapy [5]. Their diverse structural features allow for modifications that enhance their efficacy and selectivity for cancer cells. Ongoing research continues to investigate how these compounds can be optimized for clinical applications in cancer treatment [6].

2.2 Chemical Properties of Thiazole

Thiazole is a heterocyclic compound consisting of a five-membered ring containing both sulfur and nitrogen atoms. It plays a vital role in organic chemistry due to its versatile reactivity and diverse applications. Thiazole and its derivatives are commonly found in various natural products, pharmaceuticals, and agrochemicals. These compounds exhibit significant biological activity, including antimicrobial, anticancer, and anti-inflammatory properties. The structural diversity of thiazole derivatives allows for the development of molecules with tailored characteristics, making them valuable in drug design and other industrial applications.

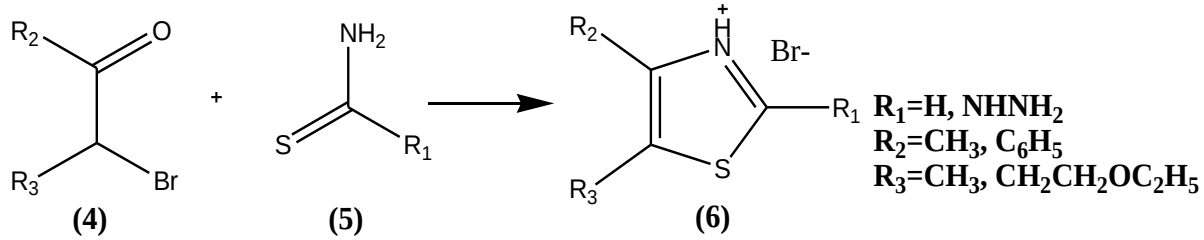
2.2.1 Synthesis of Thiazoles and its derivatives

1) Thiazole **1** can be synthesized efficiently through the condensation of α-chloroacetal- dehyde **2** with thioformamide **3**. This reaction leads to the formation of the thiazole ring system, with the process yielding the desired compound in good efficiency [7,8]



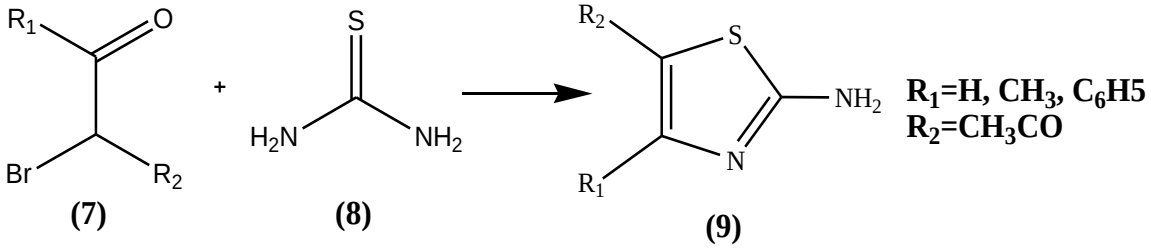
Scheme 1. Synthesis of Thiazole **1**.

2) The reaction of *N*-Monosubstituted thioamides **5** with α- halocarbonyl compounds **4** yields thiazolium salt **6** in good yields [9-13]



Scheme 2. Synthesis of Thiazolium salts **6**

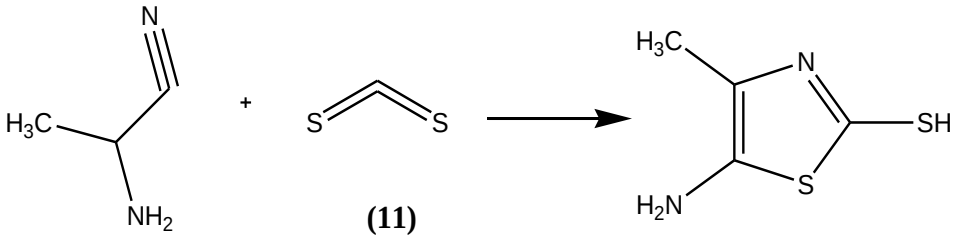
3) The condensation of one mole equivalent of thiourea **8** and one mole equivalent of α–haloketones or α–haloaldehydes **7** gives exclusively 2-aminothiazoles **9** [14]



(7) (8) (9)

Scheme 3. Synthesis of 2-aminothiazoles **9**.

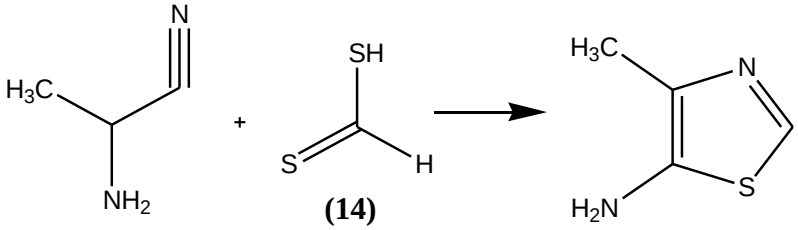
4) The reaction between carbon disulfide (CS_2) **11** and α-aminonitriles **10** leads to the synthesis of 2-mercapto-5-amino thiazoles **12** [15-18]. In this process, the carbon disulfide provides sulfur atoms, which interact with the nitrile and amine groups of the α-aminonitrile to form a thiazole ring. The resulting compound features both a mercapto (-SH) and an amino ($-NH_2$) group at key positions, which are crucial for its reactivity.



(10) (11) (12)

Scheme 4. Synthesis of 2-mercapto-5-amino thiazoles **12**.

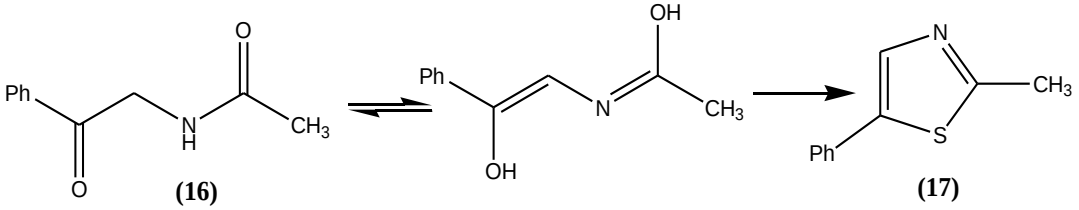
5) The reaction between dithioformic acid **14** derivatives and α-aminonitriles **13** in aqueous ether at room temperature yields 5-aminothiazoles **15** in high yields [19] This transformation involves the nucleophilic attack of the thiolate anion on the α-aminonitrile, followed by cyclization to form the thiazole ring. The procedure offers a convenient and efficient route to synthesize 5-aminothiazoles, which are valuable intermediates in drug discovery and materials science.



(13) (14) (15)

Scheme 5. Synthesis of 5-aminothiazoles **15**.

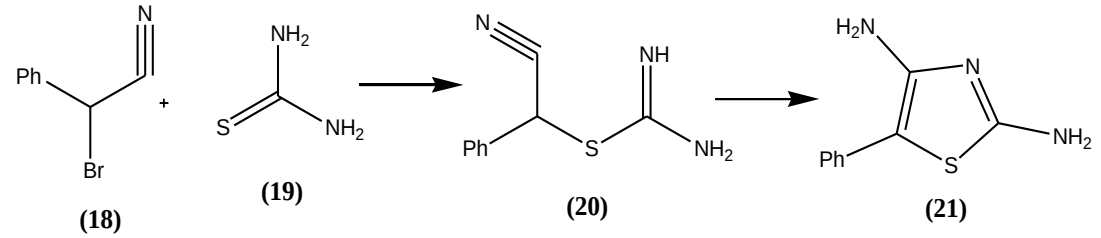
6) In 1910, Gabriel [20] described a reaction where N-(2-oxo-2-phenylethyl) acetamide **16** reacts with phosphorus pentasulfide to form 2-methyl-5-phenylthiazole **17.** The phosphorus pentasulfide replaces the carbonyl oxygen with sulfur, creating a thioamide intermediate. This intermediate then undergoes cyclization, forming the thiazole ring with a methyl group at position 2 and a phenyl group at position 5. This reaction is a key example of thiazole synthesis, widely used in organic chemistry.



(16) (17)

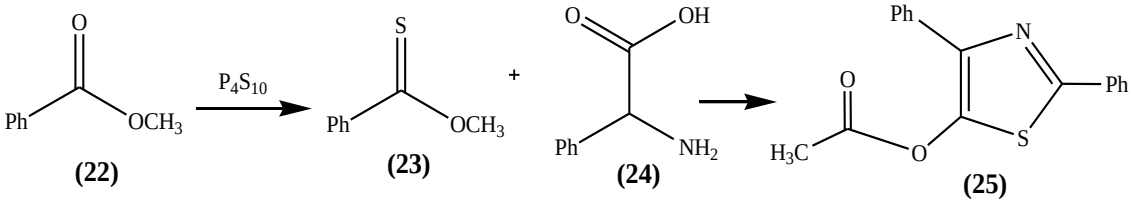
Scheme 6. Synthesis of thiazole derivatives based on diketone **17**.

7) The reaction of thiourea **19** with 2-bromo-2-phenylacetonitrile **18** in an alcoholic medium leads to the formation of 5-phenylthiazole-2,4-diamine **21** [21-23] This process involves a nucleophilic substitution, where thiourea displaces the bromine atom, followed by cyclization to form the thiazole ring.



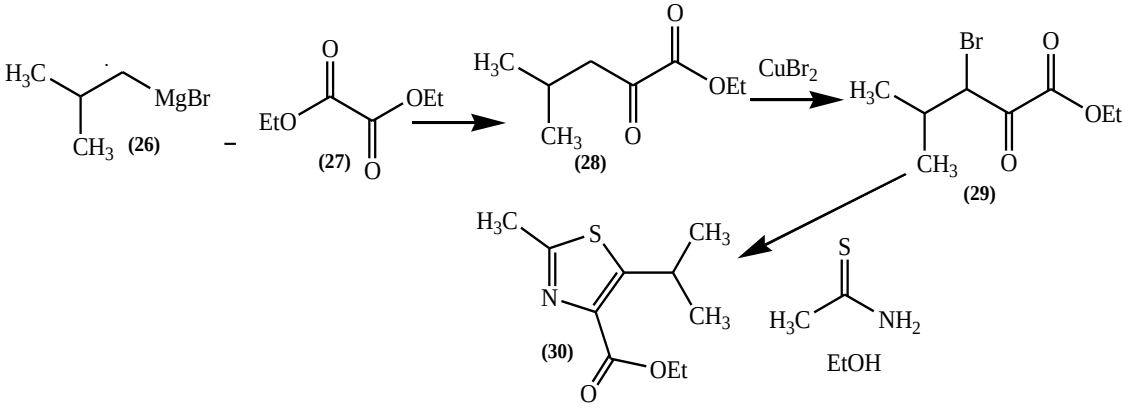
Scheme 7. Synthesis of 2,4-diaminothiazole **44**.

8) The reaction between methyl benzoate **22** and phenylglycine **24** leads to the formation of a thiazole derivative **25** through a cyclization process [24] This transformation occurs in good to moderate yields, typically under mild reaction conditions, with the involvement of a sulfur and nitrogen-containing heterocyclic ring. Such reactions are valuable in synthetic chemistry for the efficient construction of biologically active thiazole-based compounds.



Scheme 8. Synthesis of thiazole compound **50**.

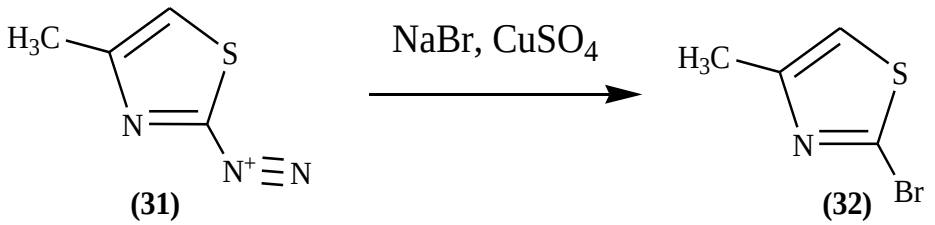
9) Bueno et al. synthesized thiazole **30** using the Hantzsch method [25], which involves the condensation of an α, β-unsaturated carbonyl compound with sulfur and an amine. This method is widely used to prepare 2,4-dihydro-1,3-thiazoles, which have important applications in pharmaceuticals and agrochemicals. The synthesis of thiazole **30** demonstrates the versatility of the Hantzsch method in creating valuable heterocyclic compounds.



Scheme 9. Synthesis of ethyl 5-isopropyl-2-methylthiazole-4-carboxylate **30**.

3) Nucleophilic Substitution Reactions of Thiazole:

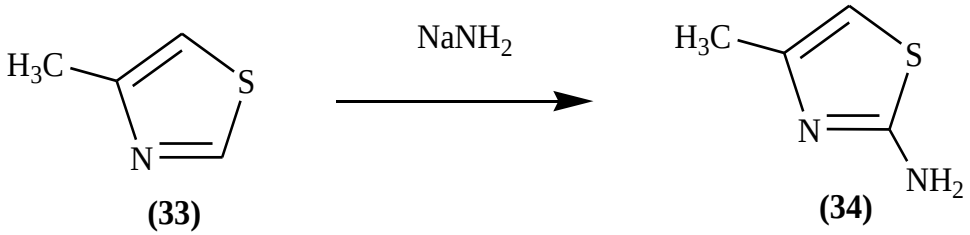
The diazonium salt of 2-aminothiazole **31** undergoes nucleophilic substitution when treated with sodium bromide in the presence of copper sulfate as a catalyst. The electron-deficient carbon center of the diazonium ion becomes highly reactive and is attacked by the bromide ion, leading to the replacement of the diazonium group with a bromine atom. Copper sulfate facilitates the reaction by stabilizing the transition state and enhancing the electrophilic nature of the diazonium ion. This results in the formation of 2-bromo-4-methyl thiazole **32** [26] (Scheme 43), a valuable intermediate for further synthetic applications.



(31) **(32)**

Scheme 10. Synthesis of thiazole compounds

High nucleophilicity reagent Sodamide on reaction with 3-methylthiazole produce 2-amino-3 methylthiazole. (Scheme 44)



(33) **(34)**

Scheme 11. Synthesis of 2-amino-3 methylthiazole

4) Biological activities of Thiazole compounds

Thiazole derivatives are a class of heterocyclic compounds containing a five-membered ring with sulfur and nitrogen atoms, which exhibit a broad range of biological activities, making them highly valuable in medicinal chemistry. These compounds have shown promising antibacterial, antifungal, anticancer, anti-inflammatory, and antiviral properties, among others.

Thiazoles possess significant antibacterial and antifungal activity, often disrupting microbial cell wall synthesis, protein function, or membrane integrity. Their ability to combat both Gram-positive and Gram-negative bacteria, along with fungal pathogens such as *Candida* and *Aspergillus*, positions them as potential candidates for novel antibiotics and antifungal agents.

In oncology, thiazole derivatives demonstrate anticancer properties by inhibiting cell proliferation, inducing apoptosis, and targeting key signaling pathways like tyrosine kinases. These compounds have exhibited effectiveness against various cancers, including breast, lung, and colon cancers, suggesting their therapeutic potential in cancer treatment.

Thiazoles also display robust anti-inflammatory effects, likely due to their ability to inhibit key enzymes such as cyclooxygenase (COX) and modulate inflammatory cytokines, making them promising for treating diseases like arthritis, inflammatory bowel disease, and psoriasis. Additionally, these compounds exhibit antioxidant activity, protecting cells from oxidative stress associated with aging and neurodegenerative conditions.

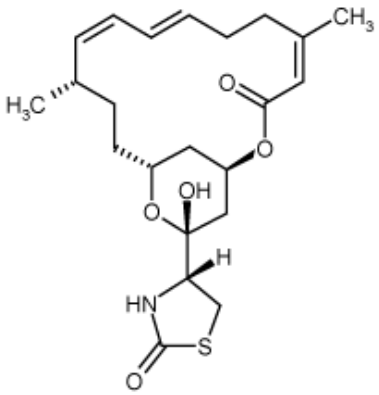
Antiviral activity is another notable feature, with thiazoles demonstrating efficacy against several viruses, including HIV and herpes simplex virus (HSV), by interfering with viral replication and entry. Furthermore, thiazoles have shown potential in managing diabetes by regulating glucose metabolism and enhancing insulin sensitivity.

These compounds also possess neuroprotective and antiplasmodial properties, opening avenues for treating neurodegenerative diseases and malaria. Their anthelmintic activity against parasitic worms further expands their scope of therapeutic applications.

Overall, the diverse biological activities of thiazole compounds underscore their importance in drug development. Their ability to target multiple disease pathways positions them as a valuable class of compounds for tackling infections, cancer, inflammation, and other challenging medical conditions.

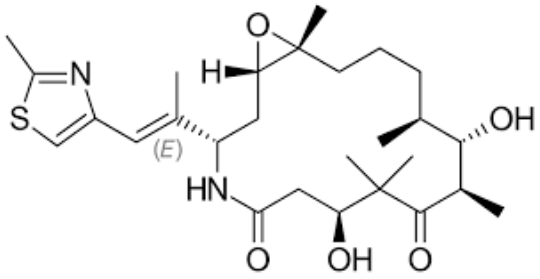
4.1 Anticancer activity:

One notable example is Latrunculin A, a thiazole-containing compound known for its potent inhibition of actin polymerization. **Latrunculin A** and its derivatives have shown promise as inhibitors for prostate tumors. [27]



(Latrunculin A use to treat prostate tumors)

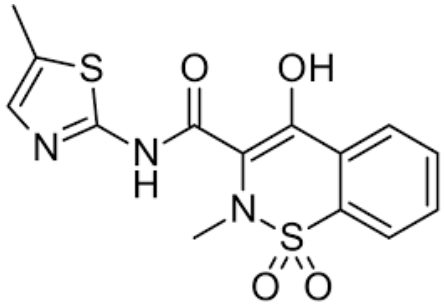
Ixabepilone, is an anti-cancer medication used for the treatment of aggressive metastatic or locally advanced breast cancer [28]



(Ixabepilone)

4.2 Anti-inflammatory activity:

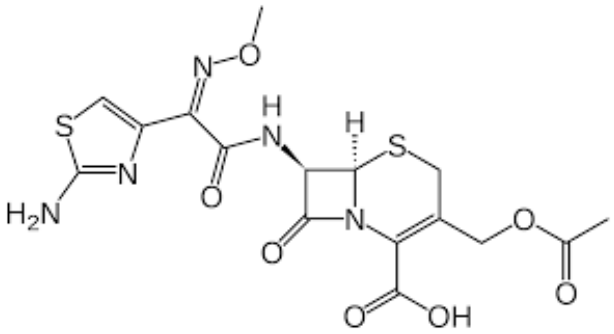
Meloxicam, is a nonsteroidal anti-inflammatory drug (NSAID) used to treat pain and inflammation in rheumatic diseases and osteoarthritis [29][30]



(Meloxicam)

4.3 Antibacterial activity

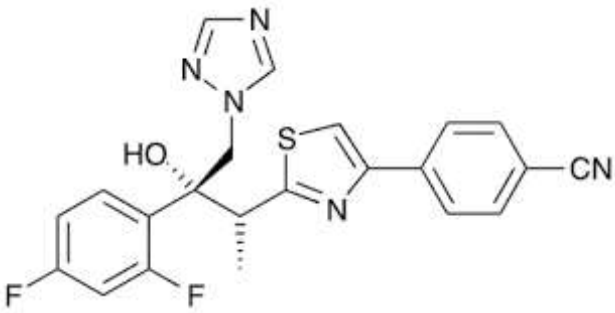
Cefotaxime is an antibiotic used to treat several bacterial infections in humans. Specifically in humans it is used to treat joint infections, pelvic inflammatory disease, meningitis, pneumonia, urinary tract infections, sepsis, gonorrhea, and cellulitis [31]



(Cefotaxime)

4.4 Antifungal activity

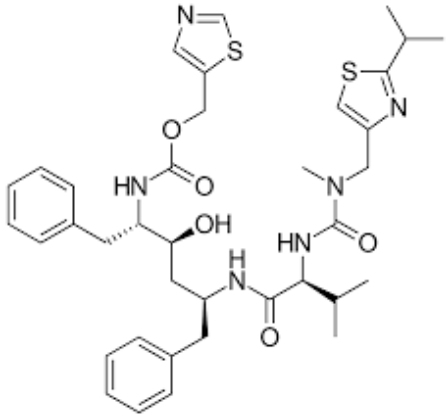
Isavuconazole is a broad-spectrum triazole antifungal medication approved for treating invasive aspergillosis and mucormycosis in adults [32]



(Isavuconazole)

4.5 Antiviral activity

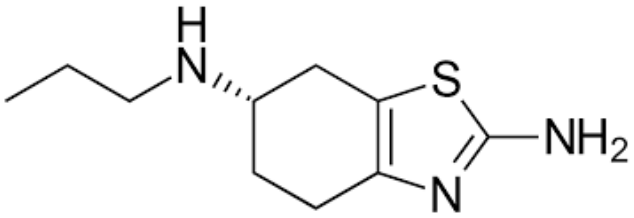
Ritonavir, is an antiretroviral medication used along with other medications to treat HIV/ AIDS. This combination treatment is known as highly active antiretroviral therapy (HAART).[33] It may also be used in combination with other medications to treat hepatitis C and COVID-19.



(Ritonavir)

4.6 Antiparkinsonian activity

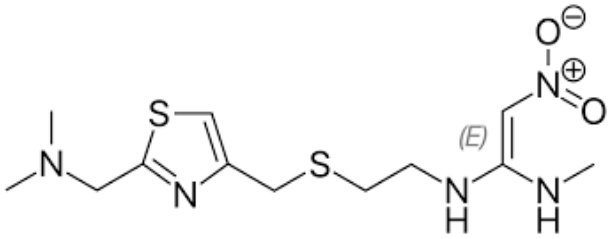
Pramipexole, is a medication used to treat Parkinson's disease and restless legs syndrome. In Parkinson's disease it may be used alone or together with levodopa [34]



(Pramipexole)

4.7 Gastrointestinal activity

Nizatidine is a histamine H_2 receptor antagonist that inhibits stomach acid production, and is commonly used in the treatment of peptic ulcer disease and gastroesophageal reflux disease.[35]



(Nizatidine)

Conclusion:

In conclusion, thiazole derivatives represent a highly promising class of compounds with significant potential in drug discovery and development due to their diverse biological activities. The various synthetic routes available for the preparation of thiazoles, including condensation and cyclocondensation reactions, offer versatility and the ability to tailor the structure of these compounds for specific biological targets. The broad spectrum of pharmacological activities exhibited by thiazole derivatives—such as antimicrobial, anticancer, anti-inflammatory, antiviral, and antidiabetic effects—demonstrates their potential as lead molecules for the development of novel therapeutics. Furthermore, the growing focus on sustainable and green chemistry approaches in their synthesis highlights the ongoing efforts to improve efficiency and minimize environmental impact. As research advances, further exploration of the mechanisms underlying the biological actions of thiazole derivatives, along with their optimization for clinical use, will be crucial for realizing their full therapeutic potential. The continued exploration of this class of compounds holds great promise for addressing a variety of unmet medical needs and advancing the field of medicinal chemistry.

Notes: The authors declare no competing financial interest.

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Antimalarial Drug Resistance: Basics and Emergence

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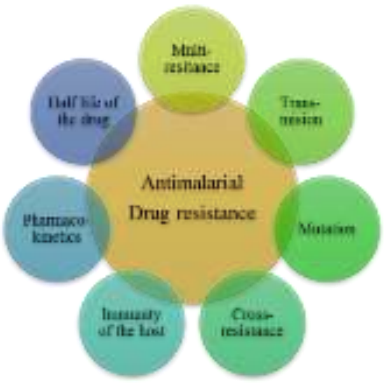
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Abstract:

Antimalarial drug resistance is a major challenge globally in our fight against malaria. Here, the authors have discussed the problem of antimalarial drug resistance, with emphasis on current trends. The epidemiology and current status of antimalarial drug resistance have been discussed in detail, with special emphasis on the development and spread of P. falciparum resistance. Authors have also summarized the factors contributing to antimalarial drug resistance. The mechanism and detection of antimicrobial resistance have also been touched upon. Finally, authors have described the upcoming modalities for preventing drug resistance, which include a reduction in overall drug pressure, improvement in the usage of drugs, and combination therapy. Finally, the conclusions and future perspective in this field are expounded upon.

Keywords: *Malaria, Artemisinin-based combination therapy (ACT), Anti-malarial drug resistance, Plasmodium falciparum, Drug pressure, Combination Therapy*

Graphical Abstract:



I. Introduction

"While keeping in mind the realities one can nevertheless be confident that malaria is well on its way towards oblivion. Already as a malariologist, I feel premonitory twinges of lonesomeness, and in my own organisation, I am now a sort of 'last survivor'. So perhaps it is fitting that I should take this backward glance at the fascinating pages of malaria history."[1]

---- Paul Russell

Malaria is a disease spread by mosquitoes affecting human beings and many other species. Its symptoms usually include tiredness, fever, headaches, and vomiting. In extreme cases, the outcome can be convulsions, yellow skin, coma, and even death[2]–[6]. Normally, the symptoms of this disease appear 10 to 15 days after being bitten by an infected mosquito. The disease can recur even months later, if not properly treated the first time. Fortunately, reinfection is usually less severe. Table 1 summarizes the different types of malaria [7], [8].

Table 1: Different types of Malaria

Name	Pathogen
Algid malaria	*Plasmodium falciparum*
Bilious malaria	*Plasmodium falciparum*
Cerebral malaria	*Plasmodium falciparum*
Congenital malaria	Various plasmodia
Falciparum malaria, *Plasmodium falciparum* malaria, Pernicious malaria	*Plasmodium falciparum*
Ovale malaria, *Plasmodium ovale* malaria	*Plasmodium ovale*
Quartan malaria, Malariae malaria, *Plasmodium malariae* malaria	*Plasmodium malariae*
Quotidian malaria	*Plasmodium falciparum, Plasmodium vivax, Plasmodium knowlesi*
Tertian malaria	*Plasmodium falciparum, Plasmodium ovale, Plasmodium vivax*
Transfusion malaria	Various plasmodia
vivax malaria, *Plasmodium vivax* malaria	*Plasmodium vivax*

Single-celled microorganisms of the Plasmodium group are responsible for causing malaria, spread by an infected female Anopheles mosquito. The parasite is introduced into a human being's blood after being bitten by an infected mosquito. It travels to the liver, matures, and reproduces [9]. As shown in Table 1, five species of Plasmodium are responsible for different types of malaria, with

maximum deaths being caused by P. falciparum, and P. ovale, P. vivax, and P. malariae causing a mild form of malaria. In addition to that, the species P. knowlesi hardly causes disease in human beings [10], [11]. Diagnosis of malaria involves the use of antigen-based rapid diagnostic tests and microscopic examination of blood using blood films or methods utilizing the polymerase chain reaction.

1.1 Current Trends in Incidence of Malaria

There has been a steady decline in the incidence of malaria, for instance, in 2019, 57 cases per 1000 population at risk were reported; in 2015, this number was 58 while in 2000, it was 80, leading one to conclude that the rate of decline has slowed[12], [13]. The mortality due to malaria shows encouraging results, with reported deaths due to malaria in 2019 being 409,000, quite less than the reported number of 736,000 for the year 2000. In the category of children under 5 years, the percentage of deaths due to malaria reduced to 67% in 2019 than 84% in 2000. Alarmingly, 28 out of 82 malaria-endemic countries reported resistance to all four of the most frequently used insecticide classes, with resistance to pyrethroids continuing to be extensive, followed by resistance to organochlorines. Carbamates and organophosphates show less prevalence of resistance[14].

1.2 Geographical Distribution:

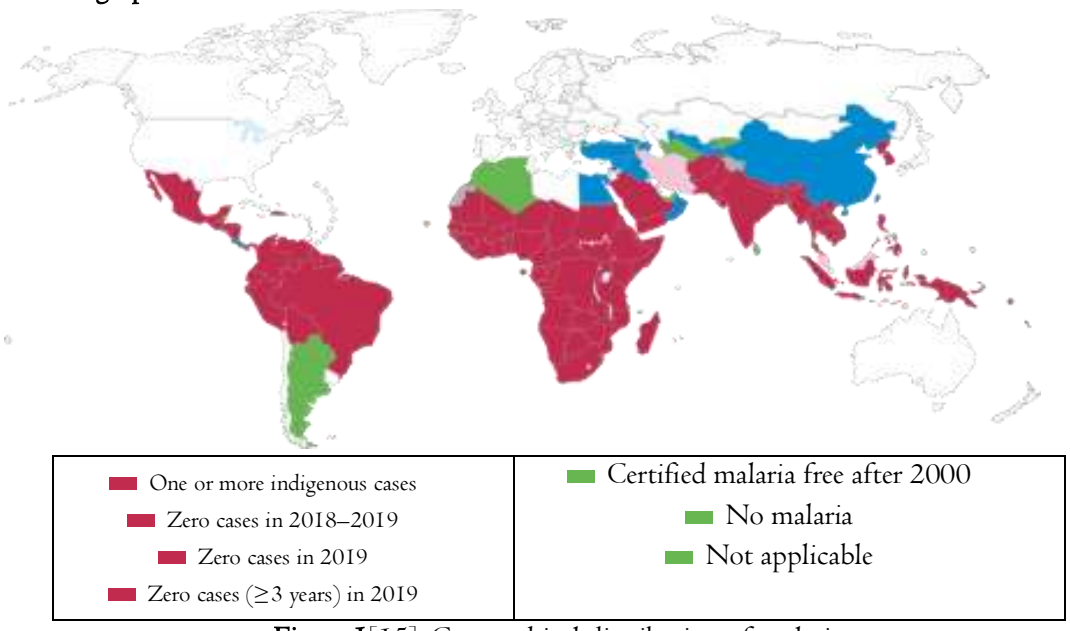


Figure 1[15]: Geographical distribution of malaria

As seen in Figure 1, "Countries with indigenous cases in 2000 and their status by 2019 Countries with zero indigenous cases over at least the past 3 consecutive years are considered to have eliminated malaria. In 2019, China and El Salvador reported zero indigenous cases for the third consecutive year and have applied for WHO certification of malaria elimination; also, the Islamic Republic of Iran, Malaysia, and Timor-Leste reported zero indigenous cases for the second time. Source: WHO database."

1.3 Drugs Available for Treatment of Malaria:

Artemisinin-based combination therapy (ACT) is the most common treatment strategy for treating malaria, chiefly for P. falciparum malaria. The aim is to make sure that the Plasmodium parasites are eliminated quickly and completely from the bloodstream of the patient so that the severity of the disease is contained. Proper treatment is also important because it helps in the

reduction of transmission of the infection. Before starting malaria treatment, a rapid diagnostic test (RDT) or microscopy should be used to confirm the presence of the parasite. If a facility for diagnosis is not available immediately, then the patient can be treated based on clinical grounds. It has been observed that oral artemisinin-based monotherapy (oAMT) contributes to resistance to artemisinins. WHO has counselled malaria-endemic countries to ensure that the production of oAMT is stopped and ACTs are recommended for the treatment of falciparum malaria. The various drugs used for treating malaria are summarized in Table 2.

Table 2: Main antimalarial drugs

Chemical Class	Drugs
Amino-alcohols	Quinine, quinidine, mefloquine, halofantrine, lumefantrine
Antibiotics	Azythromycin, clindamycin, doxycycline, tetracycline
Sulfonamides and sulfones	Sulfadoxine, sulfalene, dapsone
4-Aminoquinolines	Chloroquine, amodiaquine, piperaquine
Biguanides	Proguanil, chlorproguanil
8-Aminoquinoline	Primaquine
Sesquiterpene lactones	Artemisinin, arteether, artemether, artesunate, dihydroartemisinin
Diaminopyrimidine	Pyrimethamine
Naphthoquinone	Atovaquone

1.4 The Problem of Antimalarial Drug Incidence:

It is very important to monitor the therapeutic efficacy of antimalarial drugs regularly, as the parasite responsible for malaria is continuously evolving to develop resistance against the available drugs. This will aid in the timely detection of shifting patterns of parasite vulnerability and, thus, treatment plans and policies can be tweaked suitably. The most significant challenge in the fight against malaria has been resistance to drugs. 3 out of 5 malaria species, that is, P. falciparum, P. vivax, and P. malariae, have been reported to show antimalarial drug resistance.

According to WHO,

"Drug resistance is the ability of a parasite strain to survive or multiply despite the administration and absorption of a drug given in doses equal to or higher than those usually recommended but within the tolerance of the subject (WHO, 1967).

Later, this was modified, and the following sentence was added:

"The form of the drug active against the parasite must be able to gain access to the parasite or the infected erythrocyte for the duration of the time necessary for its normal action" [16].

Some opine that one must take into account the concentration profile of the drug while defining the problem of drug resistance. Another complicating factor in drug resistance is cross-resistance, which happens between drugs having similar mechanisms of action or belonging to the same chemical family. Then, the problem of multidrug resistance, for instance, P. falciparum shows resistance to more than two drugs belonging to different chemical families and have distinct

mechanisms of action. Because of resistance to antimalarial drugs, there is a lag or failure to remove asexual parasites from the blood of the infected patient. This allows the production of gametocytes that transmit the resistant genotype. This is a major problem and has changed the epidemiology of malaria all over the world.

2. ANTIMALARIAL DRUG RESISTANCE

2.1 Current Status of Antimalarial Drug Resistance: Epidemiology

In terms of the burden of the disease, the trends indicate an enhancement in the admissions to hospitals after the advent of chloroquine resistance in Africa[17][18]. Also, mortality was observed to increase at the community level[19], [20]. The most pertinent problem is that ineffective treatment causes low birth weight and anemia [21]. It is also to be noted that antimalarial drug resistance is responsible, at least in parts, for malaria epidemics [22] and enhanced transmission [23]. Antimalarial drug resistance also has huge economic costs. This works at two levels. On one hand, the global cost of novel drug development increases, and on the other hand, visiting health care facilities for further treatment leads to loss of working days that should be counted against economic costs[24], [25].In addition to disease burden, one has to note that changes in the distribution of malaria species are observed; for example, the proportion of P. falciparum malaria has changed, as it shows a rise with respect to P. vivax [26]. It is a vicious cycle as lack of treatment opportunities in the public sector leads to patients relying on the private sector, which is highly unregulated and thus increases drug resistance, as substandard or counterfeit medicines can be used in the private sector because of the lack of regulation.

The underprivileged, tropical and subtropical regions of the world, such as Africa, have more cases of malaria (figure 2) due to many factors, for example, very high transmission due to weather conditions and spread by Anopheles gambiae. In addition to that, socioeconomic problems lead to ineffective malaria control. Also, the prevalence of Plasmodium falciparum causes severe malaria and death.

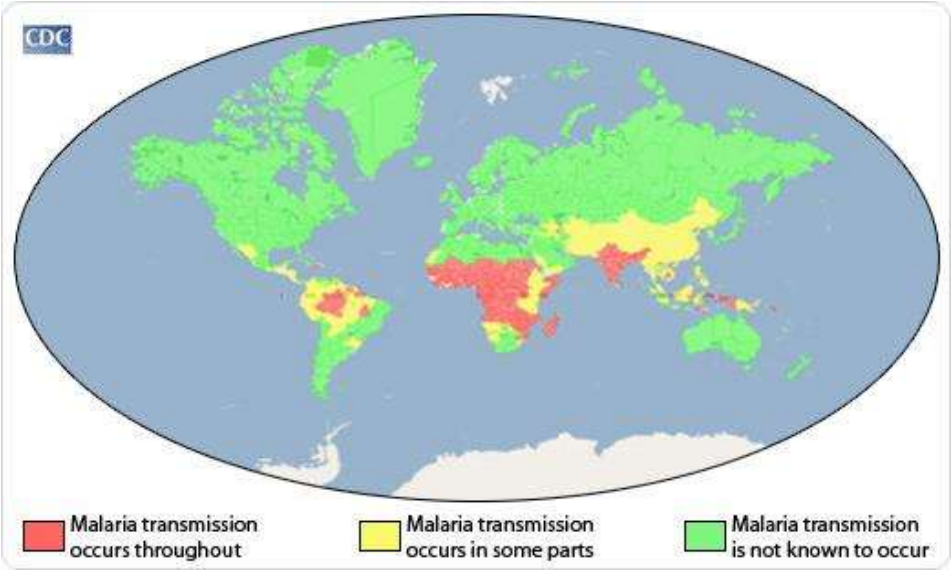


Figure 2 [27]: Malaria transmission across the globe

2.2 Development and Spread of P. Falciparum Resistance

P. falciparum causes the most damaging form of malaria. To add to this, it is resistant to traditional antimalarial drugs in most of the malaria endemic areas, increasing the morbidity and mortality due to malaria[28], [29]. For instance, it is resistant to pyrimethamine/sulfadoxine and chloroquine, which are spread throughout the malaria endemic regions, making these two ineffectual[30][31][32]. This makes artemisinin-based combination therapies (ACTs), the first-line treatments for uncomplicated malaria. The genes that are involved in the resistance to these drugs have been investigated in detail by making use of microsatellite markers that flank drug-resistance genes, and it has been revealed that these genes have very limited geographic reach. It is to be noted that the mutations that are drug resistant can arise in the preerythrocytic liver stages, sexual parasitic stages, and sexual erythrocytic parasite stages (refer to Figure 3). There is a lot of fluidity in the emergence and spread of anti-malarial drug resistance, and figuring out the exact focal point of the spread is very difficult. As an example, the dominant artemisinin-resistant P. falciparum C580Y is supposed to arise in western Cambodia. It is postulated that it then distributed to Thailand and Laos. So the only way is eliminating falciparum malaria from an area when the drugs are effective; once they develop resistance, it becomes very tough to control malaria [33]. The resistance of plasmodium falciparum parasites to artemisinins is linked with various polymorphisms in the parasite's K13-propeller gene; however, not much data is available regarding the molecular epidemiology of these artemisinin-resistant genotypes in Africa [34]. There is a need to globally sequence K13, so that ART resistance can be tracked [35]–[38]

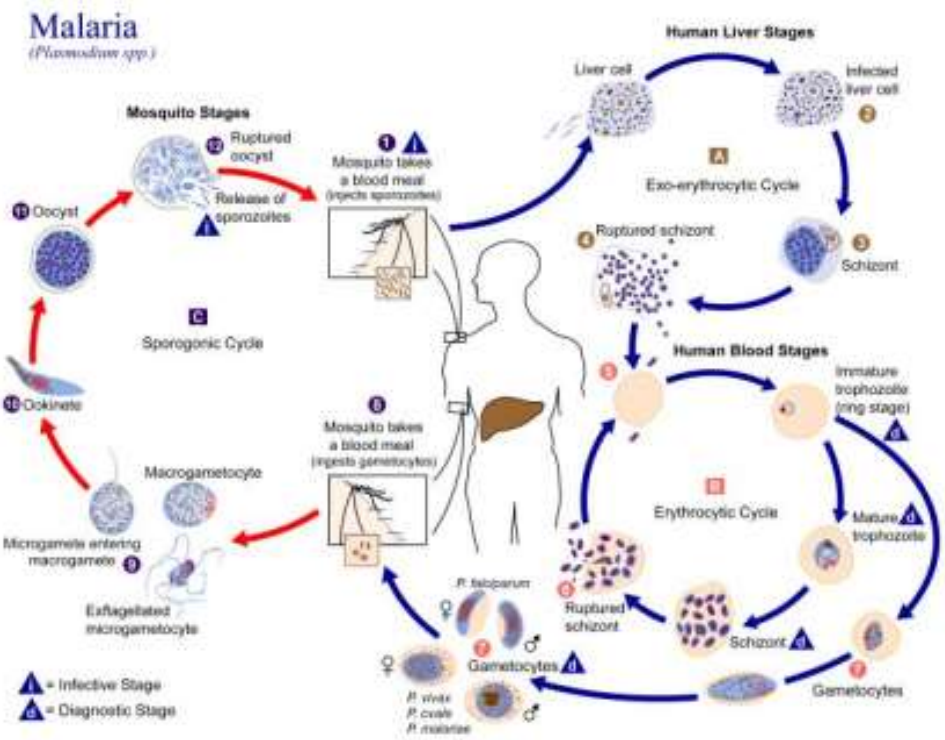


Figure 3 [39]: Life cycle of the parasites of the genus Plasmodium

2.3 Factors Contributing to Antimalarial Drug Resistance:

Malaria parasite shows de novo mutation quite frequently, typically single, and occasionally multiple. If the drug levels are not sufficient and the infection load is very high, the survival and propagation of mutations causing resistance becomes easy. It has been observed that the Southeast

Asia region shows the maximum number of cases of antimalarial resistance. There are many reasons for this. For one, this region shows low transmission where malaria cases are mostly symptomatic, so a larger number of patients receive treatment, making the selection of resistant strains of malaria more viable. Another factor is indiscriminate usage of antimalarial drugs. Interestingly, regions like Africa, where the rate of transmission is high, exhibit less number of cases of drug resistance. People of this region are partially immune to malaria as they are exposed to the malarial parasite continually throughout life, leading to asymptomatic malaria. Since patients do not present with symptoms, so chances of using antimalarial drugs for treating infection reduce, and proportionately selection of resistant strains also decreases. Also, it is to be noted that in these regions, the amount of drugs available is also less. The bloodstream of a partially immune person will have the propensity for non-selective elimination of blood-stage parasites. In addition to that, in people having partial immunity, the existence of intricate polyclonal leads to the possibility of outbreeding of multi-genic resistance mechanisms. More gametocytes are released due to drug pressure, so resistant parasites that have escaped the drugs are propagated. Features that endorse the growth of drug-resistant pathogens are more powerful with P. falciparum in relation to P. vivax, and this describes the greater frequency of resistance in P. falciparum. Primaquine should be used as a gametocytocidal agent for P. falciparum; otherwise, it will lead to the development and spread of resistance. In addition to that, if a drug has a long elimination phase, such as mefloquine, chloroquine, and piperaquine, it aids in the spread of resistance by selectively filtering some parasites but allowing infection by resistant varieties. Figure 4 summarizes the factors contributing to antimalarial drug resistance.

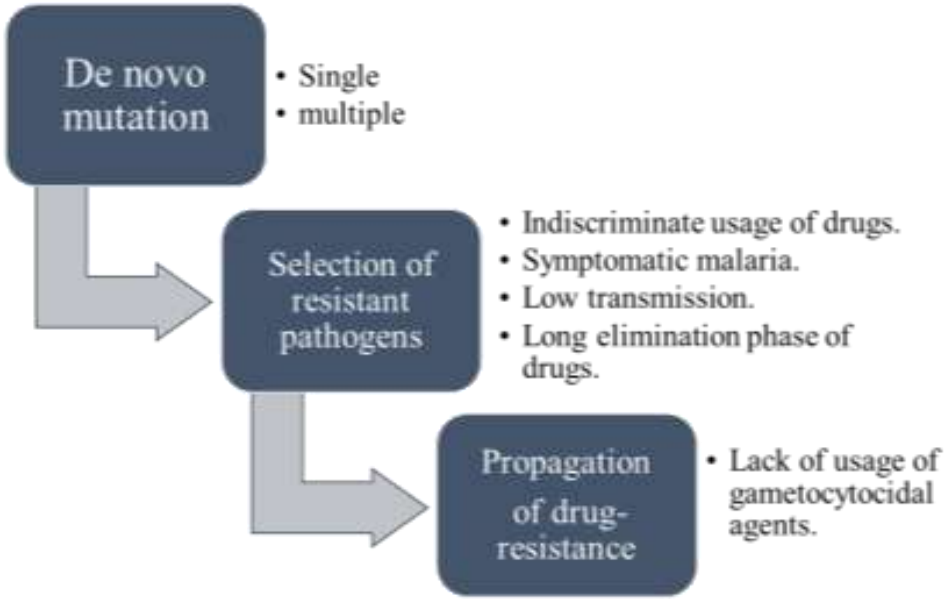


Figure 4: Spread of anti-malarial drug resistance

2.4 Mechanism of Antimalarial Drug Resistance:

In the three classes of antimalarial drugs, i.e., chloroquine, the antifolates, and atovaquone, the mechanism of drug resistance is clear. For instance, it has been reported that the strains of P. falciparum that show drug resistance to chloroquine exhibit less efficient accumulation of the drug compared to sensitive strains. Polymorphism in the pfcrt (for chloroquine resistance transporter) gene, principally the one amino acid change, K76T, is the hallmark of P. falciparum parasites

showing chloroquine resistance. Other mutations responsible for resistance in mefloquine, halofantrine, artemisinin, and probably chloroquine are at the pfmdr1 gene. Reversal of resistance to chloroquine of P. falciparum has been observed with a combination of drugs like antidepressants, phenothiazines, calcium inhibitors, and antihistamine compounds. Table 3 summarizes the mutations causing resistance to various antimalarial drugs. As mentioned in the previous section, cross-resistance occurs among the chemically similar drugs and is common among chloroquine, 4-aminoquinolines, and amodiaquine. Development of resistance to mefloquine results in resistance to halofantrine and quinine.

Table 3: Mutations causing resistance to various antimalarial drugs

Drug	Mutations
Chloroquine	*pfcrt* , *pfmdr1*
Quinine	*pfcrt*, *pfmdr1*, and *pfnhe1*
Sulfadoxine-pyrimethamine (SP)	Point mutations in *pfdhfr* and *pfdhps*
Artemisinin	Pf kelch protein gene on chromosome 13 (kelch13)
Piperaquine	*pfcrt*
Lumefantrine	*pfcrt*, *pfmdr1*
Amodiaquine	*pfcrt*, *pfmdr1*
Mefloquine	*pfmdr1*
Atovaquone	Single nucleotide polymorphisms in the cytochrome *b* gene

2.4 Detection of Antimalarial Drug Resistance:

Detection of antimalarial drug resistance entails detailed investigation of therapeutic efficacy. Three main factors decide the outcome of these studies [40]. First is the parasite factor, which would decide the curse of drug resistance, second is the immunity of the host, and finally third factor will be variations arising out of pharmacokinetics. For instance, if a person contracts malaria but lives in an area of high transmission, he or she can get rid of the parasite because of being partially immune. Another example of individual variation is reduced absorption of an antimalarial drug on account of some gastrointestinal problem. Table 4 summarizes the year in which resistance to a particular drug was seen.

Table 4: Drug and year-wise resistance

Drug	Year in which medicine was introduced	Year in which resistance was reported for the first time
Quinine	1632	1910
Chloroquine	1945	1957
Proguanil	1948	1949
Sulfadoxine-pyrimethamine	1967	1967
Mefloquine	1977	1982
Atovaquone	1996	1996
Artemisinins	1971	1998

One must bear in mind that therapeutic efficacy is only one of the many tools that are needed to confirm antimalarial drug resistance. Recrudescence in recent patients of malaria has to be proven, followed by genotyping of parasites to differentiate between recrudescent parasites and those causing novel infections. Pharmacokinetic analysis of blood samples, at least for 4 parasitic cycles, is a must. Also, in vivo valuation should be done. It will involve post-treatment monitoring of the clinical response after administration of the drug, taking into consideration case reports and detecting treatment failure. One has to be careful while attributing treatment failure to drug resistance, as treatment failure can be due to improper dosage, inadequate absorption of the drug, interaction of the drug with other substances, misdiagnosis, inferior quality of the drug, and not following the duration of the regimen completely. An important protocol that has been standardised after many revisions is the in vivo test protocol for evaluation of the sensitivity of chloroquine to P. falciparum [41].

Molecular markers, efficacy studies of clinical drugs, and in vitro and ex vivo appraisals of drug sensitivity provide information on drug efficacy of antimalarial drugs. For the trials of antimalarial drugs having long terminal half-lives, the follow-up of the patients must be adequately long [42], [43]. Figure 5 summarizes the detection of antimalarial resistance.

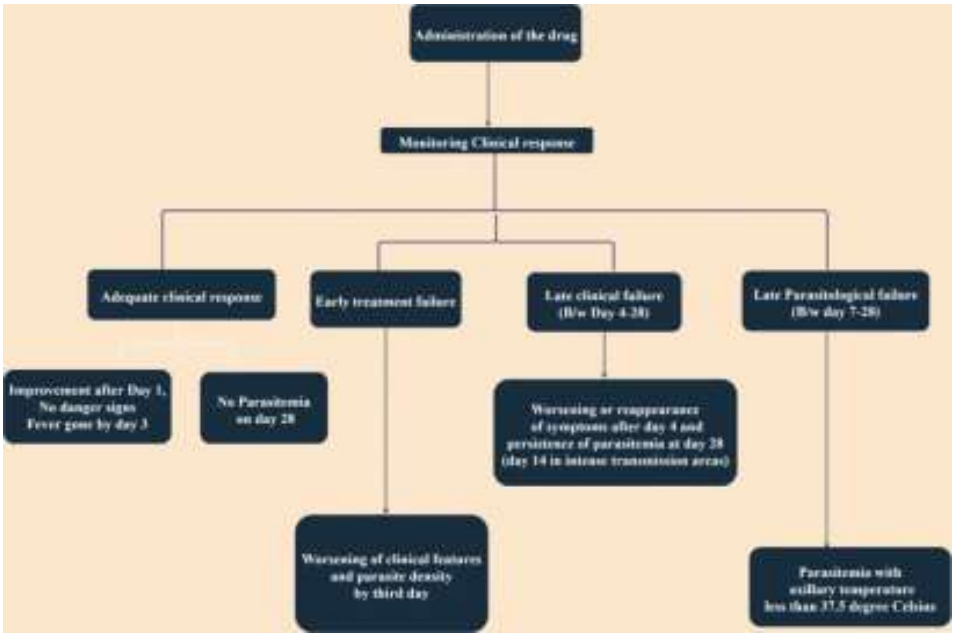


Figure 5: Detection of antimalarial resistance

3. MODALITIES FOR PREVENTION OF DRUG RESISTANCE

There are two approaches for preventing antimalarial drug resistance. First would be focused on the reduction in the development of drug resistance, and second would be aimed at preventing malaria. The first approach leads to a decrease in drug resistance as fewer cases mean less consumption of drugs and less probability of resistant parasites being passed on to new hosts.

3.1 Reduction in Overall Drug Pressure:

The most significant factor that causes drug resistance is 'drug pressure'. There is an urgent need to restrict the use of drugs. Along with this, improvement in the diagnosis of malaria is the single most important factor that can dramatically decrease drug resistance. Unfortunately, a high number of patients keep receiving drugs for malaria that can be avoided if diagnosed properly. Diagnostic tools such as rapid antigen tests or microscopy will decrease the number of unnecessary antimalarial drug treatments, which in turn will lead to a lower probability of exposure to sub-therapeutic levels of drug in the blood. The advantages of presumptive treatment have to be weighed against the problem of drug resistance that it exposes the population to. Presumptive treatment is mostly effective in areas where cost is the determining factor for using diagnostic tools. It is argued that the antimalarial drugs could be made more efficient via policy-mediated decrease in drug pressure, but defining the association among policy for drug pressure, treatment practices, and drug resistance is quite a challenge [44], [45].

3.2 Improvement in the Usage of Drugs.

The usage of drugs with single-dose regimens, such as mefloquine and SP, makes directly observed therapy (DOT) possible and helps with the issue of non-compliance. In this light, there is an urgent need to compare the benefits of single-dose drugs of drugs with long half-lives. In addition to that, there should be close follow-up of the patients undergoing treatment. Here again, the need for proper diagnostic tools has to be stressed so that treatment failure in patients can be identified quickly. These patients can be treated again, thus reducing the possibility of the spread of drug resistance [46]. The malaria treatment programme cannot be successful unless the public is educated regarding its use, as the prompt and timely use of malaria treatment leads to a reduction

in severe cases. The drug can be highly effective, but would not be of much help if not used optimally. Educating the public is also necessary because traditional beliefs, illiteracy, suspicion, and passive attitudes can act as major roadblocks for the effective implementation of these programmes [47], [48].

3.3 Combination Therapy

Another approach that has been gaining currency these days to counteract drug resistance in antimalarial drugs is using drug combinations. For instance, amodiaquine, SP, or mefloquine can be used in combination with artemisinin derivatives, which are effective against a broad range of the developmental stages of the parasite. The transmission rates of malaria in some parts of Thailand and sub-Saharan Africa have been reported to decrease upon use of combination therapy. However, there is a lot of scepticism about combining drugs having such different half-lives. Another concern is the use of individual components for monotherapy. The benefits incurred on account of combination therapy will be lost due to unofficial and indiscriminate usage of the component drug [49], [50].

4. Conclusions And Future Perspectives

The fight against malaria is an ongoing battle, and continued efforts are needed in the future against antimalarial drug resistance until malaria is completely eradicated. Also, the problem of antimalarial drugs will keep on persisting as long as drugs are being used against malaria. P. falciparum is resistant to practically all existing antimalarial drugs, and it is expected that it will ultimately develop resistance to any drug that is used broadly. The design of novel drugs against malaria is not able to catch up to the speed at which resistance is developed. For instance, in Southeast Asia, resistance to antimalarial drugs is faster compared to the 12 to 17 years it takes to develop and market a new antimalarial compound. In addition to that, in a poor country like Africa, the affordability of the drug is also a major issue. There is an urgent need to develop diagnostic tools such as rapid antigen tests or microscopy because they will reduce the number of needless antimalarial drug treatments, leading to a reduction in malaria cases. New approaches to reduce the development of drug resistance, coupled with novel strategies to prevent malaria, are needed.

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Conflict of interest: The authors declare no conflict of interest.

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Synthesis of Cerium Doped Rare-Earth Silicate Ceramic and its Characterisation

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Abstract:

Cerium doped gadolinium silicate powder in two different phases namely oxyorthosilicate (GSO) and pyrosilicate (GPS) were synthesized by solid state sintering and solution combustion method. Synthesized powder was used for making ceramic by vacuum hot-pressed method applying the pressure of 4-6 ton at temperature of 1500°C for two hoursin the vacuum of $2x10^{-6}$ mbar. Heat treatment were given to vacuumed hot pressed ceramic in different atmospheric condition and its effect on structural and optical properties were studied using XRD, photoluminescence and scintillation spectra.

Key words: *Gadolinium Silicate, Scintillation, Ceramic, luminescence*

I. Introduction

Gadolinium Silicates doped with Cerium are very good scintillation material owing to its high density, robust, non-hygroscopic properties [1-5]. Scintillating materials in the form of single crystal are ideal for the detection of nuclear radiation. However, due to high cost and time-consuming growth processes necessary for single crystals, other alternative options like glass-ceramics and composites have been explored in the past. These glass-ceramics and composites suffer from problems of low light-yield relative to crystalline materials. Polycrystalline optically transparent ceramics (OTC) having a density greater than 99.99% that of the single crystal area better option, with light output greater than glass-ceramics, composite and comparable to the single crystals [6,7]. The OTC may be useful to fabricate efficient, high resolution radiation detectors. OTCs are made by a simplified method consisting of mechanical compaction and heat treatments [8]. In addition, problems associated with the single crystals like the growth of incongruently melting materials, incorporation of the activator homogeneously, making large size and different shapes can be overcome in OTC by using the single phase, uniformly dispersed polycrystalline powder. Preparation of the OTC is economical and an easier alternative to the single crystal and research and development is being carried out to make good quality OTC of different materials [7].

For a ceramic to be transparent, it should be pore-free, optically isotropic, should have no secondary phases. Materials with a cubic crystal structure are optically isotropic and have single index of refraction. So the great deal of development has taken place in preparing OTC of materials with cubic crystal structures (e.g.Y3Al5O12,Lu2O3:Eu, CaF2: Mn, Eu, etc.) [6-8]. In ceramics from optically anisotropic crystals (non-cubic), an additional scattering of light arises on the boundaries because of their arbitrary crystallographic orientation. Modern scintillator materials of current interest that have a non-cubic crystal structure, the preparation of their OTC will be a challenging task. To fabricate an OTC of a non-cubic polycrystalline material, initial powder grain size is an important factor along with the compaction and heat treatment in different medium. Transparent ceramics requires highly dispersed and high sinterable powders [9]. It is

reported that the powder having an optimum distribution of crystallite size (submicron) demonstrated success in the development of OTC of hexagonal alumina, hydroxyapatite, monoclinic Lu2SiO5, etc. [9].

Here we tried to explore the possibility of preparing polycrystalline ceramic of gadolinium silicate materials using the polycrystalline powder synthesized by different methods and subsequent heat treatment to improve the translucency of the ceramics and their structural and optical characterizations.

2. Synthesis and Characterization

Uniaxial hot press was used to prepare pellets of Gd_2SiO_5:Ce (GSO) and $Gd_2Si_2O_7$:Ce (GPS). Initial powder materials were synthesized by two different routes to study the effect of the synthesis method on the ceramic formation. One route is solid state sintering of the mechanically mixed initial oxides [Gd_2O_3& SiO_2(Alfa Aesar, 99.99%)]having submicron grain size. Other is solution combustion route in which the nitrates of gadolinium and cerium were first dissolved in deionized water in an appropriate molar concentration and then the fuel Glycine ($C_2H_5NO_2$(Cisco Lab, India, 99.5%)) and fumed silica (Sigma Aldrich, average particle size nearly 14 nm)were added to the aqueous solution of nitrates [10-11]. The mixed solution was kept under constant stirring at nearly 70–80°C until a transparent viscous gel was formed. The resultant gel precursor was placed in a preheated furnace at 580°C. After the thermal equilibrium was reached, the gel self-ignites resulting in white powder. The Ce doping was kept as 0.5 At. % and 5 At. % for GSO and GPS respectively. The as-obtained powder was heat treated at different temperatures from 1000°C to 1600°C for different time durations in an air with a heating/cooling rate of 300°C/h.

For synthesis of ceramic 15-10 g of the synthesized powder (depending upon the material density) was taken in a graphite die (25 mm dia) and loaded inside the vacuum chamber of a Hind High Vacuum (HHV) hot-press. First, the chamber was evacuated to of 2x10−6 mbar pressure then the temperature was raised to 1500◦C in 5hours. After achieving the temperature, a load of 4-6 ton was applied on the material for two hours and the pellet was cooled down to room temperature at the rate of 500◦C/h.

The XRD measurements were carried out using Cu Kα X-ray source (λ = 1.54Å) in the 10–65 range (2θ) on a diffractometer (Rigaku Mode-lRINT-2000).Photoluminescence (PL) spectra were recorded in the range 200–700 nm in reflection geometry by positioning the samples at 45° with respect to the excitation beam. For measurements in the spectral domain, a continuous Xe lamp was used as the excitation source. The PL measurements were carried out using an Edinburghmake FLP-920 spectrometer and a low temperature measurement set-up (OxfordModel: Optistat-DN). The recorded luminescence spectra were corrected for thespectral sensitivity function of the instrument.

3. Results and Discussions

3.1 Effect of sintering

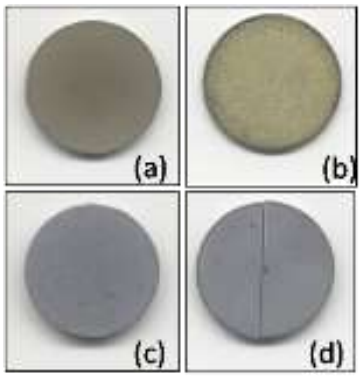


Fig.1 Photograph of GSO (a,b) and GPS (c,d) HPP prepared using powder synthesized by solid state (left) and solution combustion method (right).

Fig.1 shows photograph of the hot-pressed pellets (HPP) of GSO, GPS prepared from the powder synthesized by solid state sintering and solution combustion method. These pellets were then cut, polished and then heat treated in air, vacuum and again in air to see the effect of the annealing on the translucency of the hot-pressed pellets. Also, to see the effect of reducing and oxidizing heating environment on the luminosity, as in reducing medium percentage of the activator (Ce) going in the Ce^{3+} state which is luminescence center increases compared to the Ce^{4+} which quenches the luminescence through the non-radiative de-excitation. Hot pressed pellets without any heat treatments (unheated) are dark in color mostly due to the oxygen vacancies and may also be due to the carbon (from the graphite die) introduced during the vacuum hot pressing stage. In case of the GSO the darkness is uniform throughout the pellet, while in case of the GPS the pellets are dark only on the surface while inside it is white in color. Dark color of the HPP when heated in the air at 1100°C for 35 h turns into the white as shown in the Fig. 2 due to the refilling of the oxygen vacancies, and elimination of the carbon particles. Further these unheated and initially air heated HPP are heated in the vacuum at 1050°C for 48h shown in Fig. 3a. Vacuum heating of the pellets result in the dark pellet in both the cases of unheated and initially air heated pellets. This confirms that the darkness of the HPP is majorly due to the oxygen vacancies. This vacuum heated dark pellets again reheated in air at 1100 °C for 35 h, to check the reversibility of the creation and filling of the oxygen related vacancies and as shown in Fig.3b these reheated pellets in air turn into the white color indicating that these processes seem to be reversible in nature. Further, it needs to confirm from the structural and luminescence studies presented in following sections.

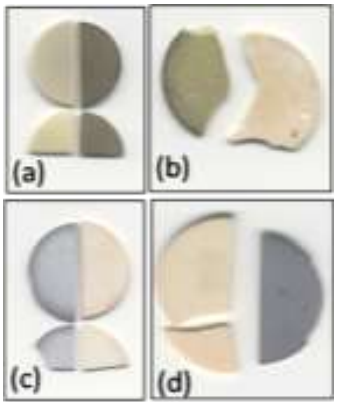


Fig.2 Photograph of GSO (a,b) and GPS (c,d) HPP heated in air at 1100°C for 35 h prepared using powder synthesized by solid state (left) and solution combustion method (right), along with the unheated pellets dark in color.

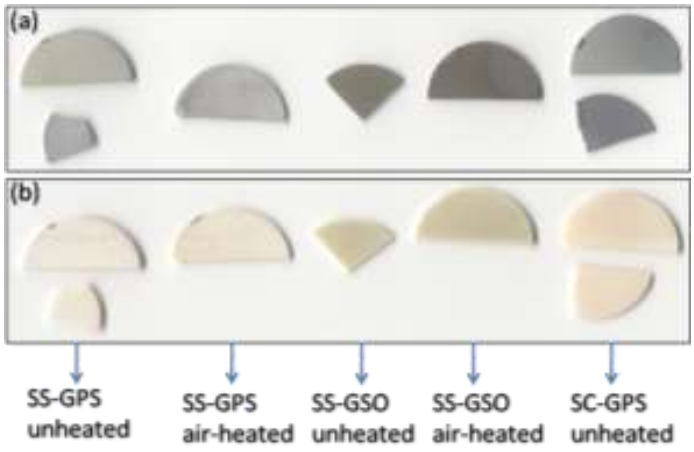


Fig.3 Figure 6.10: photographs of GSO and GPS HPP (as-prepared and air annealed) heatedin vacuum at 1050◦C for 48 h (a) and then in air at 1100◦C for 35 h (b); preparedusing powder synthesized by solid state (SS) and solution combustion (SC) method.

3.2 Structural characterization

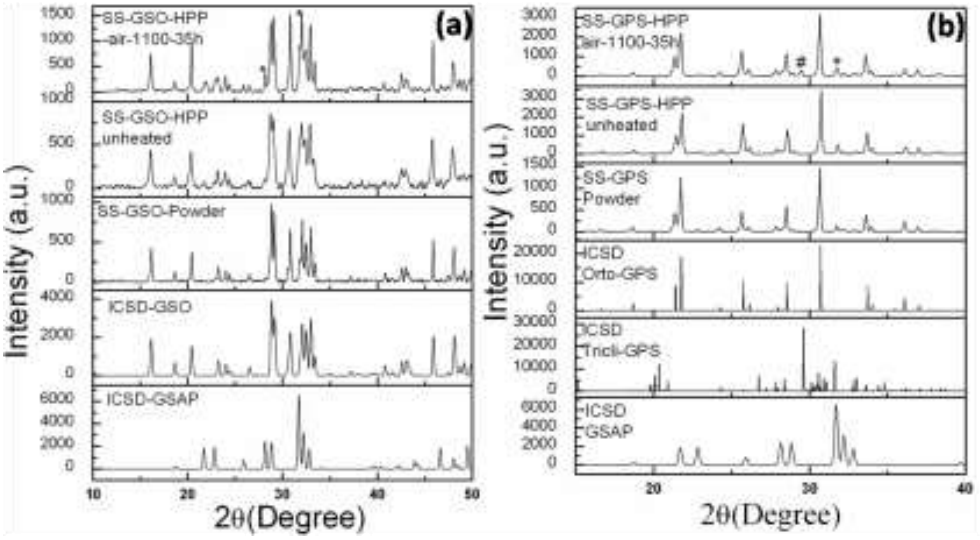


Fig.4 XRD pattern of HPP prepared using solid state sintering (SS) of (a) GSO and (b)GPS

To see the effect of fabrication processes and post sintering on structure of the HPP its XRD were carried out as shown in the Fig.4 and Fig.5 for the HPP prepared using solid state sintering (SS) and solution combustion (SC) respectively, along with the synthesized powder and ICSD for comparison. It can be seen that the unheated HPP shows the structure similar to the synthesized powder with small proportion of the additional peaks corresponding to the hexagonal $Gd_{4.67}(SiO_4)_3O$ (indicated by-*), except HPP prepared using GSO powder synthesized using the SC method showing phase other than GSO (may be due to some chemical residue in the synthesized powder). While HPP heat treated in air at 1100°C for 35 h show that peaks corresponding to (hexagonal) GSAP evolve in both the case of GSO and GPS. In case of GPS small intensity of the peak corresponding to the triclinic GPS (marked as #) is observed. Further we also studied the HPP heat treated in the Vacuum at 1050°C for 48 h shows the structural changes corresponding to the GSAP phase (which is reported to be the stable phase in the gadolinium silicate family) in both the cases of GSO and GPS [11]. During the fabrication process (1500°C for 2 h in 4-6 ton pressure) HPP did not show the structural changes but the long duration (at 1050°C for 48 h) of the vacuum heating shows the structure changes.

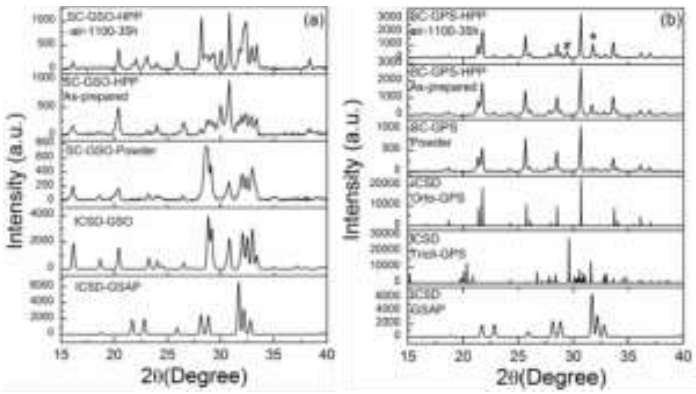


Fig.5 XRD pattern of HPP prepared using solution combustion (SC) of GSO (a) and GPS (b)

3.3Photo-luminescence and Radio-luminescence studies

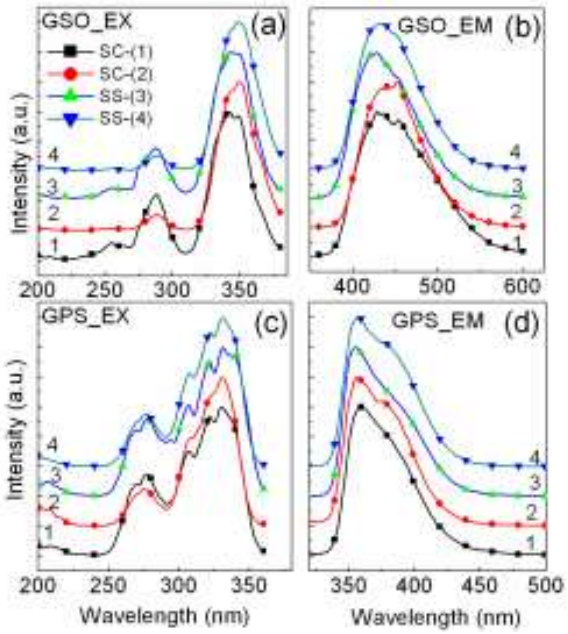


Fig.6 Excitation (left) and emission (right) spectra of the as-prepared (1, 3) and air annealed (2, 4) GSO:Ce (a, b) and GPS (c, d) HPP prepared using the powder synthesized by solid state (SS) and solution combustion (SC) methods.

Photo-luminescence studies of the as-prepared HPPs as well as of those annealed in air (at 1100°C for 35 h) are carried out. The photo-luminescence excitation (EX) and emission (EM) spectra of the samples are shown in the Fig.6. They show the characteristic luminescence of the monoclinic GSO:Ce (Fig.6.13 a and b) and orthorhombic GPS:Ce (Fig.6 c and d) phases. HPPs annealed in air show increased luminescence intensity compared to as-prepared dark pellets due to reduced oxygen related defects. In both the cases the emission peaks could be fitted in two Gaussian peaks corresponding to the transition from the lowest 5d level to two spin-orbit split 4f ground state namely $^2F_{7/2}$ and $^2F_{5/2}$ of Ce^{3+}. Annealing of pellets in air enhances the emission component at the higher wavelength, leading to a slight shift in the emission peak to the higher wavelength. The excitation spectrum shows three bands at 255, 290 and 350nm in case of GSO. While in case of GPS it shows two prominent bands at 280 and 330nm. Intensity of the higher energy excitation bands reduces after the heat treatment in air compared to the as-prepared HPP. These observations of change in luminescence properties due to annealing process are due to change in the relative numbers of $Ce^{3+}$and Ce^{4+} centers [12-14]. In addition to the photo-luminescence, radio-luminescence (RL, theX-ray excited luminescence) was also studied.

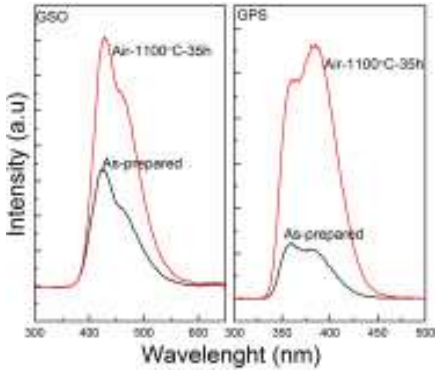


Figure 7: Radio-luminescence spectra of the as-prepared and air annealed GSO and

GPS, HPP fabricated from powders prepared using the solid-state sintering route.

The RL spectra of the as-prepared HPPs of GSO and GPS (Fig.7) shows that, the air annealing significantly affects the luminescence intensity. The annealed samples were twice more luminescent than the as-prepared samples. This can again be attributed to the reduction of the oxygen related vacancies that result in the enhancement of the luminescence intensity.

The scintillation properties of the HPP were studied by mounting them on a PMT and output pulse was recorded for the as-prepared and air annealed GSO and GPS, HPPs using a ^{137}Cs gamma-ray source. Scintillation decay of the GPS (Fig.8) shows the average decay time of 90 ns and 40 ns for the as-prepared and air annealed pellets. This further indicates that the oxygen related defects may be responsible for the longer decay time in the as-prepared HPPs compared to the air annealed pellets. In case of the as-prepared HPPs of GSO we could not obtain any detectable pulse, which may be attributed to the lower light output of the GSO than GPS.

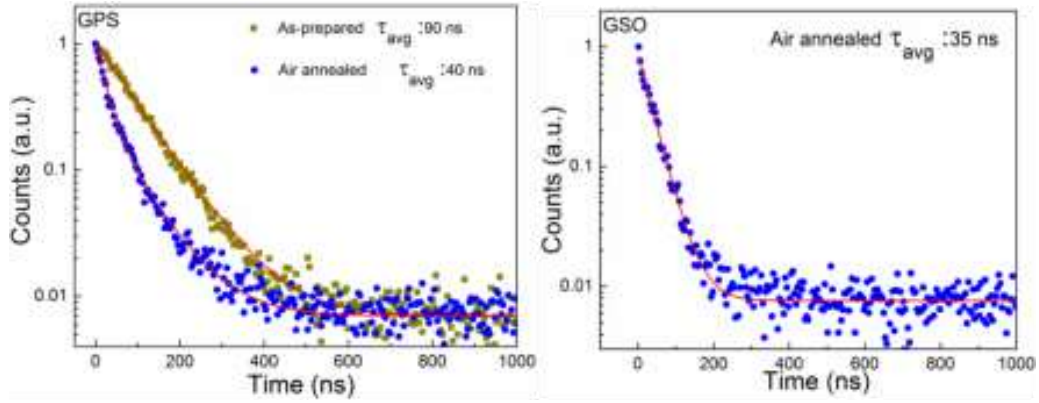


Figure 8: Scintillation decay of the GPS and GSO HPP.

4. Conclusion

The possibility to prepare optically translucent ceramics of gadolinium silicates, by uniaxial vacuum hot-pressing of the synthesized GSO and GPS polycrystalline powder (solid state and solution combustion route) was explored. Hot pressed pellets were prepared applying the pressure of 4-6 ton at a temperature of 1500°C for two hours. The hot-pressed pellets showed the phase similar to the initial synthesized phase, except for the GSO powder synthesized by solution combustion method. As-prepared hot-pressed pellets were dark in color. The darker color of pellets was traced to the oxygen related defects that reduces the luminescence intensity and increases the scintillation decay time. Oxygen defects were eliminated by a heat treatment in air that resulted in translucent ceramics. These translucent ceramics exhibited an enhancement of the luminescence intensity and faster decay time compared to the as-prepared dark pellets.

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Phytochemical Profile of Leguminous Seeds: A Comprehensive Review

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Abstract:

Leguminous seeds are a vital source of nutrition and bioactive compounds with significant health benefits. Leguminous seeds, including beans, lentils, peas, and chickpeas, are an essential component of the human diet. They serve as a primary source of protein, dietary fiber, and essential micronutrients. Beyond their macronutrient composition, leguminous seeds are rich in phytochemicals, which have garnered considerable interest due to their health-promoting properties. They contain a diverse range of phytochemicals, including phenolic compounds, flavonoids, tannins, saponins, and alkaloids, which contribute to their antioxidant, antimicrobial, and anti-inflammatory properties. This review study provides an in-depth analysis of the phytochemical composition of leguminous seeds, their health implications, and potential applications in functional foods and pharmaceuticals. This review aims to summarize current knowledge on the phytochemical constituents of leguminous seeds and their biological significance.

Keywords: *Leguminous seeds, Phytochemistry, bioactive compounds.*

Introduction:

Leguminous seeds, such as soybeans, lentils, and chickpeas, are rich sources of bioactive compounds that contribute significantly to human health. These seeds contain phenolic compounds, oligosaccharides, phytosterols, saponins, and carbohydrates, which exhibit various health-promoting properties. For instance, isoflavones found in soybeans act as phytoestrogens and have been associated with potential protective effects against hormone-related cancers. Similarly, lignans present in seeds like flaxseeds possess antioxidant properties that may help in reducing the risk of chronic diseases. Additionally, saponins in legumes have been shown to exhibit cholesterol-lowering and immune-boosting effects. The diverse array of bioactive compounds in leguminous seeds underscores their role as nutraceuticals, offering multiple health benefits beyond basic nutrition.

Comprehensive Review:

Leguminous seeds play a vital role as nutraceuticals in human health. These seeds provide proteins and other important components including minerals, B-complex vitamins and other vital

health-protective compounds (Grela *et al.*, 2017). In addition to this, these seeds have a broad range of bioactive compounds *viz.* phenolic compounds, oligosaccharides, phytosterols, saponins and carbohydrates. According to Thi and Nguyen (2021), legumes are known for their high levels of bioactive compounds. Some of these compounds are used in plant defense mechanisms against predators and environmental conditions. *Bioactive compounds* are *secondary metabolites found* in *small quantities* in *various plants (Kris-Etherton et al., 2002).*

Bioactive compounds have multiple effects on the plant itself and other organisms. They induce and regulate many physiological activities like flowering, fruit setting and abscission, signal deciduous behavior and maintain perennial growth. More than 50,000 secondary metabolites have been discovered in the plant kingdom (Teoh, 2015). Phytochemistry is the branch that takes into account plant-produced chemicals especially secondary metabolites which are synthesized as a measure of UV exposure, self-defense and environmental hazards. Phytochemical investigations provide information on secondary metabolites about their structural compositions, biosynthesis, functions and mechanisms of action in living systems and also their medicinal, industrial and commercial applications. Drug discovery and the development of novel therapeutic agents against diseases need a proper understanding of phytochemicals. The study of phytochemicals has been significant in the discovery of new plant natural products of commercial value in various industries (Egbuna *et al.*, 2018).

Thi and Nguyen (2021) stated that phenolic compounds are very commonly found in legume seeds. This is a huge group of secondary metabolites, chemically it contains at least one benzene ring with one or more hydroxyl substituents and its complexity ranges from simple phenolic molecules to highly polymerized compounds (Lin *et al.*, 2016). The primary phenolic compounds observed in the seeds of legumes are phenolic acids, condensed tannins and flavonoids (Singh *et al.*, 2020 and Amarowicz, 2020). Duenas *et al.*, 2006 observed that these compounds are primarily found concentrated on the seed coats (chiefly flavonoids).

Depending upon chemical structure Thi and Nguyen (2021) observed two types of phenolic acids hydroxybenzoic acids and hydroxycinnamic acids in legume seeds. Condensed tannins, also known as proanthocyanidins (PACs), chemically are oligomeric and polymeric flavonoids. Sancho *et al.* (2015) recorded a high concentration of condensed tannins in black beans, lentils and red beans. Singh *et al.* (2017) noted that flavonoids are the main phenolic compound found in legumes. The presence of flavonoids affects the flavor and colour of common beans (Yang *et al.*, 2018).

In legumes, saponins are found to consist of a triterpenoid aglycone (sapogenin) linked to one or more oligosaccharide moieties. They can absorb free radicals and activate antioxidant enzymes. Soyasaponins are the most common saponins among legumes (Thi and Nguyen, 2021). Guajardo-Flores *et al.* (2012) reported the highest concentration of saponins in the hilum portion than the seed coat or cotyledon part of the seeds. Saponins have been estimated in many edible legumes like chickpeas, lupins, fenugreek, soybeans, lentils, and various beans (Mercedes Muzquiz *et al.*, 2012, Barakat *et al.*, 2015, Navarro *et al.*, 2018 and Moreno-Valdespino *et al.*, 2020).

Phytosterols are structurally similar to cholesterol and occur in a variety of plants (Zhang *et al.*, 2018 and Woyengo *et al.*, 2009). A wide range of biological potentials is attributed to them. Cereal grains, grain legumes, nuts and vegetable oils are rich sources of phytosterols. Ryan *et*

al. (2007) reported β-sitosterol in lentils to be a common component in plants followed by stigmasterol and campesterol.

Carbohydrates are an essential component of legume seeds and have a bioactive property to cure chronic diseases. Barman *et al.* (2018) and Venkidasamy *et al.* (2019) stated that chickpeas are good sources of carbohydrates, such as dietary fiber, starch, and oligosaccharides. The research on Pigeon peas showed that they have a high content of carbohydrates. Black gram beans were found to possess mucilaginous polysaccharides in addition to dietary fiber.

Dietary fiber (cell wall material) is a useful food component synthesized by the combinations of polymeric non-starch substances like cellulose, hemicellulose and pectin. Khan, *et al.* (2007) stated that in the human gastrointestinal tract dietary fibers are resistant to enzymatic digestion. The content of dietary fiber in legume seeds varies from species to species. Guillon and Champ (2002) reported a lower level of dietary fiber in cotyledon than in testa.

Legume seed is the chief source of resistant starch (RS). It is an indigestible component for humans. According to Nigudkar and Madan (2017) in legume seeds, resistant starch concentrations are higher than in cereals and many tubers. Singh *et al.* (2020) studied RS content of white beans, kidney beans, peas, lentils and cowpea.

Oligosaccharides such as raffinose, stachyose, ciceritol and verbascose are found to be present in many legume seeds. These components are undigested in the human gut. Fan *et al.* (2015) discovered more concentrations of raffinose, stachyose and verbascose in seed cotyledons as compared to the seed coat.

Many leguminous seeds were screened for their bioactive constituents from time to time. Seeds of *Cajanus cajan* were analyzed for the presence of various phytochemicals. Nanna *et al.* (2013) reported the presence of bioactive compounds alkaloids, glycosides, tannins, flavonoids and steroids in various extracts used for phytochemical tests. Sahu *et al.* (2014) found the presence of alkaloids, tannins, flavonoids and saponins in various extracts derived from seed powder. Maria *et al.* (2017) carried out phytochemical screening of ethanolic extracts of various seeds belonging to different families including *Albizia multiflora* and *Piscidia carthagenensis* of Leguminosae and reported various bioactive compounds. Aswathi and Abdussalam (2020) detected the presence of saponins, cardiac glycosides, tannins, terpenoids, phenols, coumarins, flavonoids, and phlobatannins in petroleum ether extract of seeds of *Canavalia rosea.*

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Rare Earths in Clean Energy Systems: A Comprehensive Review of Applications, Supply Risks, and Alternatives

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Introduction

Rare Earth Elements (REEs) are a group of 17 chemically similar metals, including the 15 lanthanides, scandium, and yttrium. Their unique electronic and magnetic properties make them critical for various high-tech applications, particularly in clean energy technologies such as wind turbines, electric vehicles (EVs), and energy storage systems. The increasing global demand for REEs is driven by the transition towards renewable energy and electrification. However, their supply remains a significant challenge due to geopolitical constraints, economic volatility, and environmental concerns [1].

China dominates the global REE market, accounting for over 60% of global mining and nearly 90% of processing capacity. This concentration raises concerns regarding supply security, particularly for countries dependent on REE imports. In response, several nations have initiated policies to diversify their supply chains, promote recycling, and invest in alternative materials. However, challenges persist, including low recycling rates, high processing costs, and the environmental impact of extraction technologies. Conventional REE extraction is energy-intensive and environmentally damaging, often involving hazardous chemicals and generating radioactive waste. Recent advancements in bioleaching, solvent extraction, and secondary resource recovery have demonstrated potential in reducing environmental impact. However, the economic feasibility and scalability of these methods remain uncertain [2].

This review provides a comprehensive assessment of REE applications in clean energy, supply chain risks, and emerging strategies for sustainable extraction and recycling. By addressing these aspects, this study aims to highlight key challenges and opportunities in securing a stable and sustainable REE supply for the clean energy transition [3].

2. Role of Rare Earth Elements in Clean Energy

2.1 REEs in Wind Turbines and Electric Vehicles

The clean energy transition is heavily dependent on the unique magnetic properties of rare earth elements (REEs), particularly in the production of high-performance permanent magnets. Wind turbines and electric vehicles (EVs) utilize neodymium-iron-boron (NdFeB) magnets, which are essential for achieving high energy efficiency and power density. Neodymium (Nd), praseodymium (Pr), and dysprosium (Dy) are fundamental to these applications, with projected demand expected to rise significantly due to the widespread deployment of renewable energy and electrification of transportation.

Wind turbines incorporating NdFeB magnets contain approximately 171 kg of REEs per MW of capacity. This dependence on REEs is driven by the need for strong, lightweight materials that enable direct-drive turbines, which improve reliability and reduce maintenance compared to gearbox-based alternatives. The inclusion of dysprosium (Dy) in these magnets enhances thermal stability, allowing them to function under extreme operational conditions.

Electric vehicles similarly rely on NdFeB magnets for traction motors, where the combination of Nd, Pr, Sm, Dy, and Tb ensures high torque density and efficiency. Hybrid

vehicle technologies, in particular, integrate REEs for both electric propulsion and regenerative braking systems, further underscoring their indispensable role in modern transportation.

2.2 REEs in Energy Storage, Batteries, and Hydrogen Technologies

Beyond their applications in magnetics, REEs are integral to advanced energy storage technologies. Nickel-metal hydride (NiMH) batteries, widely used in hybrid electric vehicles, incorporate La, Ce, Nd, and Pr, which enhance hydrogen storage capacity and prolong battery lifespan. NiMH batteries exhibit a wide operational temperature range (-30°C to 70°C) and currently account for 57% of hybrid and electric vehicle battery usage worldwide, making them a critical component of energy-efficient transportation.

In addition to battery applications, hydrogen technologies also rely on REEs. Yttrium (Y), cerium (Ce), and lanthanum (La) are utilized in solid oxide fuel cells (SOFCs) and hydrogen storage materials, improving catalytic efficiency and long-term stability. Furthermore, REEs such as Dy, Nd, Tb, Eu, and Y contribute to high-performance lighting and fuel cells, reinforcing their role in reducing the carbon footprint of emerging energy systems.

The strategic importance of REEs in clean energy underscores the need for secure and sustainable supply chains. As demand escalates, addressing challenges related to resource availability, recycling, and alternative materials will be critical to ensuring long-term technological advancement and energy security [4].

3. Supply Risks and Economic Challenges

3.1 Geopolitical Control and Market Volatility

- China holds 48.3% of the world's REE reserves and accounts for 97% of global REE production, creating a near-monopoly.
- The United States was the leading producer of REEs until the 1980s, after which China took control, and U.S. production only resumed in recent years.
- China has implemented export restrictions and quota reductions, officially citing environmental concerns, but these policies also influence global REE prices.
- The 2010 diplomatic dispute between China and Japan over the Senkaku/Diaoyu Islands resulted in sharp reductions in Chinese REE exports, demonstrating the geopolitical sensitivity of REE supply chains.
- The European Commission and the U.S. Department of Energy have classified REEs as critical raw materials due to their economic importance and supply risks.

3.2 Price Trends and Economic Implications

- The global REE market is highly volatile, with prices experiencing dramatic fluctuations between 2008 and 2011 due to China's export restrictions.
- Between 2011 and 2019, prices of La and Ce dropped significantly from $150/kg to below $15/kg, making recycling economically less viable.
- Heavy REEs such as Dy, Nd, and Tb have seen price increases since 2020, with Tb reaching $1,450/kg in 2021.
- China's dominance in REE production and its ability to influence prices create challenges for global industries reliant on these materials.
- Market projections estimate the REE sector will grow to $9.6 billion by 2026, reflecting increasing demand from clean energy technologies [5].

4. Environmental and Sustainability Concerns

4.1 Mining and Processing Impacts

- REE mining is associated with severe environmental risks, including soil erosion, water contamination, and air pollution.
- Rare earth ores often contain radioactive thorium and uranium, posing health and environmental hazards.

- Managing and disposing of hazardous chemical byproducts from REE production is a major challenge, contributing to environmental strain.
- Extraction processes, such as leaching and solvent-based separation, require large amounts of chemicals, leading to toxic waste generation.

4.2 Life-Cycle Assessment and Environmental Footprint

- Life-cycle assessment (LCA) studies indicate that REE extraction is energy-intensive, contributing to high greenhouse gas emissions.
- REE production generates significant solid waste, requiring improved waste management strategies.
- The environmental impact of REE mining can be mitigated through advanced recycling and sustainable resource management.
- Current LCA studies mostly rely on outdated datasets from the 1990s, highlighting the need for updated, region-specific assessments [6].

5. Recycling and Secondary Sources for Rare Earths

5.1 Recycling from Spent Magnets, Batteries, and Industrial Waste

- Recycling of rare earth elements (REEs) from secondary sources such as battery waste, scrap alloys, spent magnets, spent catalysts, waste LEDs, and fly ash is gaining momentum as a sustainable alternative to primary mining.
- Hydrometallurgical processes, including chemical and bioleaching, followed by solvent extraction, are widely used for the separation and recovery of REEs.
- The recovery of REEs from end-of-life permanent magnets has been demonstrated using selective leaching and precipitation techniques.
- The recycling of Nickel-Metal Hydride (NiMH) batteries offers an efficient means of recovering critical REEs such as lanthanum (La), cerium (Ce), neodymium (Nd), and praseodymium (Pr).
- A circular economy approach can help mitigate supply risks by integrating REE recovery from industrial byproducts.

5.2 Advances in Recovery Technologies

- Recent advancements in REE recycling have focused on solvent extraction, electrochemical recovery, and plasma-based separation techniques.
- Bioleaching has emerged as a promising low-energy alternative for REE extraction from waste phosphors and industrial residues.
- The recovery of REEs from waste LEDs and fluorescent lamps is increasingly viable through selective precipitation and ion-exchange processes.
- Supercritical fluid extraction and ionic liquid-based separation methods are being explored as environmentally friendly alternatives to traditional hydrometallurgical routes [7].

6. Alternative Materials and Technological Innovations

6.1 Potential Substitutes for Critical REEs

- The European Union and the United States are actively researching alternative materials to replace rare earth elements (REEs) in magnets, phosphors, and catalysts.
- La and Ce are being tested as partial substitutes for Pr and Nd in NdFeB magnets to mitigate supply risks.
- Several iron-nitride-based and manganese-aluminum (MnAlC) magnets are under development as non-REE alternatives, though challenges remain in achieving comparable performance.
- Research on organic-based phosphors for LED applications aims to reduce reliance on REEs such as europium (Eu) and terbium (Tb).

6.2 New Materials and Emerging Technologies

- Advances in high-entropy alloys (HEAs) are being explored as potential replacements for REE-based materials in high-performance applications.
- Superconducting materials, such as yttrium barium copper oxide (YBCO), have been proposed as alternatives to REE-based permanent magnets.
- The use of artificial intelligence (AI) and computational materials design is accelerating the discovery of novel compounds that could replace or reduce the dependence on REEs.
- Graphene-based materials are emerging as substitutes for REE-containing catalysts and electronic components [8].

7. Policy Frameworks and Global Strategies

7.1 National and International Policies on REE Sustainability

- The European Commission has classified REEs as critical raw materials and has developed policies aimed at ensuring supply security and sustainability.
- The U.S. Department of Energy (DOE) and the U.S. Geological Survey (USGS) have identified REEs as essential for clean energy and have prioritized research into domestic extraction and processing.
- China, the dominant REE supplier, has imposed export restrictions and quota reductions, significantly impacting global markets.
- Policies such as REE stockpiling and strategic reserves have been implemented by Japan and South Korea to reduce dependency on imports.
- The World Trade Organization (WTO) has ruled against China's export restrictions on REEs, highlighting the geopolitical tensions surrounding these materials.

7.2 Circular Economy and Resource Diversification

- Circular economy strategies emphasize REE recovery from waste streams, including electronic waste, end-of-life magnets, and industrial byproducts.
- The European Union has introduced resource efficiency and eco-design policies aimed at reducing REE consumption through material substitution and recycling.
- The U.S. Department of Defense has invested in REE recycling programs to enhance domestic supply resilience.
- Research initiatives in REE separation and reprocessing technologies are being funded by multiple governments to support circular economy principles.
- The transition toward closed-loop supply chains is seen as essential to mitigating the environmental impact of REE extraction [9].

8. Future Perspectives and Research Directions

8.1 Innovations in REE Mining and Processing

- Advances in bioleaching have demonstrated potential for REE extraction with reduced environmental impact, utilizing microbial processes instead of harsh chemical reagents.
- The development of supercritical fluid extraction techniques has improved the efficiency of REE recovery from waste materials and ores.
- High-entropy alloys (HEAs) are being investigated as potential substitutes for conventional REE-based materials, offering enhanced performance in extreme environments.
- Selective crystallization methods using metal-organic frameworks (MOFs) have shown promise in separating individual REEs with high precision.
- Sustainable mining strategies are focusing on REE extraction from coal ash and red mud, utilizing secondary resources to reduce dependence on primary mining.

8.2 Role of Artificial Intelligence and Advanced Materials

- Artificial intelligence (AI) and machine learning (ML) are being applied to optimize REE discovery, processing, and material substitution, accelerating the identification of novel compounds.
    - Computational materials science is enabling the design of new REE-free magnetic materials, reducing reliance on Nd, Dy, and Tb.
    - AI-driven models are improving the efficiency of REE separation technologies, minimizing waste and enhancing recovery rates.
    - Research on graphene-based catalysts is exploring their potential to replace REE-containing catalysts in industrial applications.
    - Advanced recycling technologies incorporating plasma arc processing and hydrometallurgical innovations are enhancing REE recovery from electronic waste [10].

9. Conclusions

9.1 Summary of Key Findings

Rare earth elements (REEs) are indispensable in modern clean energy technologies, playing a critical role in wind turbines, electric vehicles, energy storage, and hydrogen technologies. However, their supply chain is fraught with challenges, including geopolitical control, price volatility, and severe environmental impacts. China's dominance in REE production underscores the urgency for diversified sourcing strategies, while fluctuations in REE prices pose economic risks for industries reliant on these materials.

Environmental sustainability remains a pressing concern, as REE extraction generates substantial ecological damage due to toxic waste and radioactive byproducts. Life-cycle assessments emphasize the need for more sustainable mining and processing techniques, while advances in recycling and secondary resource recovery offer promising avenues for reducing primary extraction dependence. Despite these efforts, current recycling rates remain critically low, necessitating further investment in innovative recovery technologies.

The exploration of alternative materials and technological advancements is reshaping the REE landscape. Research into high-entropy alloys, iron-nitride magnets, and organic-based phosphors presents potential substitutes, mitigating supply constraints. Simultaneously, artificial intelligence (AI) and machine learning (ML) are revolutionizing material discovery, extraction optimization, and recycling efficiency, further bolstering supply chain resilience.

9.2 Implications for the Future of Clean Energy and REEs

The transition to a sustainable clean energy future hinges on securing a stable and responsible REE supply chain. Circular economy principles must be integrated into REE management through enhanced recycling initiatives, waste recovery, and material substitution. Policymakers worldwide must foster international collaboration, develop strategic reserves, and promote R&D funding for alternative materials and advanced processing technologies.

Innovations in REE extraction, including bioleaching and supercritical fluid techniques, offer environmentally sustainable pathways for REE production. Additionally, the rise of AI-driven predictive models in mining and material science will accelerate the discovery of novel REE alternatives, reducing dependency on traditionally mined resources.

Ultimately, the intersection of policy, technological innovation, and responsible resource management will dictate the future trajectory of REE sustainability. A holistic approach—encompassing economic diversification, scientific advancements, and global cooperation—is essential to balancing clean energy demands with long-term resource security.

9.3 A Broader Perspective: Beyond REEs in Clean Energy

While the discourse on rare earth elements (REEs) primarily revolves around clean energy technologies, their significance extends far beyond wind turbines and electric vehicles. The same supply chain vulnerabilities, environmental risks, and geopolitical tensions that define the

REE industry are also shaping the future of quantum computing, space exploration, and advanced biomedical devices. As society accelerates toward a future of interconnected digital infrastructure and deep-space missions, the strategies we develop today for sustainable REE sourcing will not only determine the success of clean energy transitions but will also dictate the trajectory of next-generation technological frontiers. Addressing REE challenges now is not merely about energy security—it is about ensuring humanity's ability to innovate, explore, and redefine the limits of possibility.

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Eco-Friendly Polymers: Recent Progress in Renewable and Recyclable Materials"

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Abstract

The reliance of polymers on fossil fuels and the sustainability concerns around plastic waste have led to ongoing research advancements in the field of environmentally friendly polymers and polymer composites during the past ten years. Materials made from renewable, recycled, and waste carbon resources, as well as their mixtures, are known as sustainable polymers. These materials can eventually be recycled, biodegraded, or composted. Throughout their life cycle, sustainable polymers also show less of an impact on the environment. Biodegradable or biobased (derived from renewable resources) polymers or their composites are found in environmentally friendly polymers. Their carbon-neutral lifecycle may lessen carbon dioxide emissions and reliance on petroleum-based products, which would lessen the environmental impact of humans. The creation of environmentally friendly polymer materials, or "green materials," must undoubtedly be given top priority by both academia and industry due to the current growing environmental problems and the depletion of crude oil. In actuality, chemists, physicists, and engineers who understood the need of creating ecologically friendly materials have achieved the notable advancements in this field. These days, biopolymers are regarded as one of the most promising materials to address these environmental issues. They continue to perform worse in terms of processability and end-use application, nevertheless. At the moment, blending is a highly economical way to improve the ductility and impact resistance of biopolymers. Additionally, several lignocellulosic materials are being investigated for use as reinforcing fillers in polymer matrices in order to improve overall qualities, lessen their impact on the environment, and save money.

Keywords: sustainable polymers bio-based polymers, biodegradable polyesters, carbon-neutral lifecycle, wood plastic composites, natural additives and fillers, composites characterization,

Introduction:

In order to prepare standard polymers, a significant amount of fossil fuels, such as natural gas and oil, are typically needed as raw materials. This not only strains the finite supply of fossil energy, but it also increases resource consumption. Furthermore, a significant amount of waste materials was produced during the production and usage of conventional polymers; these materials are typically not properly handled or recycled, leading to significant pollution and adverse environmental effects. Over the past few decades, the production of plastics and polymer resins has grown dramatically [1]. There has been significant worry recently on the high toxicity and non-biodegradability of synthetic plastics due to their mass manufacture and overuse for human comfort and convenience. As a result, single-use plastics will unavoidably be banned in 2021 [2], [3], [4], and [5]. Since polymer have numerous qualities [6], such as being lightweight, having adjustable strength and elasticity, being easy to shape and color, having adjustable

transparency, being thermally and electrically insulated, and many more, polymers, or plastic items, have become a part of modern society. Numerous applications profitably take advantage of these features. Foams for cushions and mattresses or various surface coverings, flexible films for packaging, rigid sheets for completed two-dimensional items, fibers for textiles and ropes, shock-absorbing joints, and assembling agents like coatings, adhesives, sealants, and elastomers are a few examples. Different combinations of characteristics are needed for these diverse applications. Composites are created by reinforcing polymers with robust materials like glass or carbon fibers, which can further reach very demanding applications. Given the real-world applications of sustainability, it is essential to comprehend the distinctions between various polymer kinds and the established criteria that validate their environmental claims. There are more goods and materials that advertise themselves as "green" or ecologically friendly as a result of the increased focus on sustainability. However, because different standards and criteria are employed to evaluate sustainability, there is frequently uncertainty over the veracity of these statements [7]. Biodegradable plastic is a type of plastic capable of breaking down into organic compounds, CO_2, H_2O, and other biomass under the influence of microorganisms in natural conditions or under biological treatment. The degradation time of biodegradable plastic is typically much shorter than that of conventional plastics, ranging from several months to a few years. According to a 2018 UN report, 127 nations had passed legislation governing plastic bags, [8] had restricted or outlawed the production of single-use plastics (SUP) and certain plastic materials, and 63 had implemented extended producer responsibility laws for SUP (Single-Use Plastic). Thirty-five countries encouraged the use and production of biodegradable polymers as part of the particular material composition standards for plastic bags [9]. Since then, a variety of biodegradable plastics have attracted a lot of interest from the public and are frequently viewed as innovative and promising solutions to the plastic dilemma. An overview of the most popular biodegradable polymers available today will be given in this book chapter.

Different types of biodegradable plastics

Sr. No.	Name of polymer	Resources
1	Polylactic acid (PLA)	Corn starch, cassava roots, potato chips, or sugarcane
2	Polyhydroxyalkanoate	Natural fermentation of sugars or lipids by bacteria.
3	Polybutylene succinate (PBS)	biological sources.
4	Polyvinyl alcohol (PVA)	Vinyl Acetate
5	Cellulose Acetate (CA)	Cellulose, a natural polysaccharide found in plants.
6	Polyglycolic Acid (PGA)	Sugar beets, sugarcane, and corn.
7	Polymer Materials Based on Lignin	Corn starch, potatoes, and cassava, or from fossil-based materials, such as petroleum.

1. Polylactic acid (PLA)

A form of biodegradable plastic called polylactic acid (PLA) is made from renewable resources such sugarcane, cassava roots, corn starch, and potato chips. Because PLA is a thermoplastic, it can be heated and shaped into a variety of forms[10]. The application of PLA given in fig. 1

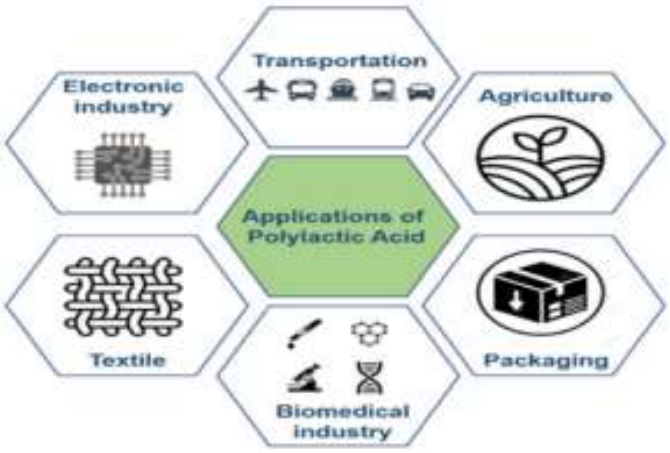


Fig. 1

2. Polyhydroxyalkanoate (PHA)

A form of bioplastic called polyhydroxyalkanoate (PHA) biodegradable plastic is produced when bacteria naturally digest carbohydrates or lipids. It is composed of R-hydroxy alkanoic acid-based polyesters. It has many advantages over traditional polymer such as,

- Biodegradability: In soil, water, or the ocean, PHA can fully biodegrade into CO_2, H_2O, and biomass. This reduces pollutants in the environment and safeguards human health.
- Renewable Raw Materials: Sugars, starches, vegetable oils, and other renewable resources are used to make PHA. This offers a long-term remedy for the problem of the depletion of fossil fuels.
- Good Physical and Chemical Properties: PHA has qualities including strength, flexibility, and resistance to impact that are comparable to those of conventional plastics. Because of this, PHA can be applied to a wide range of situations.

The different application is given in fig. 2

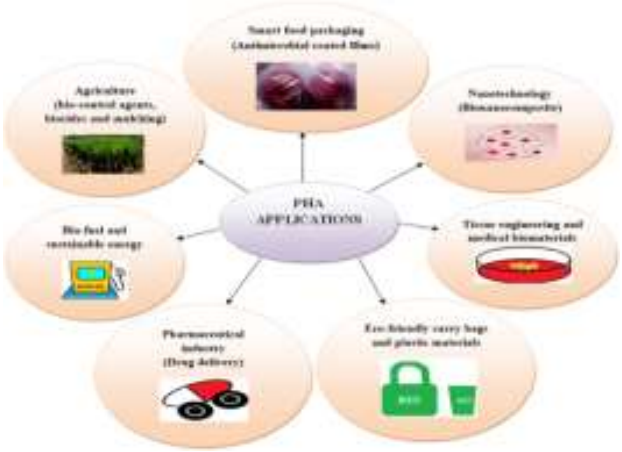


Fig. 2

3. Polybutylene succinate (PBS)

The thermoplastic biodegradable polyester known as polybutylene succinate (PBS) is made from biological sources. PBS is a kind of plastic that doesn't pollute the environment because it can be fully biodegraded by microorganisms in the natural environment into carbon dioxide and water. The natural raw resources used to make PBS include: One form of alcohol made from corn, potatoes, sugarcane, and other is, 1,4-butanediol. An organic acid made from corn, sugarcane, and other plants is succinic acid.

Applications:

- Packaging: PBS is utilized in shopping bags, agricultural mulch films, and food packaging films, Plant pots and other agricultural applications.

items for Hygiene: It can be utilized in the manufacturing of items for hygiene. Additional Uses: PBS can be used to blends and composites to enhance mechanical performance, gas-barrier qualities, and thermal conductivity.



Fig. 3

4. Polyvinyl Alcohol (PVA)

Polyvinyl alcohol (PVA) is a water-soluble, synthetic polymer with a wide range of applications, including in adhesives, coatings, textiles, and biomedical applications, known for its biocompatibility and biodegradability. Vinyl acetate is used to make polyvinyl alcohol (PVA), a biodegradable material. Since it is a synthetic polymer, smaller chemical units are used to create it. Vinyl acetate, which has the chemical formula CH_2=CHOCOCH$_3$, is the unit of measurement for PVA. It is used in various applications, including:

- Paper manufacturing
- Paint and coating production.
- Textile fibre production

- Glue and adhesive manufacturing.
- Production of medical products
- Packaging product manufacturing



Fig. 4

5. Cellulose Acetate (CA)

A form of biodegradable plastic called cellulose acetate (CA) is made from cellulose, a naturally occurring polymer that is present in plants. Cellulose is processed with acetic acid and acetic anhydride to create CA. By creating acetate bonds between cellulose molecules, this method renders them soluble in organic solvents like tetrahydrofuran and acetone. CA is a flexible and adaptable material because of its many special physical and chemical characteristics. It is a material that is flame-resistant, waterproof, strong, and lightweight. It is a good option for electronic applications because it is also a poor electrical conductor.



Fig. 5

5. Polyglycolic Acid (PBA)

   The most basic linear aliphatic polyester is polyglycolic acid. It is a thermoplastic and biodegradable polymer. It can be made from glycolic acid via ring-opening polymerization or polycondensation. Polyglycolic acid has been recognized as a potent fiber-forming polymer since 1954.

   PGA has various applications, including:

- Packaging: PGA can be used to manufacture bags, boxes, and other packaging materials. It is a sustainable alternative to traditional plastic packaging because it can biodegrade and does not contain harmful chemicals.
- Medical: PGA is used in various medical applications, such as sutures, screws, and patches. It biodegrades within the body, eliminating the need for surgical removal.
- Industrial: PGA finds use in industrial applications, including electronic components and construction materials. It boasts high strength and corrosion resistance.

6. Polymer material based on Lignin.

   Numerous benefits were demonstrated by lignin, including a high carbon content that may be converted into carbon materials and composites, a large number of functional groups, strong biocompatibility, and low toxicity. Lignin-based materials are frequently utilized in electrical devices, energy storage, the environment, and other sectors. They are typically inexpensive and environmentally friendly. An organic polymer called lignin has the potential to be imported as a raw material for the chemical and biological sciences sectors. With a heating value comparable to carbon, lignin, the second most abundant renewable biopolymer on Earth, is the second-biggest renewable source of carbon and one of the largest natural renewable sources of aromatic structures.

   Examples of lignin-based polymers:

- Phenolic Resins: Lignin can be used as a substitute for phenol in the production of phenol-formaldehyde resins, which are used as wood adhesives.
- Polyurethanes (PUR): Lignin can be used as a macromonomer or a blending filler for PURs, improving their performance and reducing reliance on petroleum-based polyols.
- Epoxy Thermosets: Lignin can be used to create high-performance epoxy thermosets from biomass.
- Other Applications: Lignin can also be used in the production of other bio-based polymer materials, including carbon fiber, hydrogels, and nanocomposites.



Fig. 6

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Integration of Smart Technologies in energy conservation: a path towards sustainable development

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Abstract:

Understanding the significance of sustainable development is essential for tackling pressing global issues, including climate change, resource scarcity, and inequality. These challenges are at the core of global agendas like the United Nations Sustainable Development Goals (SDGs), which emphasize the need for clean, affordable energy and immediate climate action. In response, smart technologies have gained prominence as innovative tools to improve energy efficiency and minimize environmental impact. The decline of traditional energy sources, coupled with growing ecological concerns, has accelerated the shift toward greener alternatives. Smart systems—ranging from IoT devices and AI-powered analytics to automated energy management and smart grids—are central to this transformation. By harnessing real-time data and intelligent automation, these technologies help reduce energy waste and support sustainable practices. This paper explores how adopting smart technology contributes to energy conservation and advances key SDGs, demonstrating a vital link between technological innovation and sustainable development.

Keywords: *Sustainable Development, Sustainable Development Goals, Energy Conservation, Smart Technology.*

Introduction:

The concept of sustainable development gained global prominence through the Brundtland Commission's 1987 report, which emphasized the importance of balancing economic progress, environmental care, and social well-being to support both current and future generations. This approach integrates economic development, social inclusion, and environmental stewardship into a unified framework. Contemporary global issues such as climate change, biodiversity decline, and rising inequality underscore the urgency of sustainable policies and long-term planning. In response, the United Nations launched the 2030 Agenda in 2015, introducing 17 Sustainable Development Goals (SDGs) to guide nations in addressing global challenges including poverty, climate change, gender equity, clean water, and sustainable energy.

A critical component of achieving these goals is energy conservation, which plays a key role in protecting the environment, fostering economic resilience, and ensuring social fairness. Strategies such as enhancing energy efficiency, embracing renewable sources, and encouraging responsible energy behavior are essential. In this context, smart technologies—enabled by real-time data, automation, and intelligent systems—emerge as powerful tools to streamline energy use, minimize waste and advance sustainability across various sectors.

Literature Review :

Researchers like Gungor, V. C., Sahin, D., Kocak have presented a comprehensive review of the communication technologies and standards essential for the development and deployment of smart grids for optimizing energy use, reducing waste, and enhancing the efficiency of energy systems across residential, commercial, and industrial sectors. [1]

The paper written by Batty in 2012 provides an interdisciplinary vision of smart cities, exploring how urban systems can be enhanced through ICT, data analytics, and sensing technologies. It frames the "smart city" as a complex system driven by real-time data, modeling and digital interaction between citizens and infrastructure. [2]

Fang et al. (2012) emphasize that intelligent grid technologies enhance demand-side management, allowing consumers to make informed decisions and reduce unnecessary energy consumption. [3]

Borgia (2014) explains how centralized control systems in smart cities manage traffic flow, street lighting, waste management, and public utilities in a more energy-efficient manner. These systems not only reduce the urban energy footprint but also improve quality of life for residents. [4]

Automation leads to significant reductions in energy waste. Home Energy Management Systems (HEMS), as examined by Zhou et al. (2016), utilize these smart devices to monitor usage patterns and recommend energy-saving behaviors to users. [5]

IoT-enabled sensors and actuators collect real-time data and automatically adjust lighting, temperature, and appliance usage based on occupancy and environmental conditions explained by Alam et al., 2017. [6]

Khan et al. (2018) note that through advanced analytics, organizations can benchmark energy performance, identify inefficiencies, and develop tailored conservation strategies. Predictive analytics, in particular, enables proactive system maintenance and load forecasting, preventing energy losses associated with equipment failure or peak demand surges. [7]

Ahmad et al. (2020) demonstrate that AI algorithms can forecast energy demand, detect anomalies, and suggest efficient energy distribution strategies. These technologies are particularly beneficial in industries, where energy-intensive processes can be dynamically controlled to minimize energy consumption without compromising productivity. [8]

Overall, the literature affirms that smart technologies offer immense potential for improving energy conservation across sectors. By enabling real-time monitoring, intelligent control and predictive optimization, these technologies align with global sustainability goals. Future research should focus on addressing implementation challenges and exploring cross-sectoral integrations of smart technologies to maximize their impact.

Research Methodology : Secondary data will be acquired from government reports, academic publications, research papers, and energy databases. Data on renewable energy capacity, energy generation, investment patterns, and environmental implications will be obtained to assist the quantitative study.

Discussion:

I. Smart Technologies and their role in energy conservation:

Smart technologies refer to advanced systems and devices that utilize sensors, data analytics, automation, smart grids, artificial intelligence (AI), machine learning (ML) and Internet of Things (IoT) to perform tasks autonomously, adaptively and efficiently. These technologies are integral to enhancing the functionality, sustainability and responsiveness of modern infrastructures.

All these smart systems rely on vast data collected from interconnected devices, which are processed through cloud platforms and edge computing to support instant decision-making. Overall, smart technologies represent a paradigm shift toward automation, connectivity and sustainability, offering transformative potential across multiple sectors by promoting resource efficiency, cost reduction and enhanced quality of life. The role of smart technology in energy conservation is described below.

A. Role of Sensors in Energy Conservation:

Sensors are fundamental to improving energy efficiency, as they generate essential data used to track and optimize energy consumption in real time. Whether in homes or industrial facilities, they monitor variables such as temperature, light intensity, movement, electrical flow, and room occupancy. This information supports smart energy management systems (EMS) that adapt lighting, heating, and ventilation based on actual conditions and user behavior. For instance, motion detectors can deactivate lighting or HVAC systems when a space is unoccupied, helping to reduce unnecessary energy use. In industrial settings, sensors aid in predictive maintenance by identifying irregularities—like unusual heat or vibrations—that might indicate inefficient machinery operation. Additionally, sensors are a key component of the Internet of Things (IoT), allowing devices to work together seamlessly to implement energy-saving actions. When paired with artificial intelligence and analytics, these systems can anticipate energy needs, spot inefficiencies, and refine consumption habits. Overall, sensors promote smarter energy use, greater efficiency, and environmental responsibility.

B. Role of Data Analytics in Energy Conservation:

Data analytics plays a transformative role in modern energy systems by turning vast volumes of data from smart meters, IoT devices, and digital infrastructure into actionable insights. These insights support energy usage monitoring, enabling the identification of peak demand periods, abnormal consumption patterns and energy-intensive operations. Through advanced techniques like time-series analysis and machine learning, stakeholders can optimize energy use, promote off-peak consumption, and implement effective load management strategies. Predictive maintenance powered by data analytics also allows for early detection of equipment inefficiencies, helping to avoid breakdowns and reduce energy losses. Moreover, demand forecasting helps align energy generation with real-time needs—especially crucial when integrating renewable energy sources like wind and solar—by improving storage and grid management.

Beyond operational optimization, data analytics enhances the functionality of smart buildings and grids through dynamic energy control based on occupancy and real-time conditions. Energy dashboards offer users insights that drive behavior change, while benchmarking tools identify underperformance and guide upgrades for greater efficiency. Real-time analytics also enable demand response initiatives, reducing grid stress during peak hours. Additionally, organizations can use data to link energy consumption to emissions, tracking and reducing their carbon footprint to meet sustainability targets and regulatory requirements. In essence, data analytics empowers a smarter, greener, and more efficient energy ecosystem.

C. Role of Automation in Energy Conservation:

Automation significantly contributes to energy efficiency by allowing systems to manage energy use intelligently without constant manual oversight. Technologies such as smart sensors, AI-driven controllers, and IoT-enabled devices ensure that energy is delivered only where and when it's

necessary. Examples include intelligent lighting systems, motion-activated controls, and adaptive climate systems that adjust based on occupancy and environmental conditions. In manufacturing and commercial settings, automation enhances operational workflows, controls motor speeds, and minimizes idle times to reduce energy use and costs.

Automated building systems also monitor and adjust lighting, HVAC, and other utilities in real-time by analyzing usage trends and external factors like weather. These systems support broader infrastructure goals, such as balancing energy demand in smart grids and shifting high-load activities to off-peak periods. Additionally, AI-enabled predictive maintenance monitors equipment health, allowing timely intervention before inefficiencies escalate. By reducing reliance on human intervention, automation enforces energy-saving behaviors consistently and helps embed sustainability into everyday operations.

D. Role of Smart Grid in Energy Conservation

A smart grid is a modernized electricity network that uses digital communication, sensors, automation, and real-time data analytics to improve how electricity is generated, distributed, and consumed. Unlike traditional grids, which operate in a one-way flow from producers to consumers, smart grids support two-way communication between energy providers and users. This interactivity allows for better energy management, enhancing both efficiency and conservation. Key features of smart grids include real-time monitoring and demand response. Through the use of smart meters and sensors, energy usage can be tracked continuously, enabling supply adjustments based on demand fluctuations. This minimizes electricity overproduction, especially during peak hours, and reduces strain on the grid through automated demand response programs. Additionally, smart grids play a pivotal role in integrating renewable energy sources such as solar and wind. By leveraging predictive analytics and weather forecasts, they can manage variability and optimize storage, reducing dependence on fossil fuel-based systems.[3,7]

E. Role of AI in Energy Conservation:

Artificial Intelligence (AI) plays a broad and transformative role in energy conservation, going beyond machine learning by incorporating decision-making, optimization, and automation. One of its key applications is in smart energy management systems that monitor real-time energy consumption and autonomously reduce or shut down non-essential loads, optimizing both the timing and quantity of energy used. In power grid management, AI is instrumental in analyzing large datasets from smart meters, historical trends, and weather forecasts to predict demand accurately. This enables efficient balancing of supply and demand while enhancing the integration and storage of energy. AI also supports smart homes by coordinating IoT-enabled devices such as thermostats, lights, and appliances, learning user behavior to automate and optimize energy-saving actions like running appliances during off-peak hours. [8]

In industrial settings, AI improves energy efficiency by identifying equipment faults or inefficiencies and adjusting operational schedules through reinforcement learning to conserve energy without impacting productivity. It also facilitates the use of renewable energy by forecasting outputs from sources like solar and wind, managing storage, and ensuring efficient energy flow within hybrid systems. In transportation, AI helps reduce energy consumption through traffic optimization, smart EV charging during non-peak times, and improved route planning for public and commercial transit. Additionally, AI empowers consumers by analyzing energy usage and billing data to offer personalized savings strategies. Some platforms even introduce gamified

approaches to encourage sustainable habits, promoting user engagement and long-term behavioral shifts toward energy conservation.

F. Role of Machine Learning in Energy Conservation:

Machine learning (ML) plays a pivotal role in advancing energy conservation by optimizing how energy is produced, distributed, and consumed across sectors. In smart grids, ML algorithms analyze data such as weather patterns, time of day, and historical consumption to forecast energy demand accurately. This predictive capability helps utility providers manage supply more efficiently, reduce overproduction, and facilitate the integration of renewable energy sources like solar and wind. Within buildings, ML enhances the efficiency of HVAC systems by recognizing occupancy patterns and adjusting temperature settings accordingly, thereby reducing unnecessary energy use and improving comfort. Additionally, ML is key to improving the performance of renewable systems by forecasting output, managing energy storage, and ensuring energy is dispatched at optimal times.

In industrial environments, ML algorithms help identify energy inefficiencies, detect malfunctioning equipment early, and optimize energy-intensive operations. This proactive approach minimizes energy waste and supports predictive maintenance strategies. The transportation sector also benefits, as ML improves route planning for logistics fleets, reduces fuel consumption, and enhances energy management in electric vehicles (EVs). On the consumer side, ML-based applications provide personalized energy-saving tips by analyzing individual usage trends. These tools can recommend optimal appliance usage times based on electricity pricing and detect high-energy-consuming devices. Collectively, machine learning empowers intelligent, data-driven energy management that significantly contributes to sustainability and carbon reduction efforts.

G. Role of IoT in Energy Conservation:

The Internet of Things (IoT) plays a vital role in promoting energy conservation by enabling real-time monitoring and automated control across residential, commercial, and industrial sectors. Through the deployment of smart meters and sensors, IoT systems can track electricity consumption as it occurs, offering both users and utility providers valuable insights into energy usage patterns. This real-time visibility allows for prompt adjustments to reduce waste. Additionally, IoT enables responsive control of lighting, heating, cooling, and appliances based on occupancy, time of day, and environmental conditions, ensuring energy is used only when necessary and improving overall efficiency.[4]

In industrial and commercial settings, IoT technology enhances operational performance by optimizing machinery use, reducing idle times, and streamlining energy-intensive processes. Smart building systems powered by IoT manage HVAC, lighting, and elevators more efficiently by operating them only as needed. IoT also facilitates two-way communication between consumers and the power grid, which supports demand response strategies by shifting or lowering energy use during peak periods. Moreover, the data collected by IoT devices can be analyzed using AI and machine learning to forecast energy demand, suggest conservation measures, and optimize energy storage. Overall, IoT provides the essential infrastructure for implementing intelligent, adaptive, and data-driven energy conservation strategies across diverse sectors.

2 .Contribution of Smart technologies to achieve sustainable development goal :

Smart technologies are strategically aligned with the United Nations Sustainable Development Goals (SDGs), offering innovative solutions that drive progress toward a more equitable,

sustainable, and efficient world. By leveraging artificial intelligence (AI), the Internet of Things (IoT), big data, and automation, these technologies contribute to multiple SDGs in transformative ways.

SDG 6: Clean Water and Sanitation

Smart technologies ensure more effective and sustainable water use. IoT devices embedded in water supply systems detect leaks early and continuously monitor water quality, preventing contamination and water loss. In agriculture, AI is used to optimize irrigation systems by adjusting water use based on weather and soil data, minimizing overuse. Additionally, smart sanitation solutions such as sensor-equipped toilets enhance hygiene in public spaces by monitoring cleanliness and usage. Together, these technologies improve water management, reduce wastage, and support better sanitation practices.

SDG 7: Affordable and Clean Energy

Smart technologies significantly contribute to the advancement of affordable and clean energy. Smart grids optimize the distribution of electricity by reducing transmission and distribution losses, improving system reliability. IoT sensors enable real-time monitoring of energy consumption, helping users and utilities to identify inefficiencies and reduce unnecessary usage. Additionally, AI is used to forecast the availability of renewable energy sources like solar and wind, allowing for their seamless integration into the power grid. These innovations collectively enhance access to energy, lower energy costs, and accelerate the shift toward renewable sources.

SDG 9: Industry, Innovation, and Infrastructure

Smart technologies are revolutionizing industries by making infrastructure more resilient and efficient. Predictive maintenance in smart factories minimizes equipment failures, reducing both downtime and energy waste. Digital twins—virtual replicas of systems—allow engineers to test and refine designs before physical implementation, saving resources and improving outcomes. The integration of 5G networks and edge computing enhances the responsiveness and efficiency of industrial IoT applications, driving innovation and facilitating the creation of sustainable, forward-thinking infrastructure.

SDG 10: Reduced Inequalities

Technology also plays a role in bridging social and economic divides. Smart platforms facilitate remote access to education and healthcare in rural and underserved areas, expanding essential services to those who need them most. AI-powered translation tools break down language barriers, supporting inclusion for marginalized communities. Mobile microgrids powered by renewable energy provide reliable electricity to remote regions, fostering energy equity. These initiatives ensure that technological progress benefits all segments of society, promoting broader social inclusion.

SDG 11: Sustainable Cities and Communities

In the pursuit of sustainable urban development, smart technologies play a vital role. Smart traffic management systems use real-time data to reduce congestion and vehicle emissions by dynamically rerouting traffic. Smart buildings use occupancy sensors and environmental data to adjust lighting, heating, and cooling automatically, minimizing energy waste. Furthermore, advanced waste management technologies track the fill levels of bins, allowing for efficient collection schedules and reducing fuel consumption. These innovations enhance urban living by boosting operational efficiency, reducing pollution, and improving residents' quality of life.

SDG 13: Climate Action

AI and sensor-based technologies provide powerful tools for addressing climate change. AI-driven models simulate future climate scenarios, helping policymakers craft effective environmental strategies. Sensor networks are deployed to monitor environmental indicators such as deforestation, carbon dioxide emissions, and urban heat levels. In industrial settings, automation and optimization technologies reduce energy consumption and emissions, supporting efforts to decarbonize production processes. These tools empower mitigation and adaptation initiatives through precise, data-driven insights.

3. A path towards sustainable development:

The Sustainable Development Goals (SDGs) function as a strategic blueprint for advancing sustainable development globally. Therefore examining the path toward sustainable development, it is evident that Sustainable Development Goals (SDGs) 6, 7, 9, 10, 11, and 13 collectively form an interconnected framework that addresses the essential pillars of environmental protection, social equity, and economic progress. Each of these goals tackles a distinct but complementary aspect of sustainability, making them pivotal to achieving a balanced and resilient future.Collectively, these goals address the complex interdependence between ecological sustainability, social equity, and economic development. By targeting key systems such as water, energy, industry, urban infrastructure, and climate, while simultaneously tackling inequality, these SDGs create an integrated pathway toward achieving a truly sustainable and inclusive global future.

4. Conclusion:

The integration of smart technologies into energy systems represents a transformative approach to addressing the global challenges of resource efficiency, climate change, and sustainable development. This research has highlighted how technologies such as artificial intelligence (AI), the Internet of Things (IoT), big data analytics, and smart grids are not only enhancing energy conservation efforts but are also enabling more intelligent, adaptive, and decentralized energy management. These innovations contribute significantly to reducing energy waste, optimizing renewable energy integration, and empowering consumers through data-driven decision-making.

Furthermore, the adoption of smart technologies aligns closely with multiple Sustainable Development Goals (SDGs), notably SDG 7 (Affordable and Clean Energy), SDG 9 (Industry, Innovation, and Infrastructure), and SDG 13 (Climate Action). By enhancing energy efficiency, supporting low-carbon transitions, and fostering inclusive innovation, smart energy systems serve as foundational enablers of sustainability across economic, environmental, and social dimensions. However, realizing their full potential requires addressing challenges related to digital equity, infrastructure investment, policy alignment, and data governance.

Despite these benefits, several challenges hinder the full-scale deployment of smart technologies. High initial costs, interoperability issues, cybersecurity risks, and the digital divide remain significant barriers. There is a need for robust policy frameworks, investment incentives, and public awareness campaigns to accelerate adoption and ensure equitable access.

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Photocatalytic Degradation Of Dyes

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Introduction

Water pollution is an escalating global issue, with industrial effluents being one of the major contributors. Many synthetic dyes are known to be toxic, carcinogenic, and mutagenic. When released into aquatic ecosystems without adequate treatment, they can significantly reduce light penetration, disrupt photosynthetic activity in aquatic plants, and pose serious health risks to aquatic organisms and humans alike. Therefore, the removal of dyes from wastewater before discharge into the environment is a critical step in sustainable water management.

In recent years, photocatalytic degradation has emerged as a highly promising technique for dye removal. This advanced oxidation process (AOP) harnesses light energy—typically from UV or visible light sources—to activate a semiconductor catalyst. The activated catalyst generates reactive oxygen species (ROS) such as hydroxyl radicals, which are powerful oxidants capable of decomposing dye molecules into harmless end products like carbon dioxide and water.

This book chapter aims to provide a comprehensive overview of the principles, materials, mechanisms, and applications of photocatalytic degradation for dye removal.

Mechanism of Photodegradation of Dyes

The generalized mechanism using a semiconductor photocatalyst (e.g., TiO2) is outlined below:

1. **Photon Absorption:** $TiO_2 + h\nu \rightarrow TiO_2 (e^- + h^+)$ (A photon excites an electron from the valence band to the conduction band, generating an electron-hole pair)
2. **Charge Carrier Migration and Reactions:**
   - $e^- + O_2 \rightarrow \bullet O^{2-}$ (Superoxide radical)
   - $h^+ + H_2O \rightarrow \bullet OH + H^+$
   - $h^+ + OH^- \rightarrow \bullet OH$ (Hydroxyl radical)
3. **Dye Degradation Reactions:**
   - Dye + $\bullet OH/\bullet O^{2-} \rightarrow$ Intermediates $\rightarrow CO_2 + H_2O$ + Mineral by-products

Each reactive species generated during the process contributes to the breakdown of dye molecules by attacking chromophoric groups and disrupting the molecular structure. This ultimately leads to decolorization and mineralization of the dye.

The photodegradation process is influenced by various factors including the nature of the dye, the type and properties of the catalyst, light intensity and wavelength, solution pH, temperature, and the presence of other substances such as salts or organic matter. Understanding the fundamental chemistry and physics of photodegradation is essential for designing efficient systems for dye removal.

Natural and Artificial Light Sources

The effectiveness of photodegradation processes is highly dependent on the light source used to activate photocatalysts. Light provides the necessary energy to excite electrons in the photocatalyst material, initiating a cascade of reactions that lead to the generation of reactive oxygen species (ROS) responsible for dye breakdown. Light sources can be broadly classified into natural and artificial categories.

1. Natural Light Sources

Solar irradiation is the most abundant and renewable light source available for photocatalysis. It includes ultraviolet (UV), visible, and infrared (IR) components, with UV accounting for about 5% and visible light approximately 45% of the total solar spectrum. While traditional photocatalysts like TiO2 primarily utilize UV light due to their large band gaps, newer materials and modifications aim to harness the broader visible spectrum.

2. Artificial Light Sources

Artificial light sources provide controlled and consistent illumination, making them ideal for laboratory studies and industrial applications. They include:

- **UV Lamps (Mercury Vapor, Low-Pressure, Medium-Pressure):** Emit UV-A, UV-B, or UV-C light. Effective for activating wide-bandgap semiconductors like TiO2 and ZnO. Commonly used in experimental setups due to their reliability.
- **Xenon Lamps:** Emit a broad spectrum resembling natural sunlight, including both UV and visible light components. Suitable for simulating solar light in lab-scale photocatalytic studies.
- **LEDs (Light Emitting Diodes):** Offer tunable wavelength output, high energy efficiency, low heat emission, and long lifespan. Widely used for visible-light photocatalysis, especially with doped or modified photocatalysts.
- **Laser and Monochromatic Sources:** Useful for specific mechanistic studies where controlled excitation at a precise wavelength is needed.

Photodegradation Materials and Catalysts

The selection of appropriate materials and catalysts is crucial for the effective photodegradation of dyes. Photocatalysts play a central role in harnessing light energy to generate reactive oxygen species (ROS) that degrade dye molecules. The ideal photocatalytic material should exhibit high photoactivity, chemical stability, low toxicity, affordability, and recyclability.

1. Semiconductor Oxides

Semiconductor metal oxides are the most commonly used materials due to their strong photocatalytic activity and availability. These include:

- **Titanium Dioxide (TiO2):** The most studied and widely used photocatalyst. It is non-toxic, chemically stable, and active under UV light. However, its large band gap (~3.2 eV) limits its efficiency under visible light.
- **Zinc Oxide (ZnO):** Similar in band gap and activity to TiO2 but with different surface properties. It is also prone to photocorrosion under prolonged irradiation.
- **Tungsten Trioxide (WO3):** Exhibits visible light activity and strong oxidative power, though it can suffer from stability issues in basic conditions.
- **Iron Oxide (Fe2O3):** Absorbs visible light and is abundant, but has low electron mobility, leading to higher charge recombination rates.

2. Carbon-Based Materials

Carbonaceous materials enhance photocatalysis by increasing surface area and promoting charge separation.

- **Graphene Oxide (GO):** Provides excellent conductivity and surface area, often used in composite photocatalysts.
- **Carbon Nanotubes (CNTs):** Serve as electron conduits that reduce charge recombination.
- **Activated Carbon:** Primarily used for adsorption but enhances photocatalysis when combined with semiconductors.

3. Metal-Organic Frameworks (MOFs)

MOFs are crystalline materials made from metal ions and organic linkers. They offer high surface areas, tunable porosity, and unique light-absorbing properties. MOFs can serve as standalone photocatalysts or as supports for semiconductor nanoparticles.

4. Doped Photocatalysts

Doping involves the introduction of foreign atoms into the semiconductor lattice to modify its electronic and optical properties.

- **Metal Doping (e.g., Ag, Fe, Cu):** Enhances light absorption and reduces recombination by trapping charge carriers.
- **Non-Metal Doping (e.g., N, C, S):** Narrows the band gap, allowing the catalyst to utilize visible light.
- **Co-Doping:** The simultaneous doping with both metal and non-metal elements provides synergistic effects for higher efficiency.

5. Composite and Heterostructure Photocatalysts

Combining two or more materials can lead to improved performance through synergistic effects:

- **TiO2/Graphene:** Combines the stability of TiO2 with the high conductivity of graphene.
- **ZnO/CdS:** Extends light absorption into the visible range and enhances charge separation.
- **g-C3N4/TiO2:** Utilizes visible light and forms a stable heterojunction for enhanced activity.

6. Green and Biogenic Catalysts

Recent studies have explored using natural materials or plant-mediated synthesis for environmentally benign photocatalysts. These include:

- **Clay minerals and natural zeolites** as supports.
- **Plant-extract-synthesized metal nanoparticles** with intrinsic photocatalytic properties.

In summary, the design and optimization of photocatalytic materials are key to improving dye degradation efficiency. The future of photocatalysis lies in the development of visible-light-active, cost-effective, and environmentally safe materials with high stability and reusability.

Analytical Techniques for Monitoring Degradation

Monitoring degradation, especially photodegradation, is crucial for understanding the stability, durability, and long-term performance of materials. Several analytical techniques are employed to study and quantify the degradation of materials. These techniques allow for the identification of chemical changes, physical alterations, and structural modifications that occur during the degradation process. Below is an elaboration of key analytical techniques for monitoring degradation:

1. UV-Visible Spectroscopy
2. Fourier Transform Infrared Spectroscopy (FTIR)
3. Thermogravimetric Analysis (TGA)
4. Differential Scanning Calorimetry (DSC)
5. X-ray Diffraction (XRD)
6. Gel Permeation Chromatography (GPC)
7. Mass Spectrometry (MS)
8. Scanning Electron Microscopy (SEM)
9. Atomic Force Microscopy (AFM)
10. Raman Spectroscopy
11. Electron Spin Resonance (ESR) or Electron Paramagnetic Resonance (EPR)

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Photocatalytic Performance of Mn-Doped TiO_2 Nanoferrites in the Removal of Emerging Organic Pollutants.

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Abstract:

Titanium dioxide (TiO_2) is known as a leading photocatalyst due to its high stability, non-toxicity, and strong oxidative potential. The photocatalytic efficiency is limited by a wide bandgap (~3.2 eV) and rapid recombination of photogenerated electron–hole pairs. To address these limitations, this chapter focuses on functionalization of TiO_2 by preparing its ferrites and doping with manganese. This engineered material has enhanced visible light absorption and suppress recombination, and as expected improved photocatalytic activity. The underlying reason for the change is attributed to multiple oxidation states of manganese which generates oxygen vacancies and mid-gap states facilitating charge separation and redox reactions critical for the degradation of organic contaminants.

The chapter presents a comprehensive synthesis strategies where sol-gel is the method employed for its simplicity and advantages like with morphology control and crystalline structure. Advanced characterization techniques such as XRD, SEM, TEM, UV-Vis DRS, PL spectroscopy, and BET analysis are required to understand the structural and electronic transformations induced by Mn incorporation. The photocatalytic performance of Mn-TiO_2 nanoferrites is systematically evaluated for the degradation of common pesticides, antifouling agents and industrial dyes under visible light. These findings underscore significant improvement in degradation rates and the potential of Mn-doped TiO_2 nanoferrites as sustainable materials for wastewater remediation, contributing to the development of eco-friendly treatment technologies for emerging organic pollutants.

Keywords: *Mn-doped TiO_2 nanoferrites, photocatalysis, wastewater treatment, organic pollutants, bandgap engineering.*

Introduction:

Water pollution due to industrial and agricultural activities has become a significant environmental concern. The presence of harmful organic contaminants such as pesticides, antifouling agents, and synthetic dyes in wastewater not only threatens aquatic life but also poses serious health risks to humans. Conventional wastewater treatment methods often fail to effectively remove these persistent pollutants. In this context, nanotechnology offers innovative and efficient solutions for environmental remediation [1,2].

Among the various nanomaterials, titanium dioxide TiO_2 stands out due to its remarkable photocatalytic activity, chemical stability, and non-toxicity. However, pure TiO_2 suffers from certain limitations, including a wide band gap (~3.2 eV) which restricts its photocatalytic activity to the UV region. To overcome this limitation, doping with transition metals such as manganese has emerged as a promising strategy [3]. Manganese (Mn) doping narrows the band

gap of TiO_2 thereby enhancing visible light absorption. The multifunctionality is introduced by incorporating ferrite part which promotes charge separation and reduces recombination rates.

This chapter focuses on Mn-doped TiO_2 nanoferrites, a hybrid material combining the photocatalytic properties of TiO_2 with the magnetic and electronic characteristics of ferrites.
We explore their synthesis and application in the degradation of pesticides, antifouling agents, and dyes in wastewater.

Background and Rationale:

The increasing use of pesticides in agriculture and antifouling agents in marine applications has led to their widespread presence in water bodies. Similarly, dyes used in textile, paper, and leather industries are among the most challenging pollutants to remove due to their complex aromatic structures and high stability. Traditional treatment methods such as adsorption, coagulation, and biological processes often fall short in eliminating these compounds completely [4,5].

Photocatalytic degradation offers a sustainable and efficient alternative. It involves the use of light-activated catalysts that generate reactive oxygen species capable of breaking down complex organic molecules into harmless end products. TiO_2 has been extensively studied for this purpose; however, its efficiency under natural sunlight is limited. Mn doping addresses this limitation by extending the absorption edge into the visible region [6].
Furthermore, combining TiO_2 with ferrites (e.g., $MnFe_2O_4$) introduces magnetic properties [7-8] enabling easy separation and reuse of the photocatalyst. This dual functionality makes Mn-doped TiO_2 nanoferrites highly attractive for real-world applications.

Synthesis of Mn-Doped TiO_2 Nanoferrites:

The method employed for the synthesis is sol-gel.
The precursors used are Titanium tetrachloride for TiO_2, Manganese nitrate for Mn, and Ferrite formation is induced by incorporating $Fe(NO_3)_3$.

Sr. No.	Method	Key Features	Advantages	Disadvantages
1	Sol-gel	Hydrolysis of metal alkoxides	High homogeneity, control over composition	Time-consuming, high-temperature calcining
2	Hydrothermal	High-pressure, high-temperature reaction	Uniform particles, high crystallinity	Requires autoclave
3	Co-precipitation	Simultaneous precipitation of metal ions	Simple, low-cost, scalable	Poor crystallinity
4	Microwave-assisted	Microwave irradiation for synthesis	Fast reaction, energy-efficient	Equipment cost

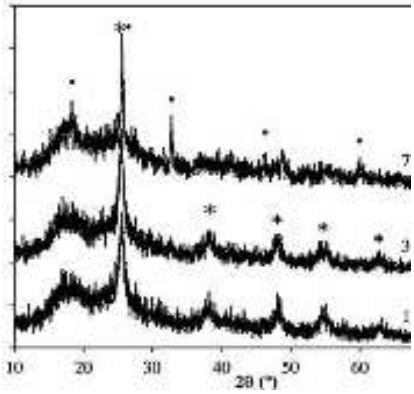
Table 1. Synthesis methods of Mn-doped TiO_2 nanoferrites.

Characterization:

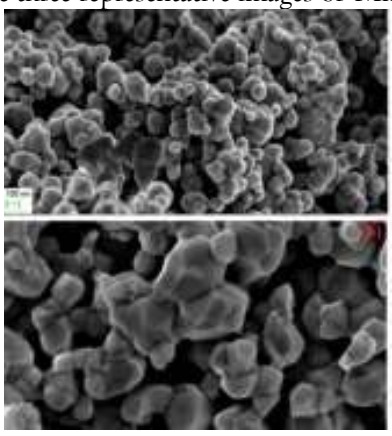
To confirm the formation of desired nanocomposite, the characterization techniques generally used are as follows:

1. **X-ray diffraction (XRD)**: Determines the crystal structure, phase purity, and crystallite size.

2. **SEM and TEM**: Provide information on morphology and particle size distribution.
3. **EDX**: Confirms the elemental composition and uniformity of Mn doping.
4. **UV-Vis DRS**: Assesses the optical properties and band gap.
5. **PL spectroscopy**: Evaluates charge carrier recombination.
6. **VSM**: Measures magnetic properties to confirm ferrite behavior.



Below are the three representative images of Mn-Doped TiO_2 Nanoferrites



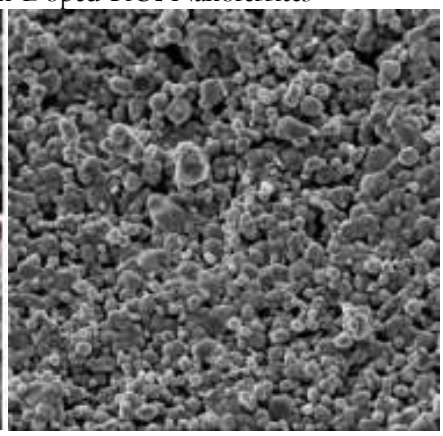


Figure 1. XRD pattern **Figure 2.** SEM **Figure 3.** TEM

To confirm successful doping and understand the physicochemical properties of Mn-doped TiO_2 nanoferrites, various characterization techniques are employed.

Application in Pesticide Degradation:

The material's performance in degrading common pesticides under visible light source is tabulated as observed.

Sr. No.	Pesticide	Time (min)	Degradation (%)
1	Chlorpyrifos	90	87
2	Atrazine	120	85
3	Carbofuran	75	81

Table 2. Photocatalytic degradation efficiency for selected pesticides.

Removal of Antifouling Agents:

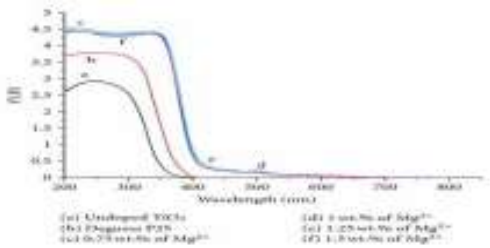


Figure 5. Degradation curve of TBT showing >80% removal under visible light.

Dye Degradation from Wastewater:

Sr. No.	Dye	Initial Conc. (ppm)	Time (min)	Degradation (%)
1	Methylene Blue	20	60	92
2	Rhodamine B	20	100	88
3	Methyl Orange	20	90	85

Table 3. Dye degradation efficiency using Mn-doped TiO_2 nanoferrites.

Environmental Impact, Reusability and Stability:

It is assumed that the synthesized material has low cytotoxicity and negligible ion leaching.
The magnetic nature of the material is beneficial in easy separation and repeated use. Though the required tests are under investigation.

Conclusion and Future Prospects:

Mn-doped TiO_2 nanoferrites combine visible-light activity, magnetic recoverability, and high photocatalytic performance. Future work is to optimize material design by optimizing synthesis methods, recyclability, exploring mechanism and biomedical applications along with the long term environmental impact needs to be thoroughly investigated.

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Foundations and Frontiers of Computational Chemistry

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Abstract:

This chapter offers a comprehensive exploration of computational chemistry, emphasizing both its theoretical foundations and modern advancements. Starting from the basic principles rooted in quantum mechanics, it outlines how methods like Hartree-Fock, Density Functional Theory (DFT), and Coupled Cluster theory enable accurate modeling of molecular systems. The discussion extends to classical approaches like molecular mechanics and molecular dynamics, which are indispensable for simulating large biomolecules and complex materials over realistic time scales. Key applications such as high-throughput virtual screening (HTVS) and machine learning–assisted property prediction are highlighted as transformative tools for accelerating drug discovery and materials design. The role of widely used platforms like Gaussian and Schrödinger is reviewed, showing how they integrate diverse computational techniques into practical workflows. Finally, the chapter stresses the importance of benchmarking and validation in ensuring the reliability of computational results, especially as AI and data-driven models become more common. Together, these methods demonstrate how computational chemistry is reshaping the way chemists approach research—moving from labor-intensive experimentation toward efficient, predictive, and scalable in silico discovery.

Keywords: *Computational chemistry, Hartree-Fock, Density Functional Theory, high-throughput virtual screening, Gaussian, Schrödinger*

Introduction:

Computational chemistry plays a pivotal role in accelerating the discovery of materials and drugs, understanding reaction mechanisms, and guiding experimental design as shown in Figure 1. For instance, high-throughput virtual screening (HTVS) and machine learning (ML) algorithms are increasingly integrated to analyze chemical space efficiently. According to von Lilienfeld et al. (2020), *"Machine learning is ushering in a paradigm shift*

in chemical research, where empirical knowledge is being supplemented by data-driven predictive models" (1).

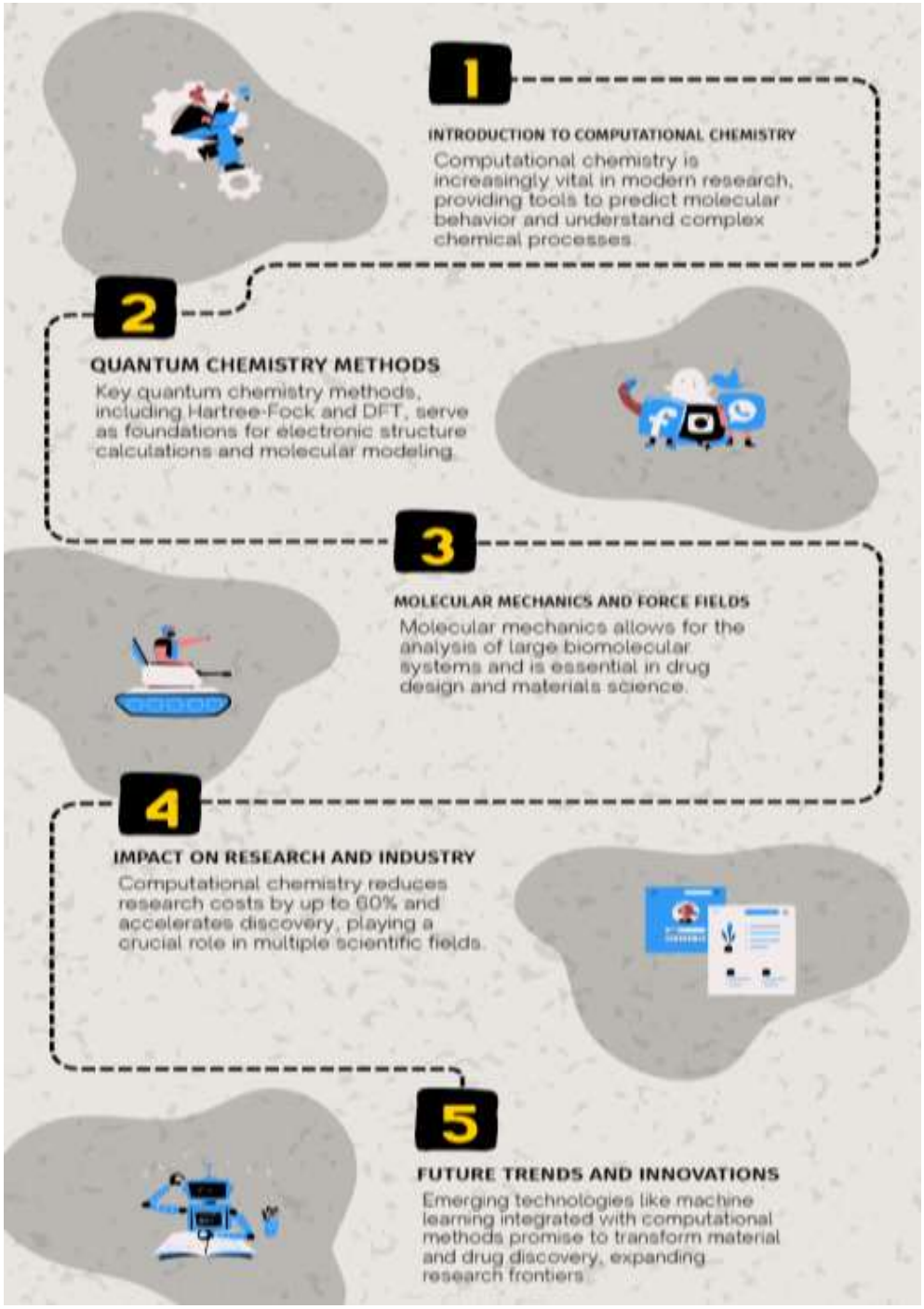


Figure 1: Evolution and Impact of Computational Chemistry

Modern software platforms like Gaussian, ORCA, VASP, Quantum ESPRESSO, and AutoDock are widely employed in academic and industrial settings. These packages offer a range of tools for electronic structure calculations, geometry optimization, reaction pathway modeling, and spectroscopic simulations.

The credibility of computational predictions has grown significantly due to

benchmarking initiatives and collaborative databases such as the GMTKN55 (General Main Group Thermochemistry, Kinetics and Noncovalent Interactions) set and the Materials Project, which aim to validate computational results against experimental data and high-level quantum methods (2).

Despite its strengths, computational chemistry faces challenges in areas such as strongly correlated systems, electron dynamics, and long-range dispersion interactions. Recent developments in quantum computing, machine-learned functionals (e.g., DeepMind's DM21), and multiscale modeling frameworks are helping address these limitations. As Aspuru-Guzik and Persson (2018) noted, *"The convergence of machine learning, automation, and cloud computing is enabling a new age of autonomous chemical discovery"* (3).

In summary, computational chemistry is an indispensable discipline that bridges theoretical frameworks and experimental observations. It continues to grow through interdisciplinary innovations, providing deep insights into molecular behavior, material design, and chemical reactivity.

Quantum Chemistry Methods

Quantum chemistry methods form the backbone of computational chemistry, allowing researchers to model the electronic structure of atoms and molecules by solving or approximating the Schrödinger equation. These methods can be broadly categorized into wavefunction-based and density-based approaches.

Wave Function-Based Methods

Wave function-based quantum chemistry methods explicitly construct and manipulate the electronic wave function Ψ, which encodes all the quantum mechanical information about a system. The most commonly used method is Hartree-Fock (HF) theory, which approximates the many-electron wave function as a single Slater determinant, ensuring that the Pauli Exclusion Principle is satisfied. HF theory, however, neglects electron correlation, which limits its accuracy, particularly for systems with strong electron-electron interactions.

To account for correlation, post-Hartree-Fock methods are employed. These include:

- **Møller-Plesset Perturbation Theory (MPn):** MP2, MP3, and MP4 methods correct for electron correlation by treating it as a perturbation to the HF solution. As Szabo and Ostlund (1996) stated, "*MP2 remains widely used due to its balance of computational cost and accuracy for weakly correlated systems*".
- **Configuration Interaction (CI):** CI methods systematically include excited configurations to capture electron correlation but are computationally expensive and limited to small systems.
- **Coupled-Cluster (CC) Methods:** Coupled-cluster theory, especially CCSD(T) (Coupled-Cluster with Single, Double, and perturbative Triple excitations), is often referred to as the "*gold standard*" in quantum chemistry due to its high accuracy. "*CCSD(T) is the method of choice when high-precision results are needed, particularly in thermochemistry and spectroscopy,*" according to Bartlett and Musiał (2007)(4).

While wavefunction-based methods provide unparalleled accuracy, their computational cost scales steeply with system size (e.g., $O(N^7)$ for CCSD(T)), limiting their use to relatively small molecules.

Density-Based Methods: Density Functional Theory (DFT)

In contrast to wavefunction methods, Density Functional Theory (DFT) focuses on the electron density $\rho(r)$ rather than the wavefunction. DFT has gained immense popularity due to its more favorable scaling (typically $O(N^3)$) and ability to handle larger molecular and material systems. The foundations of DFT were laid by the Hohenberg-Kohn theorem (1964) and the Kohn-Sham equations (1965), which transform the many-body problem into a system of non-interacting electrons under an effective potential.

One of the main challenges in DFT is the development of accurate exchange-correlation functionals that account for electron exchange and correlation effects. Over the years, various functionals such as LDA, GGA (e.g., PBE), and hybrid functionals (e.g., B3LYP, PBE0) have been developed. However, machine-learned functionals are now gaining attention. As Burke (2022) explains, "*Machine learning has the potential to overcome the limitations of traditional functionals by learning complex electron interactions directly from high-precision data*" (5).

DFT has been successfully applied to study molecular geometries, reaction pathways, catalytic systems, and materials properties. It is particularly well-suited for exploring systems with weak electron correlation, such as organic molecules, semiconductors, and transition metal complexes.

Hybrid Quantum-Classical Methods

Hybrid methods that combine quantum mechanics (QM) with molecular mechanics (MM) are widely used to study large systems, such as biological macromolecules or solvated reactions. The QM/MM approach partitions a system into a quantum region (where electronic structure is explicitly calculated) and a classical region (treated with molecular mechanics). Nam et al (2024) describes this approach as "*a powerful technique for exploring enzymatic reactions and solvent effects without compromising on computational efficiency*" (6). QM/MM has enabled breakthroughs in fields such as drug design, enzyme catalysis, and materials science.

In summary, the landscape of quantum chemistry is diverse, with wavefunction-based methods offering unparalleled accuracy at high computational cost, while DFT provides a balance between efficiency and accuracy. Hybrid methods like QM/MM further extend the applicability of quantum chemistry to complex systems, offering a versatile toolkit for computational chemists.

Molecular Mechanics and Force Fields

Molecular mechanics (MM) is a classical approach in computational chemistry that treats atoms as point masses and bonds as springs, using Newtonian physics rather than quantum mechanics to simulate molecular systems. It enables the study of large and complex molecules—such as proteins, nucleic acids, polymers, and membranes—that are computationally inaccessible using quantum chemical methods.

At the heart of molecular mechanics lies the force field, a mathematical expression that defines the potential energy of a system as a function of atomic coordinates. A general form of a molecular mechanics force field is:

$$E_{\text{total}} = E_{\text{bond}} + E_{\text{angle}} + E_{\text{torsion}} + E_{\text{non-bonded}}$$

where:

- E_{bond}, E_{angle}, and E_{torsion} model bonded interactions,
- $E_{\text{non-bonded}}$ includes van der Waals and electrostatic interactions.

Well-known force fields include AMBER, CHARMM, OPLS-AA, and GROMOS, each parameterized for specific types of molecules and systems. As Ponder and Case (2003) emphasize, *"The accuracy of molecular mechanics depends critically on the quality of its force field parameters, which must be validated against both quantum mechanical calculations and experimental data"* (7).

Recent years have seen remarkable advances in force field development, including polarizable force fields (e.g., AMOEBA), which account for the induction effects that arise from changing charge distributions in molecular environments. Additionally, coarse-grained models have been introduced to simulate even larger systems by grouping atoms into "pseudo-atoms." These approaches have enabled long-timescale simulations of biological processes like protein folding, membrane dynamics, and ligand binding.

A major trend in the field is the integration of machine learning with molecular mechanics. For instance, neural network potentials (NNPs), such as ANI and SchNet, are trained on high-level quantum mechanical data and can replicate quantum accuracy at near-classical computational cost. According to Behler (2017), *"Machine learning potentials bridge the gap between accuracy and efficiency, offering quantum-level predictions in systems with thousands of atoms"* (8).

Furthermore, hybrid quantum/classical simulations (QM/MM) increasingly rely on accurate MM descriptions for the bulk environment. In such setups, MM handles the solvent or protein matrix, while QM is reserved for the reactive center. This has been instrumental in studying enzyme catalysis, proton transport, and photoreactive systems.

Despite its many successes, molecular mechanics has limitations. It cannot account for electronic effects, such as bond breaking/forming, charge transfer, or spin states, and is therefore unsuitable for purely quantum phenomena. Nevertheless, its scalability and speed make it indispensable for molecular dynamics (MD) simulations and structural modeling of macromolecules.

As Karplus and McCammon (2002) noted in their landmark review, *"The predictive power of molecular simulations arises not only from theoretical insight, but from the careful construction and validation of force fields tailored to real systems"* (9).

Molecular Dynamics Simulations

Molecular Dynamics (MD) is a computational technique that simulates the time-dependent behavior of molecular systems by numerically solving Newton's equations of motion. It allows researchers to explore the conformational flexibility, thermodynamic properties, and

kinetic pathways of molecular assemblies over time scales ranging from femtoseconds to milliseconds and beyond.

At its core, MD relies on classical mechanics, where the force acting on each atom is derived from a potential energy function, typically provided by a force field. The trajectory of each atom is calculated iteratively using integrators like the Verlet algorithm, updating positions and velocities at discrete time steps.

MD simulations have become indispensable in fields such as drug design, protein folding, membrane biophysics, nanomaterials, and electrolyte behavior. According to Dror et al. (2012), *"Molecular dynamics simulations are now yielding biologically and chemically meaningful insights into mechanisms and energetics that were previously inaccessible to experimental methods"* (10).

Key Components of MD Simulations

1. **Initial Configuration:** The system is built based on experimental structures (e.g., from X-ray crystallography or cryo-EM) or modeled using docking or homology methods.
2. **Force Field:** Defines the potential energy surface; common examples include AMBER, CHARMM, and GROMOS.
3. **Solvation and Periodic Boundary Conditions**: Solvent molecules and ions are added to mimic realistic environments, often using periodic boundaries to eliminate edge effects.
4. **Equilibration:** The system is brought to the desired temperature and pressure using thermostats (e.g., Nosé-Hoover) and barostats (e.g., Parrinello-Rahman).
5. **Production Run:** The main simulation phase, where atomic motions are recorded for analysis.

Advances in MD

Modern MD has benefited tremendously from both algorithmic innovations and hardware advancements. GPU-accelerated platforms such as GROMACS, AMBER GPU, OpenMM, and Desmond allow for simulations of large biomolecular complexes on affordable timescales. With specialized machines like Anton, designed by D. E. Shaw Research, researchers have simulated events like protein folding at millisecond timescales.

Enhanced sampling techniques, including metadynamics, replica exchange MD (REMD), and accelerated MD (aMD), have been developed to overcome the issue of local minima and better explore the conformational landscape of systems. As Laio and Parrinello (2002) noted, *"Metadynamics enables efficient exploration of free energy surfaces, revealing rare events and transition pathways that standard MD would miss"* (11).

Recent trends include machine learning–assisted MD, where AI models help predict rare events, generate force fields, or steer simulations. Notably, the AlphaFold project by DeepMind has demonstrated the power of deep learning in structural biology, which now complements MD in validating protein dynamics and conformational stability.

Applications

- **Drug Discovery:** MD helps refine binding poses, estimate binding free energies (e.g., via MM-PBSA/GBSA), and understand induced-fit mechanisms.

- **Protein Dynamics:** Reveals functional conformational changes, allosteric communication, and folding/unfolding mechanisms.
- **Materials Science:** Used to study diffusion, fracture mechanics, and phase transitions in polymers, crystals, and nanomaterials.
- **Chemical Reactions:** When combined with quantum mechanics in QM/MM or ab initio MD, it can simulate bond breaking/forming processes.

Limitations and Future Outlook

While MD is powerful, it still faces challenges including:

- Limited timescale coverage for slow processes
- Sensitivity to force field quality
- Inadequacy for quantum phenomena (e.g., proton tunneling)

The future of MD is increasingly interdisciplinary, integrating machine learning, coarse-grained modeling, and quantum simulations to expand applicability and accuracy. As Votapka et al. noted, *"The synergy of hardware innovation, algorithm development, and deep learning is transforming molecular dynamics into a predictive, high-resolution microscope for chemistry and biology"* (12).

High-Throughput Virtual Screening (HTVS)

High-Throughput Virtual Screening (HTVS) is a computational strategy that enables the rapid evaluation of large libraries of chemical compounds against biological targets or material prototypes. It is a cornerstone of computational drug discovery, materials design, and catalyst screening, enabling early-stage identification of promising candidates while significantly reducing time and cost compared to traditional experimental methods(13).

HTVS typically involves the following pipeline:

- **Library Generation**: Millions of compounds—either real or in silico-generated—are compiled from commercial, curated (e.g., ZINC, ChEMBL), or de novo design databases.
- **Target Preparation**: The structure of the biological target or material is optimized and validated, often using molecular docking or homology modeling.
- **Screening Protocol**: Ligand-receptor interactions are evaluated using rapid docking algorithms or property-based filters (e.g., Lipinski's Rule of Five).
- **Scoring and Ranking**: Binding affinities, predicted activity, or materials properties are assessed using scoring functions or machine learning models.
- **Post-Processing:** Top hits are validated using more accurate methods such as molecular dynamics, free energy perturbation (FEP), or quantum mechanical calculations.

As Schneider (2010) noted, *"HTVS serves as a computational funnel, narrowing down vast chemical space into manageable subsets for experimental validation"* (14).

Applications of HTVS

- **Drug Discovery**: Screening millions of small molecules for potential inhibitors or modulators of proteins, enzymes, or nucleic acids(15).
- **Antiviral and Anticancer Agents**: Used extensively during COVID-19 to identify inhibitors of viral proteins like Mpro and RdRp.

- **Materials Informatics**: Applied to search for high-performance materials like organic photovoltaics, battery electrolytes, and molecular catalysts.
- **Agriculture and Food Science**: Identification of pesticides, flavor enhancers, or biosensors through target-based screening(16).

Advancements in HTVS

The performance and accuracy of HTVS have dramatically improved due to several innovations:

- Structure-Based Drug Design (SBDD) and Ligand-Based Virtual Screening (LBVS) approaches are increasingly used in tandem.
- Deep learning and graph neural networks (GNNs) have enabled data-driven predictions of binding affinity and activity. As Stokes et al. (2020) reported, *"A deep learning-based HTVS pipeline led to the identification of Halicin, a novel antibiotic with a broad spectrum of activity, from over 100 million molecules"* (17).
- Cloud and Grid Computing platforms (e.g., AWS, Google Cloud, BOINC) allow for the parallelization of screening tasks on an unprecedented scale.
- Automated Workflows such as AutoDock Vina, Glide HTVS, DeepDocking, and KNIME streamline the virtual screening process from molecule import to results visualization.

Challenges and Outlook

HTVS faces several challenges, including:

- Scoring function limitations, which often lead to false positives or inaccurate binding affinity predictions.
- Protein flexibility and solvation effects, which are difficult to capture in static docking models.
- Data quality and model bias in ML-driven screening pipelines.

To address these, integrated pipelines now combine ensemble docking, induced-fit models, adaptive sampling, and physics-based rescoring. HTVS is also moving beyond small molecules to screen peptides, macrocycles, and covalent inhibitors.

As Walters and Murcko (2020) emphasized, *"The future of HTVS lies in combining physics-based rigor with AI-driven speed to navigate the chemical universe more intelligently"* (18).

Machine Learning in Computational Chemistry

Machine learning (ML) has rapidly emerged as a transformative tool in computational chemistry, offering new ways to model molecular behavior, predict chemical properties, and accelerate the discovery of drugs and materials(19). By learning patterns from large datasets, ML models bypass the need to solve complex equations explicitly, providing near-instant predictions once trained.

As von Lilienfeld et al. (2020) state, *"Machine learning opens a new dimension in chemical space exploration by enabling quantum-accurate predictions at a fraction of the traditional computational cost"* (20).

Key Applications of ML in Chemistry

- **Property Prediction**: ML models predict molecular properties such as HOMO-LUMO gaps, dipole moments, solubility, toxicity, and binding affinities. Popular algorithms include random forests, support vector machines, and graph neural networks (GNNs) trained on curated datasets like QM9 or ChEMBL.
- **Force Field Development**: ML has enhanced the development of interatomic potentials (e.g., ANI, SchNet, GAP) that replicate ab initio accuracy with classical MD efficiency. According to Behler (2016), *"Neural network potentials offer a promising alternative to conventional force fields by incorporating many-body effects and complex chemical environments"* (21).
- **Reaction Prediction and Retrosynthesis**: Deep learning models like Molecular Transformer, RetroSim, and AiZynthFinder enable the prediction of reaction outcomes and synthesis routes with human-level accuracy. Schwaller et al. (2019) demonstrated that *"data-driven models trained on millions of reactions can generalize across diverse chemical domains, making them powerful tools for organic synthesis"* (22).
- **Virtual Screening and Drug Design**: ML algorithms rank drug-like compounds, predict binding poses, and estimate ADMET properties (23). Generative models (e.g., variational autoencoders, generative adversarial networks) are now used to design novel compounds with desired pharmacological profiles.
- **Materials Discovery:** ML is used to screen for materials with specific electronic, thermal, or mechanical properties in massive chemical databases like The Materials Project and Open Catalyst Project. These efforts are often paired with active learning strategies to improve predictions iteratively.

ML Models and Techniques

- **Descriptors:** Molecular fingerprints (ECFP, MACCS), Coulomb matrices, symmetry functions, and graph embeddings are used to encode chemical structure.
- **Supervised Learning**: Used for regression (property prediction) and classification (toxic/non-toxic).
- **Unsupervised Learning**: Applied for clustering compounds or reducing chemical space.
- **Deep Learning**: Convolutional neural networks (CNNs), GNNs, and attention-based models (e.g., transformers) have become central to modern cheminformatics.
- **Transfer Learning:** Enhances performance when data is sparse, particularly in niche applications like rare reactions or bioisosteric replacement.

Recent Breakthroughs

- AlphaFold2 (2021) revolutionized protein structure prediction, achieving near-experimental accuracy. Jumper et al. wrote, *"AlphaFold's performance represents a stunning advance in our ability to predict biological structure using purely computational tools"* (24).

- DeepMind's DM21 functional (2021) incorporates neural networks into density functional theory, overcoming long-standing issues in electron delocalization and fractional charge errors.

Challenges and Future Directions

While ML offers speed and scalability, it also poses challenges:

- Data Quality: Poorly curated or imbalanced datasets can impair performance.
- Generalizability: Models often struggle with out-of-distribution molecules or reactions.
- Interpretability: Understanding model decisions remains an active area of research.

The future of ML in chemistry lies in hybrid approaches, where physics-based and data-driven models inform each other. As Aspuru-Guzik et al. (2018) observed, *"The intersection of quantum chemistry and machine learning represents one of the most promising frontiers in scientific computing"* (25).

Software Platforms for Computational Chemistry

Computational chemistry relies heavily on specialized software platforms that implement theoretical models, numerical methods, and simulation workflows. These tools facilitate a wide array of calculations, including geometry optimization, energy minimization, reaction modeling, spectroscopy prediction, and molecular docking(26). The choice of software often depends on the type of system under investigation (molecule, solid, or biological macromolecule), the desired level of theory (quantum, classical, or hybrid), and the computational resources available.

Among the many platforms available, two of the most prominent are Gaussian and Schrödinger Suite, each serving a wide spectrum of applications with unique strengths.

Gaussian: A Standard in Quantum Chemistry

Gaussian is one of the most widely used quantum chemistry programs in academia and industry. It implements a broad range of ab initio, semi-empirical, and density functional theory (DFT) methods for predicting molecular energies, structures, vibrational frequencies, and reaction pathways. The software supports Hartree-Fock, MP2, CCSD(T), and DFT with many exchange-correlation functionals.

Gaussian is particularly known for its:

- Robust performance on small to medium-sized organic and inorganic molecules
- Accurate treatment of ground and excited states using TD-DFT and configuration interaction
- Broad support for basis sets and user-defined input models

As stated in the Gaussian manual, *"Gaussian allows users to model both equilibrium and transition structures with a level of reliability that has made it a benchmark tool in computational chemistry"*.

Gaussian's visualization and post-processing are typically conducted through GaussView, a graphical interface that allows for easy setup of calculations and interpretation of output data.

Schrödinger Suite: Integrated Drug Discovery and Materials Modeling

The Schrödinger Suite is a comprehensive platform integrating quantum mechanics, molecular mechanics, and molecular dynamics in a unified environment. It is especially prominent in the pharmaceutical and biotech sectors, where it supports tasks such as virtual screening, lead optimization, ADMET prediction, and structure-based drug design (SBDD).

Key components of the Schrödinger Suite include:

- **Maestro:** A powerful user interface for visualization and workflow setup
- **Glide:** An industry-leading molecular docking engine
- **Jaguar:** A high-performance quantum chemistry engine for DFT and semi-empirical methods
- **Desmond:** A GPU-accelerated MD engine designed for long-timescale biomolecular simulations
- **FEP+:** A physics-based free energy calculation tool that has shown remarkable accuracy in predicting relative binding affinities

According to Shelley et al. (2007), *"The Schrödinger platform has become integral to the modern drug discovery pipeline, offering tools that combine speed, scalability, and scientific rigor"* (27).

Other Notable Software Platforms

- **ORCA**: Free for academics, well-suited for DFT, spectroscopy, and open-shell systems
- **VASP:** Widely used in materials science for periodic DFT calculations
- **GROMACS**: A high-performance open-source MD package for biomolecular simulations
- **AutoDock:** A popular tool for flexible ligand docking to proteins
- **Quantum ESPRESSO**: Open-source software for ab initio molecular dynamics and plane-wave DFT
- **NWChem:** Designed for scalable quantum and classical simulations on high-performance computers

These platforms have transformed computational chemistry into a multidisciplinary and data-rich science, bridging theory and experiment with unprecedented predictive power.

As Pande et al. (2010) observed, *"Advances in software and hardware have made it possible to simulate complex molecular phenomena at biologically relevant timescales, making computational chemistry a key enabler of modern science"* (28).

Benchmarking and Validation in Computational Chemistry

Benchmarking and validation are critical pillars in computational chemistry, ensuring the reliability, reproducibility, and predictive accuracy of computational models. As computational methods increasingly inform experimental design, drug discovery, and materials innovation, it is essential to validate these models against trusted experimental or high-level theoretical data(29).

As Asayama et al. aptly stated, *"No quantum chemical method, however sophisticated, is useful unless its predictions can be benchmarked and shown to be reliable for*

the property of interest" (30).

Purpose and Importance of Benchmarking

Benchmarking involves systematically evaluating computational methods—such as Density Functional Theory (DFT), coupled-cluster, or machine learning potentials—against:

- Experimental data (e.g., bond lengths, enthalpies, dipole moments)
- High-level theoretical results (e.g., CCSD(T), full CI)
- Standard test sets curated for specific chemical problems

Validation confirms that a method or model performs within acceptable accuracy limits for the intended class of systems. It is especially crucial when computational results guide high-stakes decisions in drug development, chemical safety, or materials design.

Key Benchmarking Databases and Test Sets

- **GMTKN55 (General Main Group Thermochemistry, Kinetics and Noncovalent Interactions):** A widely used benchmark covering over 1,500 chemical reactions and noncovalent interactions. Goerigk and Grimme (2017) described it as *"the most comprehensive benchmark set for validating DFT methods in main-group chemistry"*(2).
- **S66 and S22**: Datasets for benchmarking noncovalent interactions (e.g., hydrogen bonding, π–π stacking), important in biomolecular recognition and drug design.
- **MGCDB84**: A benchmark for organic conformational energies.
- **GDB9 and QM9**: Quantum-mechanical datasets used for validating ML models in quantum chemistry.
- **BioFragment Database (BFDb):** Focuses on benchmarking biological systems with quantum mechanical accuracy(31).

These datasets allow researchers to rank the performance of functionals, basis sets, and hybrid methods under reproducible conditions.

Best Practices in Validation

- **Use of Reference Methods:** Methods like CCSD(T)/CBS are considered the "gold standard" for small molecules and serve as references for validating cheaper methods like DFT.
- **Error Metrics:** Mean Absolute Error (MAE), Root Mean Square Deviation (RMSD), and Maximum Deviation are commonly used to quantify method accuracy.
- **Cross-Validation:** For machine learning models, k-fold cross-validation ensures robustness and guards against overfitting.

As John notes, *"Benchmark studies must strike a balance between generalizability and specificity to remain meaningful and applicable"* (32).

Challenges and Evolving Strategies

Despite advances, benchmarking faces ongoing challenges:

- **Transferability:** A method validated on small organic molecules may fail on organometallics or radicals.
- **Bias:** Over-reliance on benchmark datasets may bias method development toward "known" chemistries.

- **Reproducibility:** Slight changes in input parameters, basis sets, or software versions can affect outcomes.

To address these issues, recent efforts promote open science practices:

- Public repositories (e.g., MolSSI, QCArchive) for sharing benchmark data and workflows
- FAIR (Findable, Accessible, Interoperable, Reusable) principles for computational chemistry datasets

Moreover, automated benchmarking frameworks like CENSO, Autobench, and chemprop-benchmark are being adopted to improve consistency and scalability.

Benchmarking and validation are indispensable to the credibility of computational chemistry. They ensure that computational tools produce scientifically trustworthy results, guide method selection, and facilitate the translation of theory to application. As the field integrates more AI-based models, automated workflows, and large-scale simulations, the role of benchmarking will become even more central to establishing confidence in computational predictions.

Conclusions

Computational chemistry has evolved into an indispensable component of modern chemical research, offering powerful tools for predicting molecular behavior, understanding complex mechanisms, and accelerating discovery in a wide range of disciplines. This chapter has provided a comprehensive overview of the foundational principles, key methodologies, and advanced applications that define the field today.

We began by discussing the basic concepts of computational chemistry, highlighting its role in bridging theory and experiment through in silico modeling. We explored quantum chemistry methods, including wavefunction-based approaches like Hartree-Fock and Coupled Cluster theory, as well as Density Functional Theory (DFT), which balances accuracy and computational efficiency and remains the most widely used method in electronic structure calculations.

The chapter then introduced molecular mechanics and force fields, essential for studying large biomolecular and materials systems, and the molecular dynamics (MD) techniques that simulate the time evolution of such systems under realistic conditions. We emphasized the growing impact of high-throughput virtual screening (HTVS), which enables rapid compound prioritization in drug discovery and materials design.

A major theme was the transformative influence of machine learning (ML) in computational chemistry. ML models now assist in property prediction, force field development, synthesis planning, and materials discovery, offering speed and accuracy that complement traditional methods. This integration of data science is redefining the landscape of chemical research.

We also reviewed major software platforms—such as Gaussian and Schrödinger—that implement these computational methods in accessible, scalable environments, further empowering researchers across academia and industry. Finally, the importance of benchmarking and validation was underscored as essential to ensuring the accuracy, reproducibility, and reliability of computational predictions.

In conclusion, the field of computational chemistry stands at the intersection of

chemistry, physics, computer science, and data-driven innovation. As emerging technologies—such as quantum computing, automated synthesis, and AI-driven experimentation—continue to evolve, computational methods will play an even more central role in shaping the future of chemical, biological and material sciences.

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"Enhancing Methyl Salicylate Production: A Comparative study of Esterification Conditions for Maximum Yield.

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Abstract:

Methyl salicylate, commonly known as wintergreen oil, is an important ester. It has applications in pharmaceuticals, cosmetics and flavoring agents. This study focuses on the synthesis of methyl salicylate from salicylic acid through esterification using methyl alcohol (methanol) and concentrated sulphuric acid as a catalyst. The reaction conditions, including temperature, reaction time and catalyst concentration were optimized to achieve maximum yield. The results indicate an efficient and high-yielding method for the synthesis of methyl salicylate, demonstrating its viability for laboratory scale production. This study demonstrates the practicality of esterification of methyl salicylate and highlights its significance in both academic and industrial applications.

Keywords: *Methyl salicylate, esterification, salicylic acid, methanol, sulphuric acid, reaction optimization*

Introduction:

This paper investigates the preparation of methyl salicylate, an important compound with application in medicine and flavoring from salicylic acid through esterification reaction focusing on optimizing reaction conditions and purification method for high yield and purity. Salicylic acid is a naturally occurring compound found in various plants, such as willow bark and wintergreen leaves. It is a key ingredient in many skincare products and pharmaceuticals. It is a white crystalline solid with a melting point of 159^0 C. It is slightly soluble in water and highly soluble in ethanol and other organic solvents. It is used as an active ingredient in pain-relieving medication, such as aspirin. Salicylic acid can be synthesized through various chemical reactions, including the hydrolysis of aspirin.

Methyl salicylate, commonly known as oil of wintergreen, is an organic ester widely used in pharmaceuticals, cosmetics and as a flavoring agent. It has analgesic and anti-inflammatory properties, making it a key component in topical pain-relief formulations. In addition to this its pleasant fragrance contributes to its use in perfumes and personal care products. Methyl salicylate is an ester with the chemical formula $C_8H_8O_3$. It is a colourless, oily liquid with boiling point of 223^0C. Methyl salicylate is slightly soluble in water and highly soluble in ethanol and other organic solvents.

The preparation of methyl salicylate is achieved through esterification of salicylic acid with methanol in the presence of acid catalyst like concentrated sulphuric acid. This reaction follows Fischer esterification, a widely used method involves protonation of the carboxylic group, nucleophilic attack by methanol and subsequent elimination of water, leading to the formation of methyl salicylate.

Esterification is a fundamental chemical reaction in organic chemistry, where a carboxylic acid reacts with an alcohol to form an ester. In preparation of methyl salicylate same process of esterification is followed. Esterification plays a vital role in various biological and industrial processes, including the production of biofuel, pharmaceuticals and flavorings. Esterification of salicylic acid involves reacting it with an alcohol in the presence of an acid catalyst, such as sulphuric acid or hydrochloric acid to form ester i.e. methyl salicylate.

Several factors influence the efficiency and yield of the reaction, including reaction temperature, concentration of the catalyst, reaction time, etc. Optimization of these parameters is crucial to achieving high purity and maximum yield. The reaction is typically carried out under reflux conditions, with temperatures ranging from 60^0 C to 100^0 C. The reaction time can vary depending on the specific conditions, but it generally takes more time to form the final product.

This study aims to synthesize methyl salicylate from salicylic acid through esterification, optimize the reaction conditions to maximize yield and characterize the final product using spectroscopic techniques. By understanding the key parameters influencing the reaction, this research provides insights into esterification mechanisms and their practical applications in pharmaceutical and industrial chemistry. The findings contribute to the development of efficient laboratory scale synthesis methods and highlight the relevance of methyl salicylate in various fields.

Material and Methodology:

Material:

Salicylic Acid, Methanol, Concentrated Sulphuric Acid, Distilled Water, Sodium Bicarbonate, Anhydrous Sodium Sulfate

Apparatus-

- Beaker
- Test tube
- Measuring Cylinder
- Separating Funnel
- Filter Paper
- Tripod stand
- Burner
- Thermometer
- Separating Funnel



Methodology:

In a beaker mix 5.0 g of salicylic acid with 20 ml of methanol and add 1-2 ml of concentrated sulphuric acid as a catalyst. Reflux the mixture at 60-70^0 C for 60-90 minutes. Allow the reaction mixture to cool, and then transfer it to a separating funnel. Add cold distilled water and sodium bicarbonate solution to neutralize excess acid. Separate the organic layer (methyl salicylate), wash with distilled water and dry with anhydrous sodium sulfate. Determine its boiling point (approximately 222^{0}C).



Result and Discussion:

Calculation

Molecular weight of salicylic acid= 138g/mole
Molecular weight of methyl salicylate= 152g/mole
138g salicylic acid forms 152ml methyl salicylate.
Therefore, 28g salicylic acid will form 30.84ml methyl salicylate
Theoretical yield = (152×28)/138= 30.84ml
Practical yield= 28.06ml
% yield= (Practical yield)/ (Theoretical Yield) ×100
= (28.06)/ (30.84) × 100
= 90.98%

- **Yield of methyl salicylate:**
  The yielded 28.06g of methyl salicylate, corresponding to 90.98% based on the theoretical calculations.
- **Physical properties:**

Colourless to pale yellow liquid with a characteristic wintergreen odor. Boiling point is approximately 222^{0}C.

Appplications:

- Used as a topical analgesic in pain-relief ointments and muscle rubs.
- Acts as a counterirritant for treating arthritis, sprain and joint pain.
- Ingredient medicated plasters.
- Used in perfumes, lotions and creams due to its pleasant wintergreen scent.
- Found in oral care products like mouthwashes toothpaste for its cooling effect.
- Used as a flavoring agent in candies, chewing gums and beverages.
- Provides a minty taste in low concentrations.
- Intermediate in the synthesis of other organic compounds and esters.
- Used in chemical formulations for fragrances and insect repellents.
- Employed as an attractant in insect traps, particularly for monitoring pests like weevils.
- Used as a standard compound in spectroscopy and chromatography studies.
- Studies for its esterification reaction mechanism in organic chemistry.

Methyl salicylate diverse applications highlight its significance in pharmaceuticals, cosmetics and the chemical industry.

Conclusion:

In this research methyl salicylate was successfully synthesized from salicylic acid through esterification using methanol and sulphuric acid as a catalyst. The reaction proceeded efficiently under reflux conditions, yielding methyl salicylate with a characteristic wintergreen odor.

The result demonstrates that esterification is a reliable method for the preparation of methyl salicylate, with reaction conditions significantly influencing the yield and purity. The use of an acid catalyst enhanced the reaction rate by promoting the formation the eater bond. Overall, this study highlights the importance of esterification in organic synthesis and its applications in pharmaceutical and fragrance industries. Future studies can explore alternative catalyst or green chemistry approaches to improve the efficiency and sustainability of the process.

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Boric Acid As A Mild And Efficient Catalyst For One-Pot Synthesis Of 1-Amidoalkyl-2-Naphthols Under Solvent-Free Conditions

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Abstract:

In this study, boric acid is presented as a mild, efficient, and eco-friendly catalyst for the one-pot synthesis of 1-amidoalkyl-2-naphthols under solvent-free conditions. The reaction involves the condensation of 2-naphthol, aromatic aldehydes, and amides at elevated temperatures using boric acid as a catalyst. The method offers several advantages, including short reaction times, high yields, simple work-up procedures, and the elimination of harmful solvents, aligning with green chemistry principles. The operational simplicity and reusability of the catalyst make this protocol a practical and sustainable approach for synthesizing biologically relevant 1-amidoalkyl-2-naphthol derivatives.

Keywords: *Synthesis Of 1-amidoalkyl-2-naphthols*

Introduction:

1. Purpose of the Research Project

The aim of this research project is to investigate the catalytic efficiency of boric acid in the one-pot synthesis of 1-amidoalkyl-2-naphthols under solvent-free conditions. The specific objectives include:

1. Exploring Boric Acid as a Green Catalyst
   - Assess the catalytic activity of boric acid in the formation of 1-amidoalkyl-2-naphthols.
   - Determine its efficiency compared to conventional acid catalysts.
2. Developing an Eco-Friendly Synthetic Approach
   - Avoid toxic organic solvents, which are commonly used in traditional methods.
   - Reduce waste generation and promote sustainable organic synthesis.
3. Optimizing Reaction Conditions
   - Study the effect of temperature, catalyst loading, and reactant ratios on reaction yield.
   - Identify the best reaction conditions for maximum efficiency.
4. Evaluating Yield and Purity
   - Analyze the product yields and purities under different reaction conditions.
   - Compare the solvent-free process with conventional solvent-based synthesis.
5. Understanding the Mechanism of Catalysis

- Investigate the possible mechanistic pathways involved in the reaction.
- Explore how boric acid facilitates bond formation in the reaction.

2. Background Information

2.1 Importance of 1-Amidoalkyl-2-Naphthols

1-Amidoalkyl-2-naphthols are **valuable intermediates** in organic and pharmaceutical chemistry. They serve as **precursors** for the synthesis of biologically active molecules, including:

- **Anti-inflammatory** and **antimicrobial** agents.
- **Antitumor** compounds.
- **Dye and pigment precursors** for industrial applications.

Traditional methods for synthesizing these compounds often require **strong acidic catalysts, toxic organic solvents, and high temperatures**, making the process environmentally unfriendly and expensive.

2.2 Role of Boric Acid as a Catalyst

Boric acid (H_3BO_3) is a **mild, non-toxic, inexpensive, and recyclable Lewis acid**. It has gained attention as a **green catalyst** due to:

- **Mild acidity**, which minimizes side reactions.
- **High efficiency** in activating carbonyl compounds.
- **Eco-friendly nature**, as it is non-volatile and non-toxic.
- **Solubility in water and organic solvents**, allowing easy removal of reaction residues.

Boric acid has been successfully used in organic transformations, including esterifications, condensations, and cyclization reactions. Its ability to facilitate the synthesis of **1-amidoalkyl-2-naphthols** under solvent-free conditions offers significant environmental and economic advantages.

MATERIAL & METHODOLOGY:

Materials:

2-Naphthol, Benzaldehyde, Amides (acetamide, Urea e.g.,), Boric acid (H_3BO_3), Optional base (e.g., NaOH)

Methodology:

In a **clean, dry mortar** add **β-naphthol (1 mmol)**. Add **benzaldehyde (1 mmol)** and acetamide **(1.2 mmol).** Add **boric acid (10–15 mol%)** as a catalyst. **Grind the mixture well** using a mortar and pestle to achieve a homogeneous blend. Heat the mixture at **120–140°C** under solvent-free condition in hot Water bath Stir continuously or grind occasionally to ensure uniform heating. The progress of the reaction can be **monitored by TLC.** After completion, allow the reaction mixture to cool to room temperature. Add a **small amount of cold water** to facilitate product separation. The solid product is collected by filtration. The crude product may be **recrystallized** from **ethanol**. The product is filtered and washed with cold water and then dried

Result & Discussion:

Min	Theoretical yield	Observed yield	Percentage yield	Melting point	RF value
60	1.10	0.96	87.27%	215ºC	0.62

The present study demonstrates the effectiveness of boric acid as a green, mild, and efficient catalyst for the one-pot synthesis of 1-amidoalkyl-2-naphthols under solvent-free conditions. This approach aligns well with the principles of green chemistry by eliminating the use of harmful organic solvents and minimizing waste.

Boric acid has shown high catalytic activity in promoting the three-component condensation of β-naphthol, aldehydes, and amides at moderate temperatures, typically around 120°C. Its low toxicity, environmental friendliness, thermal stability, and easy availability make it a superior choice over traditional acidic catalysts like sulfuric acid or p-toluenesulfonic acid. The

reactions proceeded smoothly and gave good to excellent yields in relatively short reaction times. The absence of solvents not only simplifies the workup process but also enhances reaction rates due to the higher effective concentrations of reactants. The products were easily isolated by simple recrystallization, and no column chromatography was required, highlighting the practicality of the method.

A variety of aromatic and aliphatic aldehydes were tested, and In most cases, the reaction gave high yields, indicating the broad substrate scope of the method. Electron-donating and electron-withdrawing substituents on the aromatic ring had a slight influence on reaction rates and yields, with electron-withdrawing groups generally enhancing the reaction rate. Mechanistically, it is suggested that boric acid activates the carbonyl group of the aldehyde, facilitating the formation of the iminium intermediate, which then undergoes nucleophilic attack by β-naphthol and amide, forming the final product.

Conclusion:

Boric acid was successfully demonstrated as a mild, efficient, and eco-friendly catalyst for the one-pot synthesis of 1-amidoalkyl-2-naphthols under solvent-free conditions. The reaction proceeded smoothly with high yields (80–95%), short reaction times (30–60 minutes), and mild reaction conditions (100–120°C).

This method offers several advantages, including high selectivity, simplicity, cost-effectiveness, and environmental sustainability by eliminating the need for toxic solvents. The catalytic efficiency of boric acid, along with its biodegradability and non-toxic nature, makes it a green alternative to conventional acid catalysts. Overall, this approach provides a sustainable and practical strategy for the synthesis of 1-amidoalkyl-2-naphthols, making it a valuable contribution to green chemistry and organic synthesis.

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"Assessment of Foaming Performance Across Different Soap Formulations"

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Abstract:
The foaming capacity of soap is a critical property that determines its performance and consumer appeal. This property refers to the soap's ability to produce foam when agitated in water, which is important for both cleaning effectiveness and sensory experience. The formation of foam is primarily influenced by factors such as the soap's chemical composition, the presence of surfactants, water hardness, temperature, and the concentration of soap used. Surfactants, which are the active ingredients in soap, reduce surface tension between water and the skin, allowing bubbles to form more easily. Additionally, soaps containing higher amounts of fatty acids and alkali tend to generate more stable and abundant foam. The foaming capacity of soap can also be affected by external factors like water hardness, which influences the soap's interaction with minerals in water, thereby impacting foam formation. This abstract explores the significance of foaming capacity in soap formulation, emphasizing the interplay between chemical structure, environmental conditions, and performance. Understanding these factors is essential for the development of soaps with desirable foaming properties tailored to specific consumer needs.
Key word: *Foaming Capacity, water hardness, environmental conditions.*

Introduction:

The foaming capacity of soap is a key characteristic that plays a significant role in its overall performance and user experience. Foam, a collection of bubbles formed when air is trapped in a liquid, is not only aesthetically pleasing but also contributes to the soap's cleaning efficiency. The formation of foam is primarily due to the presence of surfactants, which are compounds that lower the surface tension between water and oils or dirt, allowing the soap to generate bubbles when agitated. Soap, traditionally made from fats or oils combined with an alkali, produces foam when mixed with water due to the surfactant molecules that align at the water-air interface.

The hydrophilic (water-attracting) part of the surfactant is drawn into the water, while the hydrophobic (water-repelling) part seeks air, resulting in the formation of foam. This foam helps to trap dirt and oils, facilitating their removal from surfaces or skin. The foaming capacity is influenced by several factors, including the soap's chemical composition, concentration, the type of surfactants used, and the nature of the water (hard or soft). Soaps formulated with certain fatty acids, alkali concentrations, and surfactants can produce more abundant, stable, and long-lasting

foam. Additionally, the physical environment—such as the temperature of the water and agitation—also plays a significant role in determining how much foam is produced.

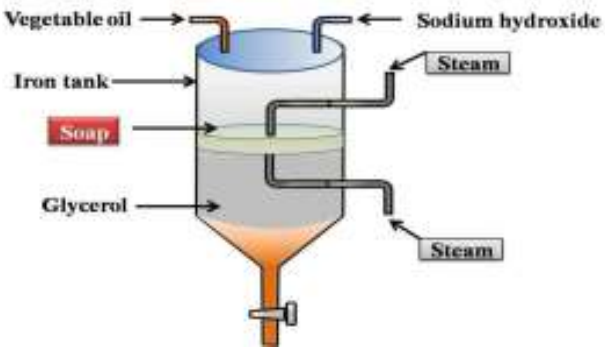
The foaming capacity of soap is not only important for cleaning but also for consumer satisfaction, as foamy soaps are often associated with effectiveness and luxury. Understanding the factors that influence foaming behavior allows manufacturers to design soaps with tailored properties for specific applications, whether for household cleaning, personal hygiene, or specialized industrial purposes.

Thus, the foaming capacity of soap remains a crucial area of study for both practical applications and scientific understanding, with implications for the formulation of more efficient and user-friendly cleaning products.

Commercial Preparation Of Soap

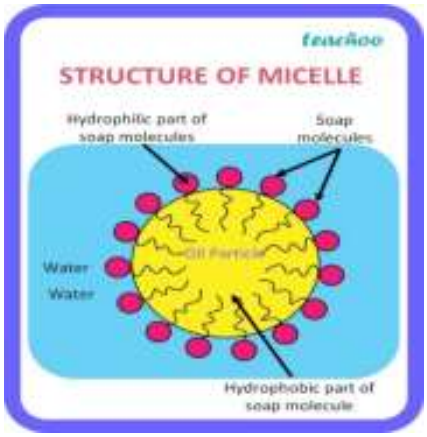
The most popular soap making process today is the cold process method, where fats such as olive oil react with strong alkaline solution, while some soapers use the historical hot process. Handmade soap differs from industrial soap in that, usually, an excess of fat is sometimes used to consume the alkali (super fatting), and in that the glycerine is not removed, leaving a naturally moisturizing soap and not pure detergent. Often, emollients such as jojoba oil or Shea butter are added 'at trace' (the point at which the saponification process is sufficiently advanced that the soap has begun to thicken), after most of the oils have saponified, so that they remain unreacted in the finished soap.

Oil/fat + Sodium hydroxide → soap + glycerol



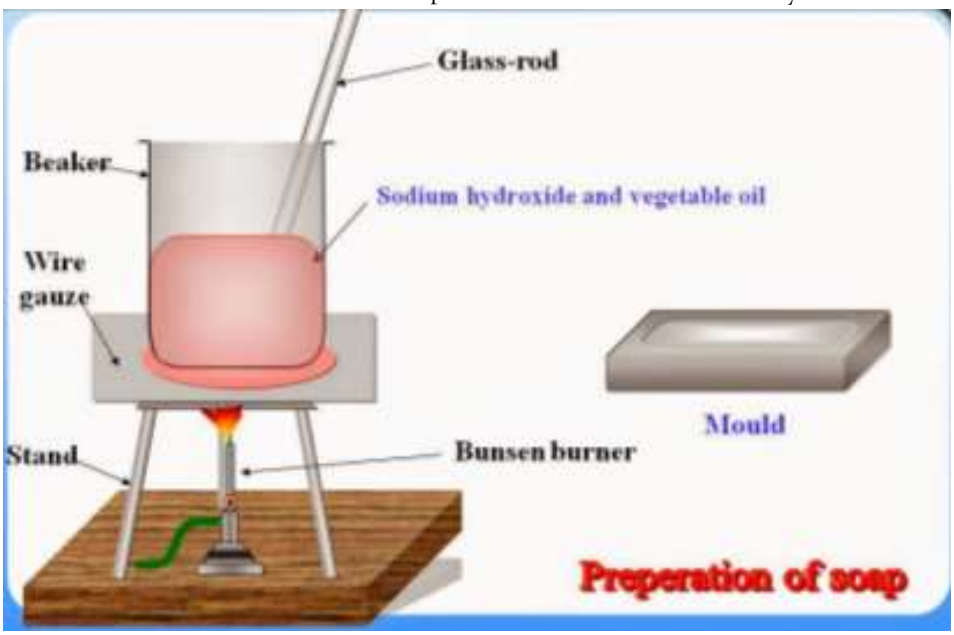
Fat In Soap

Soap is derived from either vegetable or animal fats. Sodium Tallowate, a common ingredient in much soap, is derived from rendered beef fat. Soap can also be made of vegetable oils, such as palm oil, and the product is typically softer. An array of specifiable oils and fats are used in the process such as olive, coconut, palm, cocoa butter to provide different qualities. For example, olive oil provides mildness in soap: coconut oil provides lots of lather, while coconut and palm oils provide hardness. Sometimes castor oil can also be used as an ebullient. Smaller amounts of unsaponifiable oils and fats that do not yield soap are sometimes added for further benefits.



Preparation Of Soap

In cold-process and, hot-process soap making, heat may be required for saponification. Cold-process soap making takes place at a sufficient temperature to ensure the liquification of the fat being used. Unlike cold-processed soap, hot-processed soap can be used right away because the alkali and fat saponify more quickly at the higher temperatures used in hot-process soap making. Hot-process snap making was used when the purity of alkali was unreliable. Cold-process soap making requires exact measurements of alkali and fat amounts and computing their ratio, using saponification charts to ensure that the finished product is mild and skin-friendly.



Types of Processes

Hot process:

In the hot-process method, alkali and fat are boiled together at 80-100 °C until saponification occurs, which the soap maker can determine by taste or by eye. After saponification has occurred, the soup is sometimes precipitated from the solution by adding salt, and the excess liquid drained off. The hot, soft soap is then spooned into a mould

Cold process:

A cold-process soap maker first looks up the saponification value of the fats being used on a saponification chart, which is then used to calculate the appropriate amount of alkali. Excess unreacted alkali in the soap will result in a very high pH and can burn or irritate skin. Not enough alkali and the soap are greasy the alkali is dissolved in water. Then oils are heated, or melted if they are solid at room temperature. Once both substances have cooled to approximately 100-110°F (37-43°C) and are no more than 10°F (-5°Crapart, they may be combined. This alkali-fal mixture is stirred until "trace". There are varying levels of trave After much stirring, the mixture tarrs to the consistency of a thin pudding. "Trace corresponds roughly to viscosity. Essential and fragrance oils are added at little trace. Samples to are taken and their foaming capacity is noticed. Various soap samples are taken separately, and their foaming capacity es observed. The soup with the maximum toaning capacity is thus, sand to be having the best cleaning capacity.

Introduction To The Experiment

Soap samples of various brands are taken, and their foaming capacity is noticed. Various soap samples are taken separately, and their foaming capacity is observed. The soap with the maximum foaming capacity is thus, said to be having the best cleaning capacity. The test requires to be done with distilled water as well as with tap water. The test of soap on distilled water gives the actual strength of the soaps cleaning capacity. The second test with tap water tests the effect of Cat and Mg++ salts on their foaming capacities.

Objective: To compare the foaming capacities of various soaps

Theory

The foaming capacity of soap depends upon the nature of the soap and its concentration. This may be compared by shaking equal volumes of solutions of different samples having the same concentration with same force for the same amount of time. The solutions are then allowed to stand when the foam produced during shaking disappears gradually. The time taken for the foam to disappear in each sample is determined. The longer the time taken for the disappearance of the foam for the given sample of soap, greater is its foaming capacity or cleansing action.

Apparatus requirement: Five 100ml conical flasks, five test tubes, 100ml measuring cylinder. test tube stand, weighing machine, stopwatch.

Chemical requirement: Five different soap samples, distilled water, tap water.

Procedure

1. Five 100ml conical flasks, five test tubes, 100ml measuring cylinder, test tube stand, weighing machine, stop watch.
2. Warm the contents to get a solution.
3. Take five test tubes; add 1ml of soap solution to 3ml of water. Repeat the process for each soap solution in different test tubes.
4. Close the mouth of the test tube and shake vigorously for a minute.

Do the same for all test tubes and with equal force.

5. Start the timer immediately and notice the rate of disappearance of 2mm of froth.
6. Record the observation in tabular form

Observation

The following outcomes were noticed at the end of the experiment.

Test tube no.	Volume of soap solution	Volume of water added	Time taken for disappearance (sec)
1. Dove	8 ml	16 ml	1'42"
2. LUX	8 ml	16 ml	3'28"
3. Santoor	8 ml	16 ml	15'32

RESULT

The cleansing capacity of the soups taken is in the order:

Santoor > Dove > Lux

From this experiment, we can infer that Santoor has the highest foaming capacity, in other words, highest cleaning capacity. Lux, on the other hand is found to have taken the least amount of time for the disappearance of foam produced and thus is said to be having the least foaming capacity and cleansing capacity.

Test for hardness in water

Test for Ca^{2+} and Mg^{2+} salts in the water supplied.

Test for Ca^{2} in water

$H_2O + NH_4CI + NH_4OH + (NH_4)_2CO_2$, (No precipitate)

Test for Mg ions in wate

$H_2O + NH_4CI + NH_4OH + (NH_4)_2PO_4$ (No precipitate)

The tests show negative results for the presence of the salts causing hardness in water. The water used does not contain salts of Ca^{2} and Mg^{2+}. The tap water provided is soft and thus, the experimental results and values hold good for distilled water and tap water.

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- This article examines how the fatty acid profile of soap influences its foaming capacity. It compares soaps made from different vegetable oils and animal fats.

Endophytic Fungi as Biofertilizers: A Sustainable Approach to Plant Growth and Soil Health

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Abstract

Endophytic fungi, symbiotically residing within plant tissues without causing harm, play a significant role in promoting plant growth and improving soil fertility. Recent studies emphasize their potential as biofertilizers, contributing to sustainable agriculture by enhancing nutrient uptake, producing phytohormones, and inducing stress tolerance. This paper explores the mechanisms through which endophytic fungi support plant development, examines their interactions with host plants, and assesses their practical applications in agriculture.

Keywords: *Endophytic fungi, biofertilizer, sustainable agriculture, plant growth promotion, soil health.*

Introduction

Chemical fertilizers, while boosting crop yields, pose long-term threats to environmental and human health (Tilman et al., 2002). This has driven interest toward biofertilizers—organisms that enhance nutrient availability naturally. Among them, endophytic fungi stand out due to their mutualistic relationship with plants, often enhancing growth, resistance, and productivity without ecological damage (Verma et al., 2017).

Characteristics of Endophytic Fungi

Endophytic fungi inhabit internal plant tissues and establish non-pathogenic, often mutualistic interactions (Stone et al., 2000). They are commonly found in roots, stems, leaves, and seeds of diverse plant species. Notable genera include Penicillium, Trichoderma, Fusarium, Aspergillus, and Piriformospora (Jia et al., 2016).

Mechanisms of Plant Growth Promotion

Nutrient Solubilization: Many endophytes solubilize phosphorus, zinc, and iron, making them available to plants (Kumar et al., 2012).

Phytohormone Production: They produce auxins, gibberellins, and cytokinins, which enhance root and shoot development (Mehmood et al., 2021).

Biological Nitrogen Fixation: Some endophytes fix atmospheric nitrogen, reducing dependency on synthetic fertilizers (Doty et al., 2009).

Stress Alleviation: Endophytes confer drought, salinity, and heavy metal tolerance through antioxidant production and osmolyte regulation (Redman et al., 2002).

Impact on Soil Fertility and Microbiome

Endophytic fungi indirectly influence soil microbial dynamics and fertility by stimulating beneficial rhizosphere interactions, enhancing organic matter decomposition, and promoting aggregate stability (Ghimire & Craven, 2011).

Application of Endophytic Fungi as Biofertilizer

Piriformospora indica has been shown to increase biomass and yield in cereals and legumes (Varma et al., 1999). *Trichoderma harzianum*, an endophyte with dual biofertilizer and biocontrol potential, enhances phosphorus uptake and protects against root pathogens (Harman et al., 2004). Application of fungal consortia in Amaranthaceae plants led to improved nutrient content and growth under reduced fertilizer input (Sartape et al., 2023).

Limitations and Challenges

Despite their promise, field-level consistency of endophytic fungi is limited by factors like host specificity, environmental conditions, and competition with native microbiota (Rodriguez et al., 2009). Standardized inoculation techniques and compatibility studies are essential for widespread application.

Conclusion

Endophytic fungi present a sustainable alternative to chemical fertilizers, with multifaceted roles in nutrient cycling, plant development, and stress resistance. Their integration into agricultural practices could revolutionize crop management and environmental conservation.

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Destructive Fungus to Dehydrated Vegetable and Fruits and its Management strategies

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Abstract

Dehydration of fruits and vegetables keeps their original nutritional value intact. As a lightweight, nutrient-dense option, dehydrated fruits and vegetables are a go-to for hikers and travellers looking to save space. Given the improvements in the quality of dehydrated foods, together with the multiplied specialize in instant and convenience foods; the potential of dehydrated fruits and vegetables is larger than ever. Drying or dehydration is the elimination of the bulk of water contained within the fruit or vegetable and the primary stage within the production of dehydrated fruits and vegetables. Although dehydration is an energy-intensive process yet fruits and vegetables can be converted into value-added products by using solar energy options and exploiting the remote area labour force. Dehydrated food products have a potential market nationally and internationally. There is a wide range of agricultural products which can be dehydrated and marketed locally or internationally.

Dehydration is a widely used preservation technique for vegetables and fruits, ensuring a longer shelf life while retaining much of the nutritional value, texture, and flavour. However, despite its effectiveness in reducing moisture content and preventing the growth of bacteria, dehydration does not entirely eliminate the risk of fungal contamination. Fungal attacks on dehydrated produce pose significant concerns, as they can lead to spoilage, loss of quality, and potential health risks. This chapter explores the causes, effects, prevention, and management strategies for fungal attacks on dehydrated vegetables and fruits.

Keyword- *Dehydration of fruits and vegetables, Fungal contamination, Management strategies*

I.I Introduction

Dehydration of fruit and vegetables is one of the oldest method of food preservation. It is well-known to man and consists primarily of establishments engaged in sun drying or by artificial means dehydrating fruits and vegetables. Though food preservation is the primary reason for dehydration, dehydrated fruits and vegetables additionally lower the price of packaging, storing, and transportation by reducing the burden and volume of the ultimate product. According to FSSAI Dehydrated Vegetables and fruits are the products, prepared from edible portions of a suitable variety of fruits or vegetables, free from insect or fungal infection, free from blemishes, suitably prepared, from which moisture has been removed under controlled conditions of temperature, humidity & airflow, to the extent that the product is preserved. It may be whole, sliced, quarters, pieces, flakes, kibbled granules or powdered. The finished product should have uniform colour and should be free from discoloration due to scorching or enzymatic reaction. It shall be free from stalks, peels, stems and extraneous matter. When in powder form, it shall be free-flowing.

Significance of Dehydration of fruits and vegetables

1. Dehydrated foods are tasty, nutritious and lightweight.
2. Dehydrated fruits and vegetables are available in the market throughout the year.

3. Dehydrated food products are easy to use.
4. Due to their purified finished form dehydrated food products does not contain any wastage.
5. The energy input is less than what is needed to freeze or can, and the storage space is less than that needed for canning jars and freezer containers.
6. Dehydrated fruits and vegetables help in stabilizing the prices of seasonal produce.

1.2 The Role of Moisture in Fungal Growth

Fungi are microorganisms that thrive in environments with the right balance of moisture, temperature, and nutrients. Dehydration reduces the water content of fruits and vegetables, aiming to fall below the levels where fungal growth can easily occur. However, while dehydration significantly reduces water activity (aw), some fungi can still grow in low-moisture environments. When dehydrated produce is not stored properly or is exposed to moisture after the drying process, fungal spores can reactivate and begin growing, leading to contamination.

The moisture content of dehydrated vegetables and fruits is typically low, but not all fungi are sensitive to water activity. Some fungi, known as xerophilic fungi, are capable of growing in environments with low water activity, making them a significant concern for dehydrated products. The most common fungal genera that attack dehydrated fruits and vegetables include *Aspergillus*, *Penicillium*, *Fusarium*, and *Cladosporium*.

1.3 Common Fungal Species

1. Aspergillus spp.- Particularly *Aspergillus flavus* and *Aspergillus niger*, are commonly found in dehydrated produce. *A. flavus* is notorious for producing aflatoxins, which are potent carcinogens and can be hazardous to human health. These fungi thrive in warmer temperatures and relatively dry conditions, making them a concern for dried fruits, nuts, and grains.

2. Penicillium spp.- This fungi are also prevalent in dried fruits and vegetables. While not all species produce mycotoxins, some, like *Penicillium expansum*, can cause soft rots in fruits like apples and pears. *Penicillium* spp. are responsible for characteristic blue-green mold growth and are often found on dehydrated products stored improperly.

3.Fusarium spp- Including *Fusarium oxysporum* and *Fusarium solani*, are common in dried vegetables, particularly in dried tomatoes and peppers. They produce mycotoxins, such as fumonisins, that can contaminate food products and affect both food quality and safety. *Fusarium* spp. thrive in slightly moist environments and can also cause discoloration and off-flavors in dried produce.

4.*Cladosporium* spp.-This fungi are less harmful in terms of mycotoxin production, but they can still cause unsightly mold growth and degradation of dried produce. They are commonly found in dried fruits like apricots, raisins, and figs. These fungi thrive in environments with moderate humidity and temperature, often leading to surface mold growth.

1.4 Factors Influencing Fungal Growth on Dehydrated Produce

Several factors contribute to the susceptibility of dehydrated vegetables and fruits to fungal contamination:

1.Moisture Content and Water Activity -The primary determinant of fungal growth is water activity (aw). As a rule, fungal growth is typically restricted in products with an aw of 0.60 or lower. However, if dehydrated produce absorbs moisture from the surrounding environment during storage, its water activity increases, enabling fungal growth. Even small amounts of moisture can be enough for fungi to begin colonizing the product.

2. Storage Conditions-Improper storage of dehydrated produce is one of the leading causes of fungal contamination. Exposure to fluctuating temperatures and humidity levels can cause rehydration of the produce, making it more vulnerable to mold. It is essential to store dehydrated fruits and vegetables in airtight containers in cool, dry, and dark environments to prevent moisture absorption.

3. **Quality of Dehydration Process** -The method and efficiency of the dehydration process can also influence fungal susceptibility. Under-drying, where moisture content remains too high, provides an environment for fungi to grow. Inadequate drying can also cause uneven moisture distribution within the product, further promoting fungal development.

4. Handling and Packaging -Poor handling practices during the post-dehydration phase, such as improper packaging or contamination during processing, can lead to fungal spore introduction. Packaging materials should be moisture-proof and durable to ensure that fungi do not gain access to the produce once it has been dehydrated.

I.5 Signs of Fungal Contamination

Fungal contamination can manifest in various ways, depending on the species involved. Common signs of fungal attack on dehydrated fruits and vegetables include:

- **Visible Mold Growth**: The most apparent sign of fungal contamination is visible mold growth on the surface of the dried produce. This can appear as blue, green, white, or black patches.
- **Discoloration**: Mold growth can cause discoloration of the product, such as dark spots, faded areas, or a dull appearance.
- **Off Odours**: Fungal contamination often leads to unpleasant odour. These may be musty, earthy, or sour, indicating the presence of mold.
- **Texture Changes**: Fungi can soften the texture of dehydrated produce, causing it to feel mushy or damp. This can result from fungal hyphae invading the cellular structure of the produce.

I.6 Prevention and Management strategies of Fungal Attacks

I.Optimal dehydration technique- Proper dehydration is critical to reducing fungal risks. Dehydrated fruits and vegetables should be dried to the correct moisture levels, generally aiming for a water activity of 0.60 or lower. Efficient drying methods, such as air-drying, freeze-drying, or using heat-based dehydrators, should be employed, with particular attention to the evenness of drying.

2. Controlled Storage-Dehydrated produce should be stored in airtight containers made from moisture-proof materials. Vacuum-sealing is an effective method for minimizing moisture exposure. Storing in cool, dry, and dark environments, such as a sealed cupboard or storage room with controlled humidity levels, is essential. Ideal storage conditions typically maintain a temperature of 15-20°C (59-68°F) and a relative humidity of 50-60%.

3. Use antifungal agents- Some antifungal treatments, such as sulfur dioxide (SO_2) or organic acids like ascorbic acid, can be applied during the dehydration process to inhibit fungal growth. These agents help prevent spoilage and can be particularly useful for fruits like apricots and figs, which are highly susceptible to fungal attacks.

4.Good Manufacturing Practices (GMPs)-Proper sanitation and hygiene practices during the handling, drying, and packaging of produce are critical to minimizing fungal contamination. Ensuring that all equipment, storage areas, and packaging materials are clean and free from contamination is essential.

5. Regular Quality Control -Regular inspection of dehydrated products during storage is important for early detection of fungal contamination. If mold is detected, affected items should be discarded immediately to prevent contamination from spreading to other batches.

I.7 Conclusion

Fungal contamination remains a significant concern for dehydrated vegetables and fruits, but with proper knowledge and practices, it can be managed effectively. By understanding the conditions under which fungi thrive and implementing appropriate preventive measures such as proper drying, storage, and handling, it is possible to significantly reduce the risks associated with fungal attacks. Maintaining stringent hygiene practices and monitoring the quality of dehydrated produce will ensure that these products remain safe for consumption and retain their desired quality.

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Effect of electron irradiation on ZnO nanoparticles prepared by microwave assisted technique

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Abstract:

The nanoparticles of zinc-oxide (ZnO) were synthesized by microwave method followed by calcination at 200°C for the two hours. After characterization with XRD, SEM and EDAX methods, it was observed that the synthesized particles were of ZnO with size ~50 nm. These nanoparticles were irradiated with 6 MeV electrons made available from the Race-Track Microtron of this laboratory. The electron fluence was 2.5 x10^{15} e^- / cm^2. The average particle size reduced from ~ 50 nm to ~20 nm at an electron fluence of 2.5x10^{15} e^- / cm^2.As revealed from the UV measurements, the band gap of ZnO increased from the virgin value of 3.33 eV to 3.45 eV at an electron fluence of. ~ 2x10^{15} e^- / cm^2 .The results indicate that by electron irradiation the particle size of ZnO can be tailored to suit for the applications in the field of photovoltaics and photo cells.

This study provides a comprehensive understanding of how electron irradiation can be used to fine-tune the properties of ZnO nanoparticles prepared via the microwave-assisted technique, offering insights for future applications in various technological fields.

Keywords: *ZnO nanoparticles, electron irradiation, microwave-assisted synthesis, structural properties, X-ray diffraction (XRD), scanning electron microscopy (SEM), UV-Vis spectroscopy.*

Introduction:

Nanotechnology and nanoscience are the study and application of extremely small objects with dimensions ranging from one to one hundred micrometers. Nanotechnology is being used in fields such as chemistry, biology, physics, materials science, and engineering [1]. Nanoparticle synthesis the term to refers the process of making nanoparticles by combing two or more ingredients into one [2, 3]. Nanoparticles exhibit unique physical, chemical, and green features that are not found in bulk materials [4]. This unique physicochemical property, along with other specific features of metallic nanoparticles such as small size, high surface to volume ratio, surface charge, and surface chemistry, provide a significant opportunity to design diagnostic agents for diagnostic purposes and targeted drug delivery systems, in addition to benefiting from the intrinsic pharmaceutical potential of these nanoparticles [5–7].

Zinc Oxide (ZnO) is a widely studied material known for its exceptional properties, including a wide band gap (~3.37 eV), high electron mobility, high surface area, biocompatibility, and chemical stability, making it suitable for a wide range of applications such as photocatalysis,

sensors, optoelectronics, and environmental remediation [8,9]. The increasing interest in ZnO nanoparticles (ZnO-NPs) is attributed to their enhanced properties compared to bulk ZnO, particularly at the nanoscale, where their high surface-to-volume ratio and tunable size and morphology are crucial factors influencing their performance in various applications [10, 11]. ZnO-NPs are commonly used in environmental remediation, UV-blocking, and electronic devices because of their unique optical and electrical properties [12, 13]. The synthesis of ZnO-NPs has been carried out using various techniques such as sol-gel, hydrothermal, and chemical vapour deposition. Among these, the microwave-assisted synthesis method has gained prominence due to its simplicity, cost-effectiveness, and rapid processing time. This method allows precise control over the size, morphology, and crystallinity of the nanoparticles [14, 15]. The microwave-assisted technique also provides energy-efficient and environmentally friendly processing, which makes it ideal for large-scale production of ZnO nanoparticles [16, 17]. Electron irradiation is a widely employed technique for modifying the properties of nanomaterials. When exposed to electron beams, ZnO nanoparticles undergo changes in their structural and functional properties due to the introduction of defects, such as vacancies, interstitials, and dislocations [18]. These defects can significantly affect the optical, electrical, and photocatalytic properties of ZnO, leading to enhanced performance in various applications, including photocatalysis and electronic devices [19, 20]. Electron irradiation can also induce lattice strain, which influences the photoluminescence and absorption characteristics of ZnO [21].

In recent years, studies have shown that electron irradiation can be used to modify the electronic band structure and enhance the conductivity of ZnO, making it more suitable for applications in electronic and optoelectronic devices [22]. For example, irradiation can introduce shallow donor states in ZnO, improving its electronic conductivity [23]. However, the impact of electron irradiation on ZnO nanoparticles synthesized through the microwave-assisted technique remains underexplored, particularly with regard to the interplay between irradiation dose and the structural, optical, and electrical properties of the material.

This study aims to investigate the effects of electron irradiation on ZnO nanoparticles synthesized via the microwave-assisted method. By exposing these nanoparticles to varying doses of electron irradiation, we seek to understand how the structural defects, optical absorption, and electrical conductivity are influenced by the irradiation process. The findings from this study are expected to provide valuable insights for tailoring the properties of ZnO nanoparticles for advanced technological applications, such as optoelectronics, photocatalysis, and sensors.

Experimental

Reagents

Zinc acetate, sodium hydroxide and ethylene glycol were used for the synthesis. All solutions were prepared in distilled water only. Zinc oxide nanorods were prepared by the reaction of 0.1M of zinc acetate with 1:1 NH_3. The ethylene glycol used as a capping agent for particle stabilization. pH of the solution was controlled by the addition of 1:1 NH_3 into the reaction mixture. A commercial microwave oven with adjustable power output upto 750W was used.

Preparation of nanoparticles

The nanosized ZnO nanorods were prepared by microwave-assisted method. Aqueous solution of zinc acetate (0.1M) and ethylene glycol (2-3 ml) was added. The solution thus prepared was set to stir constantly with addition of solution 1:1 NH_3 simultaneously for half an hour. After completion of the reaction, white precipitate of zinc hydroxide was produced. The precipitated zinc hydroxide solution was kept for 10 minutes under microwave irradiation with a power output of 750W by following on-off cycle. The solution was allowed to cool upto room temperature. The cooled solution was then centrifuged in presence of water and acetone to remove all the impurities. The process of centrifugation was repeated three times to remove most of the impurities from the solution and allowed to dry naturally. Annealing of the product was carried

out at 200°C for three hours in temperature controlled furnace. The pure annealed powder of ZnO was used for the irradiation.

The schematic flow chart for preparation of nanocrystalline ZnO is given in Fig.1.

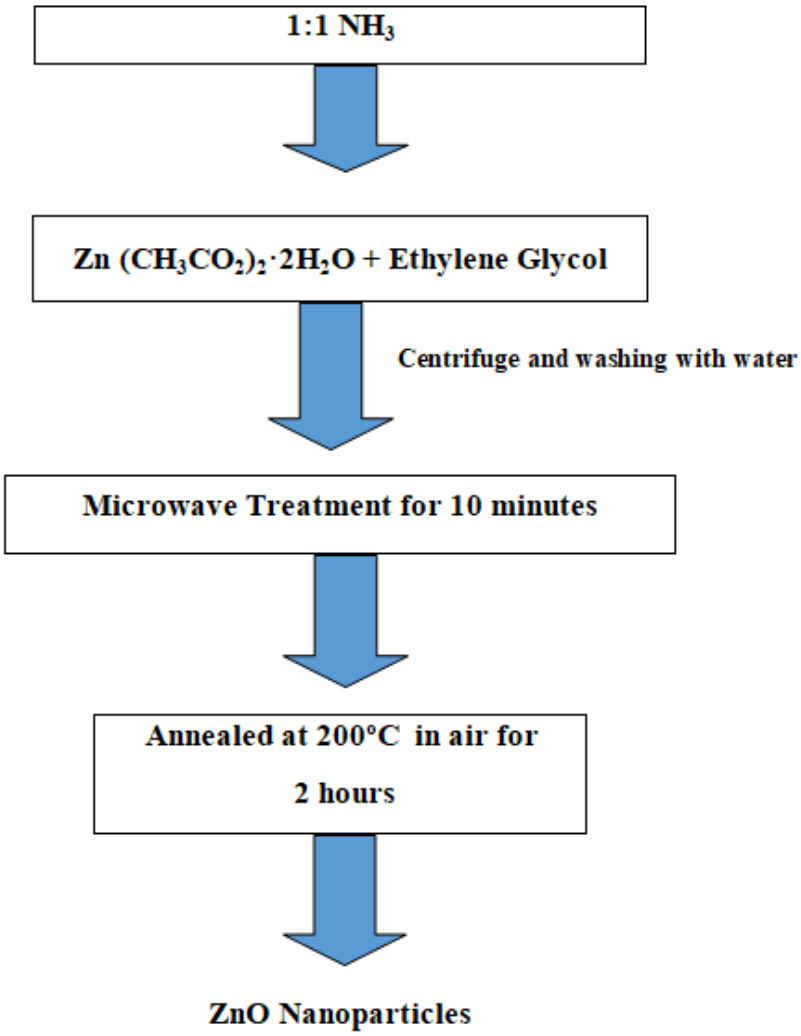


Fig.1. Schematic flow chart for the preparation of nanocrystalline ZnO

Irradiation of nanoparticles

The electron irradiation facility, designed and fabricated in this laboratory [24], was used in the present study. A schematic diagram of the experimental set-up is shown in figure 1. The main parts of this system are a multi-port cylindrical shape S.S chamber, electron gun, electron collimators, Faraday cup/sample holder, current meter, high and low voltage power supplies and isolation transformer. The electron gun assembly was mounted to one of the closing flanges of the chamber. A Faraday cup/sample holder (10 mm × 10 mm) was attached to one end of the S.S rod, which could be displaced linearly through the Wilson seal, which is fixed to one of the ports of the chamber. This Faraday cup was connected to a current meter through one of the feed-through mounted on the ports of the S.S chamber. Using a rotary-diffusion pumping system, along with a LN_2 trap, a pressure of $\sim 10^{-6}$ mbar was maintained inside the S.S chamber during the measurements. The electron gun can provide electrons of different energies in the range of 1–20 keV, beam diameter varied from 5 to 120 mm and beam current from 10 nA to 50 μA. The electron collimator could refine the shape of the electron beam on the Faraday cup/sample holder.

An electron beam of energy in MeV was used in this study. To begin, one ZnO sample was fixed on the Faraday cup mounted inside the chamber of the electron irradiation system. The electron beam was incident on the sample by keeping the beam diameter ~15 mm and energy in MeV and the sample was irradiated. During the irradiation, the beam current was kept constant at 100 nA and the electron beam was turned off as soon as the coating sample received an electron fluence ~$2.5X10^{15}$ e cm^{-2}. The chamber pressure was brought to atmospheric conditions and the electron-irradiated coating was removed from the chamber. Another ZnO sample was then mounted on the Faraday cup and the system was evacuated and the sample were irradiated with to the fluence of $2.5X10^{15}$ e cm^{-2} .

Characterization of ZnO nanomaterials

ZnO samples irradiated with electrons of 6MeV energy at the fluence of 2.5 $x10^{15}$ e^- / cm^2 were characterized by the UV–vis, XRD, SEM and FTIR techniques. Typical UV–vis spectra of the electron-irradiated samples are shown in figure 2. The structure of the ZnO particles was studied by the XRD technique and the recorded spectra of the samples irradiated at different doses are shown in figure 3. The X ray diffraction (XRD) pattern of the final ZnO nanoparticles was obtained with Cu Kα radiation (λ = 1.5418 ° A) on a Bruker axs D8 Advanced diffractometer (CuK_α radiation) at a continuous scan rate of $1\text{-}2^0$ /min with 0.1^0 resolution.and the mean grain size (D) of the particles was determined from the XRD line-broadening measurement from the Scherrer equation

$$D = 0.89\lambda/(\beta \cos \theta)$$

Where λ is the wavelength (Cu Kα), β is the full width at the half-maximum and θ is the diffraction angle. The peak positions and relative intensities were characterized by comparison with the Joint Committee for Powder Diffraction Standards (JCPDS) card no 36-1451 for examining the phase structure and purity.

Result and Discussion

UV-Visible

The absorbance maxima and corresponding band gap values are presented in table. It can be clearly seen from the figure that the maximum of the absorbance shifts toward lower wavelength. Consequently, the band gap increases gradually as compared to that of pure ZnO.

This could be mainly attributed to quantum size effect as well as the strong interaction between the surface oxides of zinc and irradiation electrons. This observation strongly suggest that the irradiation significantly affects the particle size and hence the absorption properties. Moreover, these results are in good agreement with the conclusion derived from the XRD results.

Sample	λ_{max} (nm)	Bandgap (eV)
Pure ZnO	372	3.33
Irradiated ZnO ($2.5X10^{15}$ e^- / cm^2)	365	3.45

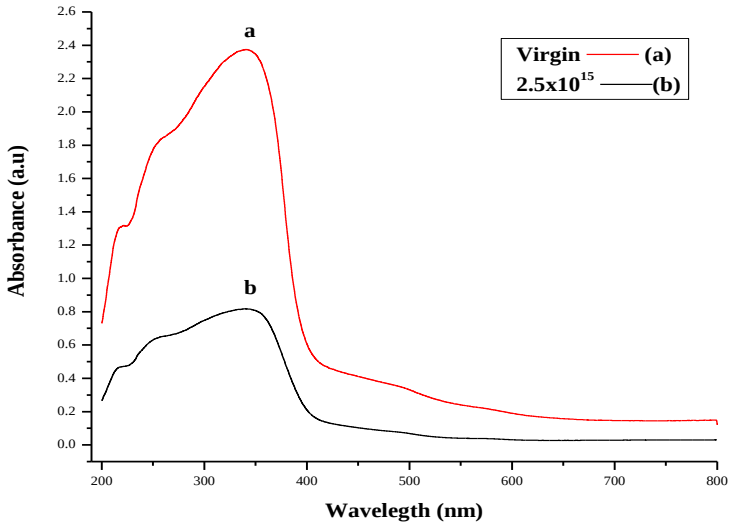


Fig. 2. UV-Visible spectrum of (a) ZnO virgin and (b) ZnO irradiated with $2.5x10^{15}$ e^- / cm^2

X-Ray diffraction

As prepared ZnO nanoparticles irradiated at different temperatures were characterized by XRD analysis shown in Fig.3 All peaks are identical to those of hexagonal phase with wurtzite structure and were closed to JCPD data (JCPDF No. 36-1451) [25]. Diffraction peaks at the scattering angles 2□ = 31.71, 34.49, 36.24, 47.52, 56.69, 62.87, 66.38, 67.85, and 69.07° to the reflections from the planes [100], [002], [101], [102], [110], [103], [200], [112], [201].The lattice parameters were found to be a = 3.25 Å and c = 5.23 Å. The amorphous nature of the ZnO formed at room temperature is due to the non-availability of sufficient thermal energy for the diffusion of atom on the surface for nucleation. It is observed that crystallinity of the ZnO increases by increasing the irradiation dose. At irradiation dose of $2.5x10^{15}$ e^- / cm^2, Fig.1 (b), the ZnO forms a well nanosized rod of optimum 25 nm size of the particles.

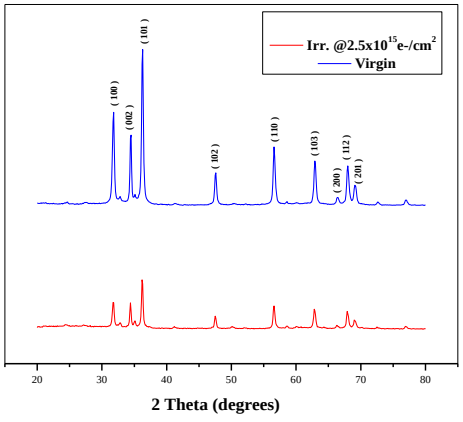
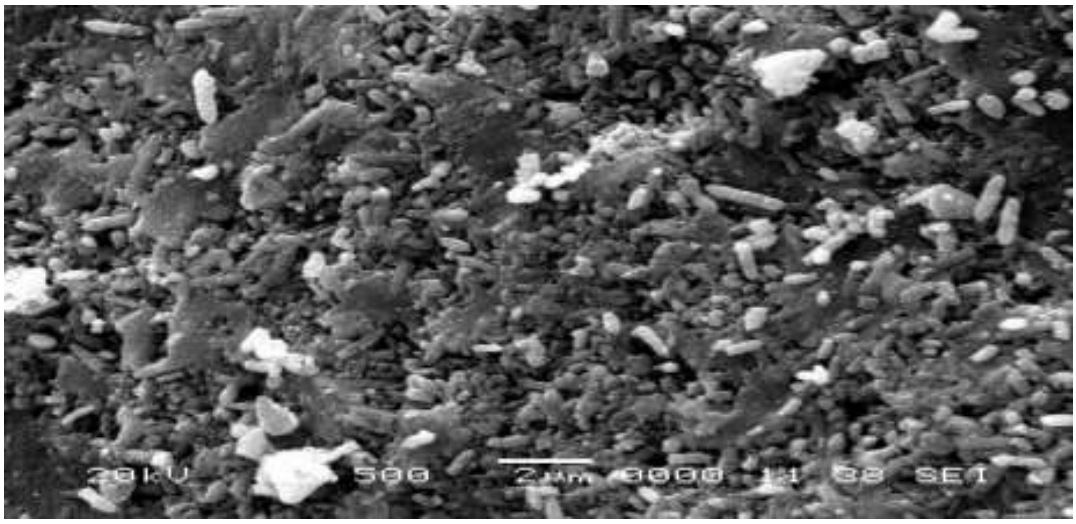


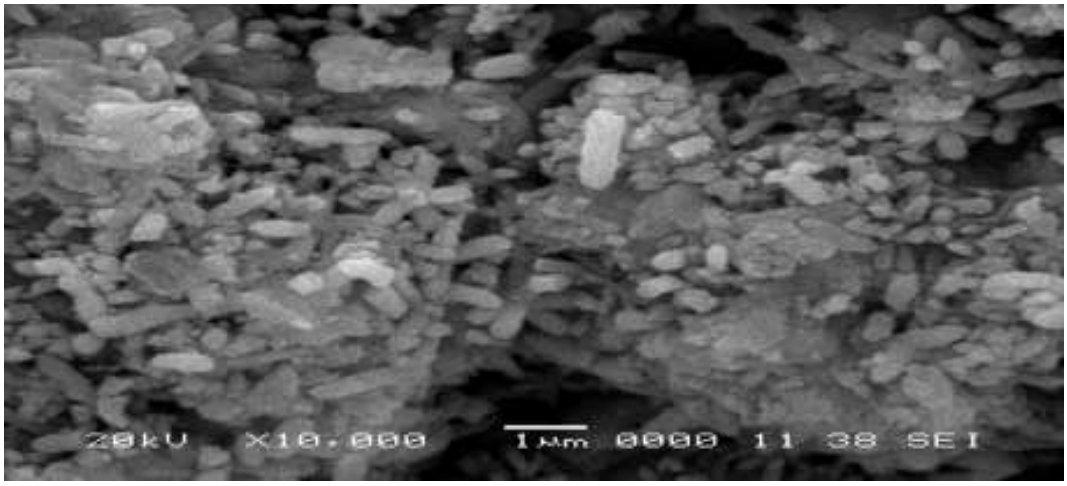
Fig. 3. XRD spectra of ZnO virgin (and ZnO irradiated with $2.5x10^{15}$ e^- / cm^2

Scanning electron micrographs

The SEM photographs of samples irradiated with 6 MeV electrons at a fluence of 2.5 x10^{15} e^- / cm^2 are shown in figure 4. From the SEM photographs, it is observed that the average size of the ZnO particles is 25 nm in the 2.5x10^{15} e^- / cm^2 irradiated sample.



(a)



(b)

Fig. 4. SEM photographs of (a) ZnO virgin (c) and ZnO irradiated with 2.5x10^{15} e^- / cm^2

Conclusion

We have developed a new, rapid, eco-friendly and energy saving microwave assisted method for the synthesis of ZnO nanorods. The microwave method is very simple to implement, and can be easily extended to the preparation of other oxide nanoparticles. Nanosized ZnO particles are synthesized followed by 6Mev electron. The irradiation dose must be carefully controlled to optimize the performance of ZnO nanoparticles for specific applications, such as photocatalysis, sensors, and optoelectronic devices. The creation of defects, including oxygen vacancies and zinc interstitials, plays a crucial role in modifying the properties of the nanoparticles. The shape of particle was nanorods with wurtzite structure. The size of nanorods reduced from 50nm to 20 nm after the electron irradiation. The particle size determined by SEM were well agree with the XRD studies.

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Synthesis & Characterization of Asian Pigeon (Clitoria Ternatea) Derived Dye as Phyto-Based Substitute for Synthetic Methylene Blue ($C_{16}H_{18}ClN_3S$)

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Abstract:

Methylene Blue is a widely used redox indicator in chemical and biological applications due to its reversible oxidation-reduction properties. This study focuses on the extraction and analysis of Methylene Blue-like compounds from the Asian pigeon flower (Clitoria ternatea), a plant known for its rich anthocyanin and flavonoid content. The extraction process involved solvent-based techniques to isolate the pigment, followed by spectroscopic and chromatographic analyses to determine its chemical composition and redox behavior. UV-Vis spectrophotometry confirmed absorption peaks characteristic of Methylene Blue. The study also evaluated the indicator's stability, colorimetric response to pH variations, and potential applications in analytical chemistry. The findings suggest that Clitoria ternatea could serve as a natural source for redox-active compounds, offering sustainable alternatives for synthetic indicators in various scientific and industrial applications.

Keywords: *Anthocyanin, Flavonoids, Methylene Blue, Absorbance, pH , Spectroscopy.*

Introduction:

Methylene Blue is a well-known redox indicator widely used in analytical chemistry, biology, and medical applications due to its reversible oxidation-reduction properties. It serves as a vital tool in redox titrations, biological staining, and even as a therapeutic agent. However, the growing demand for sustainable and eco-friendly alternatives has led researchers to explore natural sources of similar compounds.

The Asian pigeon flower (Clitoria ternatea), commonly known as the butterfly pea, is a rich source of anthocyanins, flavonoids, and other bioactive pigments. Its deep blue coloration, which shifts with pH variations, suggests potential redox activity similar to Methylene Blue. Traditional applications of C. ternatea include natural food coloring, herbal medicine, and pH-sensitive dyes, but its potential as a redox indicator remains underexplored.

This study aims to extract and analyze Methylene Blue-like compounds from Clitoria ternatea, evaluating their chemical properties, stability, and indicator potential. Through spectroscopic and chromatographic techniques, the study seeks to determine whether the plant-based extract can serve as a viable alternative to synthetic Methylene Blue. The findings could contribute to the development of sustainable natural indicators for use in chemical analysis, environmental monitoring, and various industrial applications

Literature Reviews:

•Methylene Blue and Its Applications -

Methylene Blue is a synthetic heterocyclic aromatic compound widely used in analytical chemistry, biology, and medicine due to its reversible oxidation-reduction properties (Gorman et al., 2010). It is commonly employed in redox titrations, where it shifts between its oxidized (blue) and reduced

(colorless) forms. Additionally, Methylene Blue is used in microbial staining and as a therapeutic agent in conditions such as methemoglobinemia and neurodegenerative diseases (Wainwright & Crossley, 2002). However, synthetic dyes like Methylene Blue pose environmental risks due to their non-biodegradable nature, leading to interest in plant-based alternatives (Lyon et al., 2020).

•Natural Pigments as Chemical Indicators -

Natural plant pigments, particularly anthocyanins, flavonoids, and betalains, have been extensively studied for their potential use as pH and redox indicators. Anthocyanins, commonly found in flowers, fruits, and vegetables, are known for their color variability depending on pH. They transition from red in acidic conditions to blue or green in alkaline environments (Harborne & Williams. 2000).

A study by Torskangerpoll and Andersen (2005) demonstrated that anthocyanins extracted from red cabbage and hibiscus could function as pH indicators in various applications. Similarly, research by Zhang et al. (2014) explored the use of flavonoid-rich plant extracts in redox titrations, finding that some flavonoids exhibit reversible redox behavior similar to synthetic indicators.

•Chemical Composition and Properties of Clitoria ternatea -

The Asian pigeon flower (Clitoria ternatea) is well known for its deep blue pigments, which are primarily composed of anthocyanins, particularly ternatins (Kazuma et al., 2003). These compounds are responsible for the flower's characteristic color and exhibit significant pH-dependent behaviour. Research by Srivastava et al. (2018) confirmed that C. ternatea anthocyanins exhibit colour changes from blue in neutral and alkaline solutions to purple and pink in acidic conditions.

A study by Lim et al. (2021) analyzed C. ternatea extracts using UV-Vis spectroscopy and HPLC, identifying major anthocyanins and flavonoids responsible for their stability and color-changing properties. Wong et al. (2019) further investigated the redox properties of C. ternatea anthocyanins and found that they can undergo oxidation-reduction reactions, making them potential alternatives to synthetic indicators.

•Spectroscopic and Chromatographic Studies on Clitoria ternatea -

Various spectroscopic and chromatographic methods have been used to analyze Clitoria ternatea pigments.

UV-Vis Spectroscopy: Studies have shown that C. ternatea extract exhibits strong absorbance in the visible region (500-700 nm), similar to synthetic dyes like Methylene Blue (Lim et al., 2021).

High-Performance Liquid Chromatography (HPLC): HPLC analysis has revealed that ternatins are the primary anthocyanins responsible for the blue coloration and redox properties (Kazuma et al., 2003).

Fourier Transform Infrared Spectroscopy (FTIR): FTIR studies have identified functional groups associated with flavonoids and anthocyanins, confirming the structural similarities between C. ternatea pigments and synthetic indicators (Wong et al., 2019).

•Stability and Practical Applications of Clitoria ternatea Extracts -

One of the key considerations for using natural pigments as indicators is their stability. Studies by Kumar et al. (2020) showed that C. ternatea anthocyanins exhibit high thermal and oxidative stability compared to other plant-derived indicators. This makes them suitable for use in food quality monitoring. Environmental testing, and analytical chemistry.

Additionally, C. ternatea extracts have been tested as biosensors in environmental applications. A study by Roriz et al. (2017) demonstrated that anthocyanin-based sensors from C. ternatea could detect pH changes in food and water samples.

•Comparison of Clitoria ternatea with Other Natural Indicators -

Several plant sources have been studied for their potential as chemical indicators, including:

Red Cabbage (Brassica oleracea): Contains anthocyanins that shift from red (acidic) to green (alkaline) (Torskangerpoll & Andersen, 2005).

Hibiscus (Hibiscus sabdariffa): Rich in flavonoids and anthocyanins, with pH-sensitive color variations (Zhang et al., 2014).
Beetroot (Beta vulgaris): Contains betalains with pH-dependent color changes but lacks strong redox activity (Sreekanth & Nair. 2019).
Comparatively, Clitoria ternatea offers superior stability and a well-defined color transition range, making it a strong candidate for replacing synthetic redox indicators.

•Conclusion from literature -

The literature highlights Clitoria ternatea as a promising natural alternative to synthetic redox indicators like Methylene Blue. Its rich anthocyanin content, stability, and reversible color changes make it a strong candidate for use in analytical chemistry and environmental monitoring. However, further research is required to refine extraction methods, ensure long-term stability, and validate its effectiveness in industrial applications.

Theory:

•Redox Indicators -

A redox indicator is a compound that undergoes a distinct colour change due to an oxidation-reduction (redox) reaction. These indicators function by shifting between their oxidized and reduced forms, which have different colours, making them useful for titrations and electrochemical analysis.

•Methylene Blue as a Redox Indicator -

Methylene Blue is a synthetic redox indicator with the following oxidation-reduction reaction:

$MB^+ + 2e^- + H^+ \rightarrow MBH$

Where:

Oxidized form appears blue. Reduced form is colourless.

Methylene Blue is widely used due to its stability and sharp colour transition, but its synthetic nature raises environmental concerns, leading to interest in plant-based alternatives.

•Chemistry of Natural Pigments in Clitoria ternatea -

The Asian pigeon flower (Clitoria ternatea), also known as butterfly pea, contains natural anthocyanins, specifically ternatins, which exhibit pH-sensitive and redox-responsive color changes. Anthocyanins are flavonoid compounds with a core flavylium ion structure, making them highly reactive in oxidation-reduction processes.

•Redox Properties of Clitoria ternatea -

The anthocyanins in C. ternatea exhibit similar redox behavior to Methylene Blue:
Oxidized state: Deep blue colour.
Reduced state: Lighter or colourless depending on the medium.
These redox-sensitive changes indicate that C. ternatea extracts could function as natural alternatives to Methylene Blue.

•pH-Dependent colour Transitions -

Anthocyanins are known for their pH-dependent color variation, which is also relevant for their redox activity:
Acidic pH (<4): Red (flavylium ion)
Neutral pH (5-7): Deep blue (quinonoidal base)
Alkaline pH (7): Green/yellow (chalcone form)
These properties make C. ternatea an ideal candidate for replacing synthetic indicators in titrations and biochemical applications.

•Extraction of Pigments from Clitoria ternatea -

Solvent Extraction Method:

The extraction of anthocyanins from Clitoria ternatea involves solvent-based techniques to isolate the active pigments. The most commonly used solvents include:
Ethanol-water mixtures (with mild acid) to enhance anthocyanin solubility. Methanol and acetone for stronger pigment extraction.

The steps for extraction include:

1. Flower Collection and Drying: Fresh C. ternatea flowers are collected and air-dried.
2. Grinding: Dried petals are ground into fine powder.
3. Solvent Extraction: The powder is mixed with ethanol (pH-adjusted), stirred, and filtered.
4. Concentration: The solvent is evaporated, leaving behind the anthocyanin-rich extract.

•Spectroscopic and Chromatographic Analysis -

UV-Vis Spectroscopy:

UV-Vis spectrophotometry is used to determine the absorption spectrum of the extract. Methylene Blue typically shows a strong absorption peak at 660 nm, whereas C. ternatea anthocyanins exhibit peaks in the 500-700 nm range, confirming their redox activity (Lim et al., 2021).

•Redox Behaviour Testing -

The extract is tested in oxidation-reduction reactions to evaluate its indicator potential. This includes:

Titration with reducing and oxidizing agents to observe colour changes

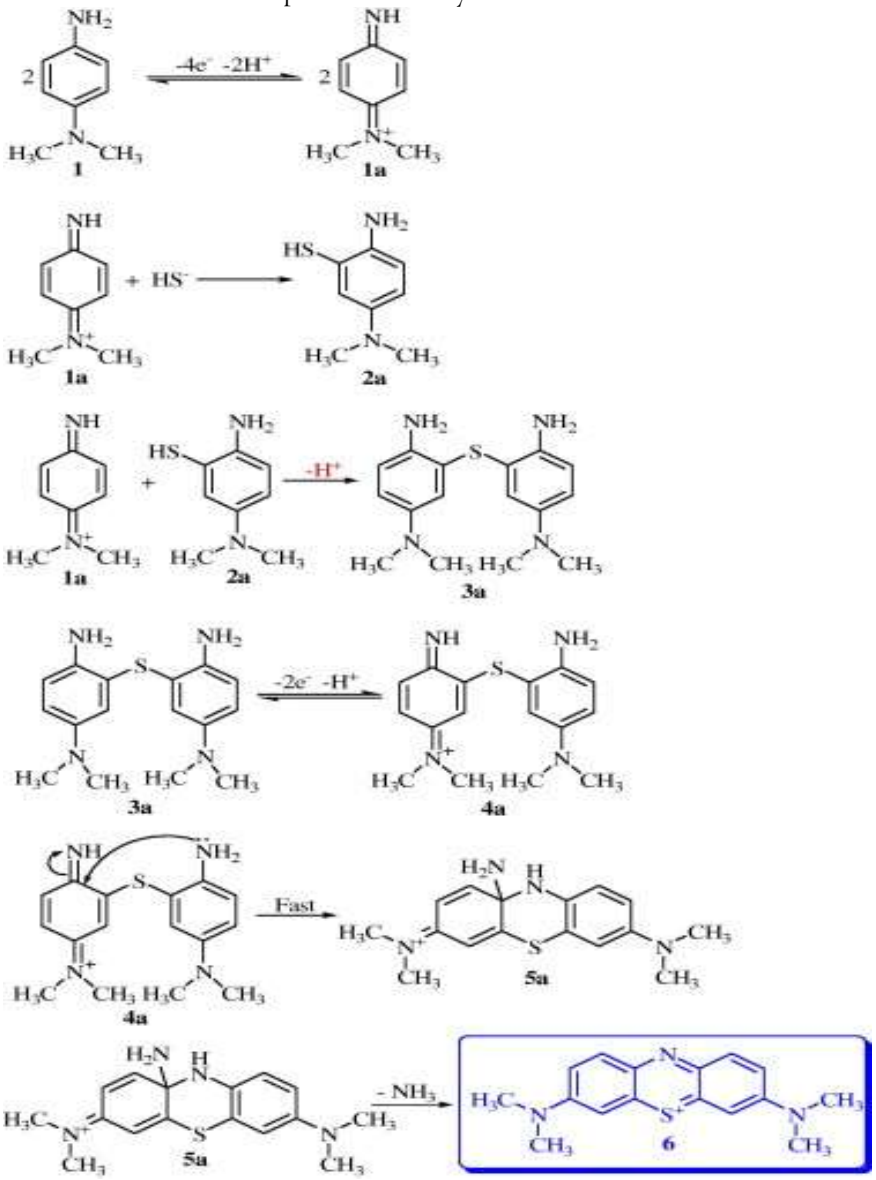
Electrochemical analysis to measure oxidation-reduction potential.

Methodology:

Synthesis of Methylene Blue from Asian Pigeon (C. Ternatea):

1. Collection and Pre-treatment of Floral Material:
   Fresh and healthy blue-colored flowers (such as Clitoria ternatea, commonly known as butterfly pea) are carefully collected, preferably in the morning hours when the pigment content is at its peak. The flowers are gently washed with clean water to remove any dust, dirt, or other impurities. The cleaned flowers are then air-dried slightly on a paper towel to remove excess surface moisture.
2. Homogenization:
   The cleaned flowers are then transferred to a clean mortar and crushed using a pestle to form a coarse paste. Alternatively, a blender can also be used for better homogenization. This process helps in breaking down the cellular structure of the petals, allowing the release of pigments and other bioactive compounds.
3. Filtration:
   To the crushed floral paste, approximately 50–100 ml of distilled water is added. The mixture is stirred thoroughly to extract the water-soluble pigments into the liquid phase. This mixture is then filtered using a filter paper or a clean muslin cloth to remove solid plant residues. The clear blue extract thus obtained is collected in a clean beaker or container.
4. Storage:
   The freshly prepared floral extract is sensitive to light and temperature. To preserve its color and chemical integrity, it is stored in an amber-colored glass container to protect it from light exposure. The container is then kept at 4°C (refrigerator temperature) until further use.
   Commercial Synthesis of Methylene Blue (Electrochemical Method):
1. Starting Materials:
   The process begins with N,N-dimethylaniline as the primary aromatic amine. This compound serves as the core structure for methylene blue. Other chemicals used include sodium thiosulfate, sodium nitrite, and hydrochloric acid.
2. Oxidation Reaction:
   The synthesis involves oxidative coupling of two molecules of N,N-dimethylaniline. This step is carried out in an acidic medium, where the amine undergoes an electrochemical oxidation at the anode, forming a reactive intermediate.
3. Thiosulfate Involvement:
   Sodium thiosulfate is introduced into the reaction mixture. It acts as a sulphur donor, helping to form the characteristic thiazine ring of methylene blue.

4. Ring Closure and Colour Development:
   A complex reaction sequence follows, involving ring closure and further oxidation, eventually forming the phenothiazinium core of methylene blue. The intense blue colour starts to develop as the final structure is stabilized.
5. Electrochemical Cell Setup:
   An electrochemical cell is used for controlled oxidation, with a graphite or platinum electrode as anode and a stainless steel or inert electrode as cathode. A DC power supply drives the redox reactions efficiently and in a controlled manner.
6. Crystallization and Purification:
   After synthesis, the reaction mixture is cooled and the methylene blue is precipitated by adjusting the pH. The crude product is filtered, washed, and then purified by recrystallization, typically using water or alcohol to yield high-purity methylene blue crystals.
7. Drying and Packaging:
   Finally, the pure methylene blue crystals are dried under vacuum or mild heat and then packed in light-resistant containers to preserve stability.



Comparison:

While floral extraction offers an eco-friendly, simple approach for natural pigments, commercial electrochemical synthesis of methylene blue is a precise, multistep process that ensures high purity and large-scale production.

Comparative Analysis of Methylene Blue(MB) Extracted from Asian Pigeon and Commercially Synthesized:

1) **pH**

- pH of MB extracted from Asian Pigeon:



Shows a Neutral pH of 7.0:

The natural extract obtained from Clitoria ternatea exhibits a stable and neutral pH value of approximately 7.0. This pH level is ideal for most biological and analytical applications, as it does not interfere with cellular structures or biochemical reactions, ensuring safety and compatibility.

Free from Synthetic Additives or pH Modifiers:

The extract is purely natural and does not contain any artificial chemicals, stabilizers, or pH-altering substances. This makes it highly suitable for experiments or products where chemical purity and natural composition are of critical importance.

Derived from Biological Sources (i.e., Clitoria ternatea):

This pigment is extracted from the petals of Clitoria ternatea, a flowering plant known for its vibrant blue anthocyanin compounds. Being plant-derived, it is a renewable and sustainable source of colorant, offering a natural alternative to synthetic dyes.

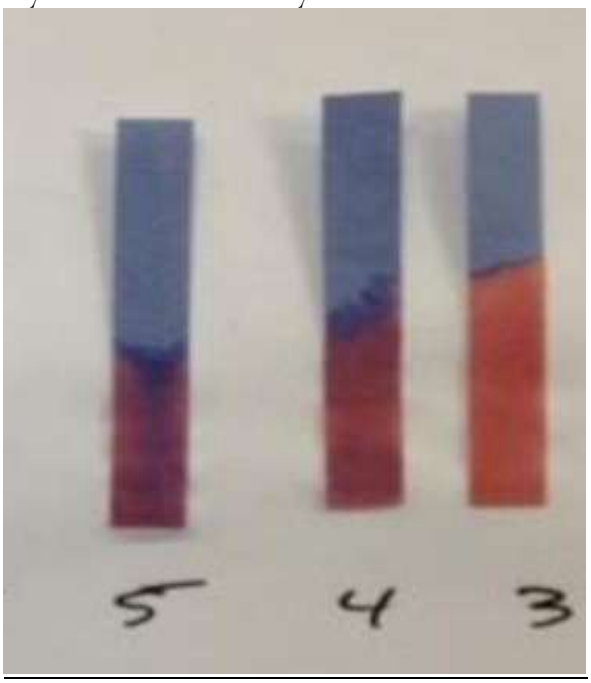
Biocompatible and Suitable for Direct Biological Use:

Due to its natural origin and non-toxic composition, the extract demonstrates excellent biocompatibility. It can be used in biological assays, live-cell staining, or educational demonstrations without causing harm to living organisms or delicate experimental systems.

Eco-Friendly Due to Its Natural and Neutral Nature:

The extraction and use of this floral pigment have minimal environmental impact. The process involves simple, water-based methods and does not generate hazardous waste, making it an environmentally responsible choice for both research and commercial applications.

•pH of Methylene Blue Synthesized Commercially from Electrochemical Method:



pH Usually Ranges from 4.0 to 6.0 (Slightly Acidic):
Commercial methylene blue solutions often exhibit a pH in the slightly acidic range, typically between 4.0 to 6.0. This is due to the nature of the synthesis process and the chemical environment required for its stabilization and storage.
Contains Preservatives and Stabilizers that may alter pH:
In order to enhance shelf-life and maintain dye stability, various preservatives, surfactants, and stabilizing agents are added during manufacturing. These chemical additives can influence the overall pH and may cause variations between different batches.
Chemically synthesized may involve acidic intermediates:
Methylene blue is synthesized via multi-step chemical pathways that often utilize acidic intermediates and strong oxidizing agents. This makes the process highly controlled but also chemically intensive, involving materials that can be corrosive or reactive.
May need pH adjustment for biological applications:
Due to its acidic nature and chemical content, methylene blue often requires pH adjustment before being applied in biological or clinical settings to avoid damaging sensitive cells, tissues, or organisms.
Can produce acidic waste, affecting the environment:
The synthetic production and use of methylene blue generate chemical waste, which may include acidic by-products and harmful reagents. Improper disposal or handling of these materials can lead to environmental pollution and ecological imbalance.
•Comparative Summary:
Natural floral extract from Clitoria ternatea is eco-friendly, biocompatible, and pH-neutral, making it ideal for direct biological use without modification; whereas commercial methylene blue, though precise and widely used, is chemically synthesized, slightly acidic, and may require pH adjustments and careful disposal due to potential environmental impact.

2) **Conductivity**

•Conductivity of Methylene Blue extracted from Asian Pigeon flower :
In our investigation, the electrical conductivity of the naturally extracted blue dye from Clitoria ternatea was measured and found to be approximately 0.61 μS/cm. This relatively low conductivity is indicative of its mild ionic character, as expected from a water-based plant extract that lacks

added salts or ionic compounds. The minimal conductivity suggests the absence of strong electrolytes and highlights the extract's natural purity, making it favorable for use in bioelectrical systems, sensors, or electrochemical studies where minimal background interference is desired. Moreover, such low conductivity ensures reduced electrochemical noise, making it potentially suitable for applications in biological environments where electrical stability is crucial.

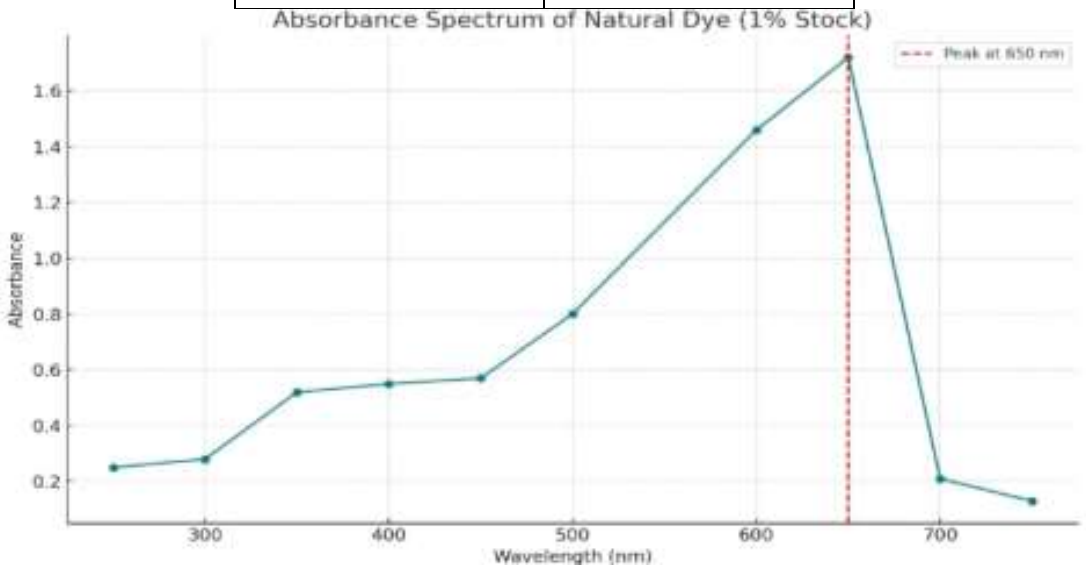
•Conductivity of Commercially Synthesized Methylene Blue-

In contrast, commercially synthesized methylene blue typically exhibits significantly higher conductivity, often in the range of tens to hundreds of μS/cm, depending on concentration and the presence of ionic stabilizers, such as chlorides or sulphates. This is due to the ionic nature of the synthetic dye, which is commonly stabilized in salt form (e.g., methylene blue chloride). While this enhances solubility and shelf-life, it also introduces electrolytic activity, which can interfere with sensitive biological assays or electrochemical measurements.

3) **Absorbance:**

• Absorbance of Methylene Blue Extracted from Asian Pigeon:

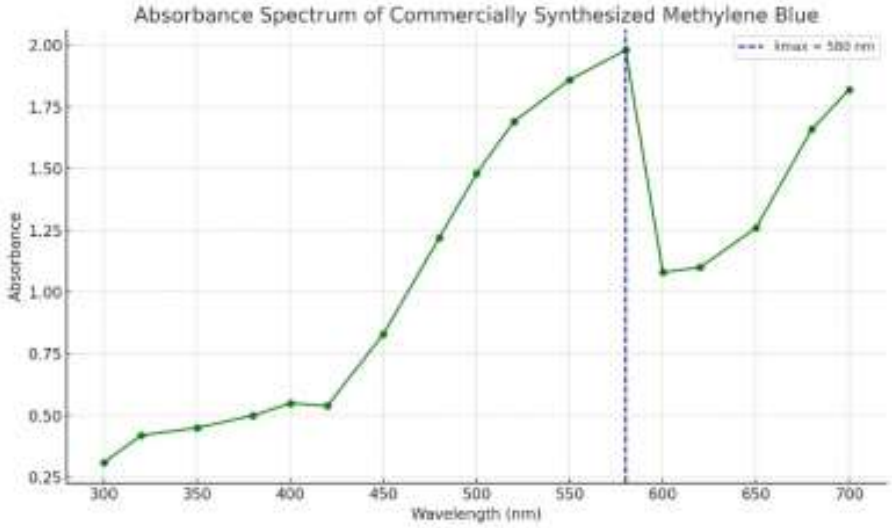
Wavelength (nm)	Absorbance
250	0.25
300	0.28
350	0.52
400	0.55
450	0.57
500	0.80
600	0.46
650	**1.72**
700	0.21
750	0.13



This graph represents the absorbance profile of a naturally extracted dye from Clitoria ternatea flowers across wavelengths ranging from 250 nm to 750 nm. A significant peak is observed at 650 nm, indicating maximum absorbance in the visible region, characteristic of methylene blue chromophores. The spectrum confirms the presence of anthocyanin-based blue pigments, supporting the effectiveness of Clitoria ternatea as a natural, plant-derived alternative to synthetic dyes.

•Absorbance of Methylene Blue Extracted from Asian Pigeon:

Wavelength	Absorbance
300	0.31
320	0.42
350	0.45
380	0.50
400	0.55
420	0.54
450	0.83
480	1.22
500	1.48
520	1.69
550	1.86
580	**1.98**
600	1.08
620	1.10
650	1.26
680	1.66
700	1.82



In the above graph, the commercially synthesized methylene blue exhibits a prominent absorbance peak at 580 nm, which corresponds to its characteristic electronic transitions within the phenothiazine ring structure. This sharp peak confirms its high purity and strong absorption in the visible region, making it suitable for various analytical, medical, and industrial applications.

•Comparative Summary:

The natural methylene blue extract from Clitoria ternatea shows peak absorbance at 650 nm, indicating a plant-based anthocyanin profile, while the commercial methylene blue peaks at 580 nm, reflecting its synthetic phenothiazine structure. This spectral difference highlights their distinct molecular compositions and potential applications.

Results & Discussion:

The present study focused on evaluating Clitoria ternatea (Asian pigeon flower) as a natural and sustainable source of methylene blue-like dye. The extracted pigment exhibited promising characteristics in terms of pH stability, absorbance spectrum, and electrical conductivity.

pH Analysis revealed a neutral pH of 7.0 for the Clitoria ternatea extract, making it biocompatible and well-suited for biological applications without the need for chemical adjustments. In contrast, the commercial methylene blue showed a slightly acidic pH (4.0–6.0) due to synthetic intermediates and added preservatives, which may require buffering for safe biological use.

Conductivity measurements further highlighted the natural extract's gentle chemical profile. The Clitoria ternatea extract recorded a low conductivity of 0.61 μS/cm, pointing to its minimal ionic load and making it ideal for electrochemical applications where background interference must be minimal. In comparison, the commercial dye showed much higher conductivity, indicating the presence of ionic salts like chlorides or sulfates, which can interfere with delicate electrochemical systems.

Spectrophotometric analysis using UV-Vis spectroscopy confirmed key optical properties. The natural extract demonstrated a major absorbance peak at 650 nm, typical of anthocyanin-rich compounds. This peak supports the extract's identity as a plant-based chromophore, distinct from synthetic dyes. Conversely, the synthetic methylene blue presented a sharp peak at 580 nm, which aligns with its phenothiazine structure and confirms its commercial purity.

Together, these results suggest that Clitoria ternatea possesses properties similar to commercial methylene blue in terms of optical response and redox potential- yet differs favourably in environmental and biological compatibility. Its natural origin, low toxicity, and eco-friendly profile make it a strong candidate for future applications in analytical chemistry, biological staining, and possibly pharmaceutical fields.

Conclusion:

This study successfully demonstrated that Clitoria ternatea can serve as a viable phyto-based substitute for synthetic methylene blue. Its neutral pH, low conductivity, and strong absorbance in the visible region validate its potential as an environmentally responsible and biologically compatible dye. While commercial methylene blue offers high purity and standardization, its acidic nature, chemical residues, and environmental load remain concerns. In contrast, the natural extract offers a cleaner and greener alternative with promising applications in redox-based systems and scientific analysis. Future work may focus on stability optimization, long-term storage and integration into real-world analytical systems.

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Succinic Acid: An Efficient Catalyst For Synthesis Of 1-Amidoalkyl 2- Naphthol

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Abstract:

A green, general and efficient synthesis of amido-alkyl-naphthols using succinic acid as an efficient catalyst for the three-component condensation reaction of 2-naphthol, aldehyde and amide under thermal solvent-free conditions is described. The reactions proceed easily at low temperatures for a reaction time of 60 minutes to observe the yield and progress of reaction without the use of harmful and evaporative organic solvents. The advantages of this protocol are high-yielding, short reaction time, simple work-up, higher availability economical attraction, low-cost catalyst, lack of harmfulness and more eco-friendly catalyst.

Keywords: *Succinic Acid, Eco-friendly, 1-Amido Alkyl 2-Nephthol, Solvent Free Reaction.*

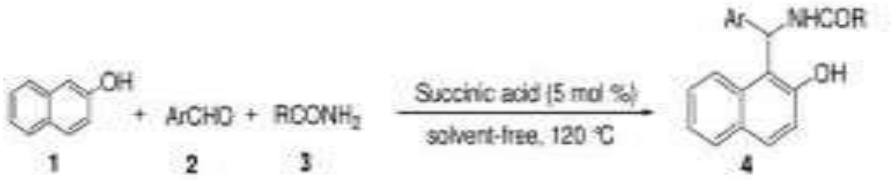
Introduction:

Multi-component reactions, or MCRs, have become a crucial tool for creating complex and varied chemical compounds. They are naturally superior to two component reactions in a number of ways, such as the ease of one-pot processes and the potential for structural change. Multiple cooperative bond formation processes in MCRs provide the synthetic competency, saving raw materials, time, and energy. A wide range of physiologically significant natural products and potent medications, including as many nucleoside antibiotics and HIV protease-liability drugs like lopinavir and ritonavir, include compounds with 1,3-Amino oxygenated functional groups. Additionally, amidoalkyl naphthols are synthetic building blocks with low, hypotensive, and weak cardiac activity that may be transformed by an amide hydrolysis process into significant physiologically active 1-aminomethyl-2-naphthol derivatives.

Ortho-quinone methides (O-QMs) feature an activated carbon-carbon double bond and are utilized in several combined procedures. However, because of their interactions with nucleophiles, they have not been used to their full potential. Such O-QMs have been utilized in the accumulation of dibenzoxanthenes and are known to be produced when 2-naphthol reacts with aromatic aldehydes in the presence of methane sulfuric acid. With 2-naphthol acting as a nucleophile, the identical O-QMs that were produced in situ also interacted with amides to yield amidoalkyl naphthols. Acids offer several advantages, including simplicity of handling and environmentally safe ejection. By creating cleaner synthetic pathways, waste and byproducts may be reduced or eliminated.

Since 1-amidoalkyl-2-naphthol and its derivatives have significant biological and pharmacological characteristics, including bradyarrhythmia and depressor effects in humans, synthetic researchers have been very interested in their production. Nevertheless, the majority of these techniques have disadvantages, including toxic catalysts, environmental contamination from the use of organic solvents, costly catalysts or challenging preparation, unavailability of reagents, irreversible reaction durations, and unsatisfactory yields. Thus, an effective one-pot multi-component synthesis of amidoalkyl naphthols free of these issues has to be further developed. It is commonly known that acid catalysis has become more popular recently because of its low cost, stability, ease of preparation and handling, lack of toxicity, ease of operation, and consideration of economic and environmental factors. Succinic acid is one of these acid catalysts. A ubiquitous metabolite found in microbes, plants, and animals, succinic acid has found extensive application in the culinary, pharmaceutical, and agricultural sectors. This acid has a wide range of industrial uses, including ink, paints, resins, polymers, and cosmetics.

Long reaction periods, the use of costly reagents, low product yields, high catalyst loading, caustic agent conditions that are extremely acidic, and the requirement for an extra microwave oven are some of the drawbacks of several described procedures. The development of a novel, readily accessible catalyst with high catalytic activity and a quick reaction time for the synthesis of amidoalkyl naphthols is therefore still helpful in order to get over these restrictions. A three-component one-pot condensation of 2-naphthol, amides, and aldehydes in the presence of methane sulphonic acid was attempted as a result of these discoveries. We now present a straightforward, universal, and effective protocol for the synthesis of 1-amidoalkyl-2-naphthols by one-pot condensation reaction of 2-naphthol, aldehydes, and acetamide using catalytic amounts of succinic acid because increasing our interest in the creation of workable, secure, and eco-friendly processes for a number of significant organic transformations.



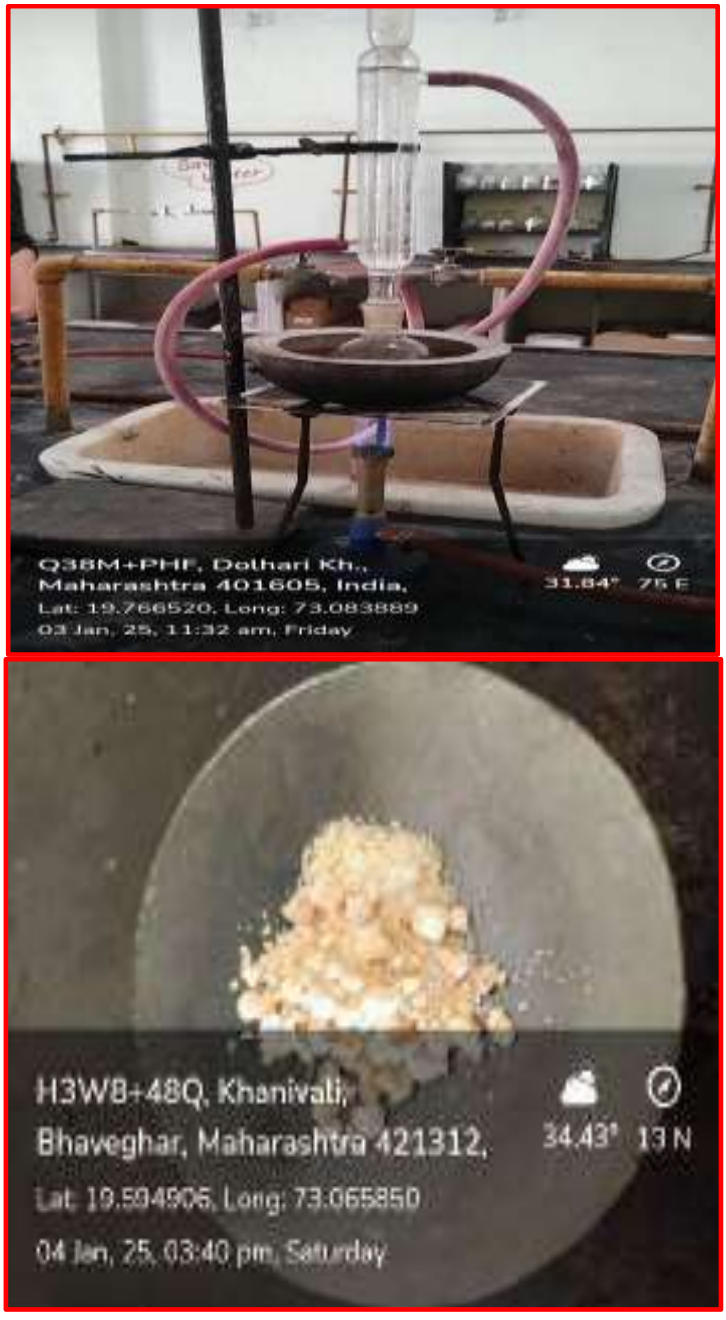
Material & Methodology:

Materials:

2-naphthol, Benzaldehyde, Acetamide, succinic acid

Methodology:

The preparation of 1 amidoalkyl 2 naphthol using succinic acid as an efficient catalyst. A mixture of 2 naphthol, aldehyde, amide and succinic acid was refluxed and stirred at 100°C in a hot water bath for 60 minutes. Then the reaction mixture is placed in ice bath for half an hour with constant stirring. The progress of the reaction was monitored by TLC. The crude product was cooled to room temperature and washed with ice cold water and stirred well. The catalyst is soluble in water and removed from the reaction mixture. The pure products were obtained by recrystallization using ethyl alcohol.



Result & Discussion:

Calculation for yields:

1. Theoretical yield:

Mole on product × Molecular weight

0.0025×309.36=0.773 g

2. Observed yield: 0.659 g

3. Percentage yield:

$$\frac{\text{Observed yield}}{\text{Theoretical yield}} \times 100$$

$$\frac{0.659}{0.773} \times 100$$

=85.25 %

4. R*f* value:

$$R_f = \frac{\text{distance travelled by the compound}}{\text{distance travelled by the solvent}}$$

$$R_f = \frac{4.9}{7.8}$$

$R_f = 0.63$

Reaction time in min.	Theoretical yield	Observed yield	Percentage yield	M.P.	RF value
60	0.773g	0.659g	85.25%	210 ºC	0.63

To improve the reaction conditions, the reaction of 2-naphthol, aldehyde and amide under thermal solvent-free conditions. Reactions at different conditions and various ratio uses in the presence of catalyst revealed that the both conditions were solvent-free at 100°C and catalytic an acid slight because of the acetamide was found to be advantageous. The 1-amidoalkyl-2-naphthol is likely to undergo electrophilic aromatic substitution, where the hydroxyl group on the naphthalene ring attacks the benzoyl group, resulting in the formation of benzoyl derivatives at the 2-position of the naphthalene ring

Conclusion:

In summary, we have developed an efficient, mild and clean synthetic protocol for the Synthesis of amidoalkyl naphthols. In this protocol, attempt has been made to exploit catalytic Activity of cobalt (II) chloride in organic synthesis. and succinic acid catalyzed the reaction efficiently Without using any other harmful organic reagents/solvents.

High yields, clean reaction conditions, shorter reaction times, and a simple experimental procedure combined with the easy purification of the product makes this method convey- net and environmentally benign for synthesis of 1-amido-or1-aminoalky-2-naphthol-derivatives.

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Assessment of plant diversity to describe ecotourism potential of sacred groves from Guhagar Taluka, Maharashtra India

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Abstract:
Sacred groves play a crucial role in biodiversity conservation and gene pool preservation and also provide ecological services such as carbon sequestration and water conservation. This study assessed the plant diversity of selected Sacred Groves from Guhagar Taluka, Maharashtra. Comprehensive field surveys were conducted to document the plant diversity at these sites. The findings highlight the role of sacred groves as reservoirs of endemic and rare species. By integrating ecological data with possibilities of community-based tourism strategies, this paper outlines a sustainable approach to conserving sacred groves while harnessing their potential to attract nature-based tourism. The research underscores the need for policy interventions to support the dual objectives of biodiversity conservation and local economic development.
Keywords: Sacred groves, Plant diversity, Endemic plants, threatened plants, Ecotourism

Introduction:

The sacred groves are patches of forests protected for various reasons, which include the existence of a deity, the religious practices, burial grounds etc. According to the estimation by Malhotra et al. (2001), there are about 100000-150000 sacred groves throughout the country. The size of the sacred groves varies from a few trees to a few hectares.

They are thought to be dating back to the pre-agrarian times (Kosambi, 1962) Any kind of interference in the forest is supposed to be restricted. The sacred groves hence show a vegetation in its climax stage (Gadgil and Vartak, 1976). Generally, sacred groves are believed to be treasure houses of medicinal, rare and endemic plants and also act as refugia for relic flora of a region. (Chandran et al, 1998). This is a very crucial role in preserving the plant diversity in isolated patches while the areas surrounding them undergo alterations as a result of anthropogenic activities. Sacred groves attract many researchers and conservationists because of the tremendous diversity they harbour, the ecosystem services they provide and the threats that they are facing.

Sacred groves are disappearing due to cultural changes and pressure to use the natural resources that they harbour(Chandrakanth et al. 2004). Due to changing socioeconomic conditions as well as land-use systems many sacred groves are now threatened and altered in terms of size, vegetation structure and species composition. (Chandrashekara& Sankar, 1998)

To protect sacred groves, it is essential to consider their ecological services and contributions to biodiversity conservation. At the same time, their eco-tourism potential should also be taken into account. By integrating these aspects, we can ensure that these groves are preserved not just as ecological habitats but also as sustainable attractions that generate awareness and income for local communities.

The **IUCN** defines Ecotourism as: "Environmentally responsible visiting of relatively unspoiled natural areas, to enjoy and appreciate nature (and any accompanying cultural features - both past and present), that promotes conservation, has low negative visitor impact, and provides for beneficially active socio-economic involvement of local populations". Responsible tourism planned as per the conditions given in this definition can help in conservation along with generating revenue for the local people. Patel and Adhvaryu (2021) explored how ecotourism could contribute to the sustainable development of sacred groves of Parnera hills in the Valsad District of Gujarat, India. The authors stated that the prospect of an increase in Tourism at this location could encourage the residents in the area to protect nature. The authors also stated that tourism could make people aware of the importance of preserving the natural environment.

Das and Chatterjee (2015) presented both the success stories and the failures of ecotourism practices. They discussed the management of conflicts between ecotourism and biodiversity conservation. The success stories that the authors described had responsible tourism which also supported the communities through livelihood generation and it adhered to the principles of biodiversity conservation by avoiding the malpractices that disturbed the habitats.

Ormsby(2012) studied the perceptions of tourism at sacred groves in two countries, Ghana and India. The work included ethnographic studies at five sacred forests where tourism was allowed, out of which two sites were in Ghana and three were from Meghalaya, India. This study states the possible linkages between the economic gains from tourism and protection of the sacred groves. The study also recommends the community resource management and the education prgrams linekd with sacred groves.

The risks of unchecked tourism and its impact on nature and wildlife have been described by many authors before

Materials and Methods:

Study Area: Three sacred groves from Guhagar Taluka were chosen for the study. Three sacred groves from Guhagar Taluka were selected for this study. The area of these three sacred groves ranges from a maximum of 4 hectares to a minimum of 2 hectares. Although these three sacred groves are relatively small, studying their plant diversity is crucial for assessing their conservation potential. Table 1 gives the details of these sacred groves.

Village Name	Deity	Area	Coordinates
Patpanhale	Manai, Mahalaxmi	2.08	17°28'49.98"N 73°14'57.66"E
Chikhli	Vaghai Zoali	4.1 Ha	17°29'36.63"N, 73°17'25.73"E
Malan	Bhanoba	2.28 Ha	17°28'18.62"N 73°16'9.29"E

Table 1: Details of three sacred groves in Guhagar Taluka considered for the study

Data Collection:

The sites were visited every season in the year 2022-23 to record the plant diversity. The tree diversity was studied once a year and surveys for lower strata were conducted every season.

Quadrant method was selected to study the plant diversity. 10m*10m quadrant were laid randomly for trees, 5m*5m for shrubs and herbs were studied in randomly laid quadrants of 1m*1m.
The trees were identified with the help of the Flora of Maharashtra and field guides for plants identification.

Results:

80 species of flowering plants belonging to 52 families were recorded in this study. 35 species of trees, 14 species of climbers, 6 species of shrubs and 24 species of herbs were recorded. Tables 2, 3, 4 and 5 give the list of all the plants recorded in the current study.

Species	Family
Blumea paniculata	Asteraceae
Chromolaena odorata	Asteraceae
Lepidagathis lutea	Acanthaceae
Aegenetia indica	Orobanchaceae
Aerides crispa	Orchidaceae
Amorphophallus commutatus	Araceae
Asystasia dalzelliana	Acanthaceae
Begonia crenata	Begoniaceae
Chlorophytum tuberosum	Asparagaceae
Curculigo orchioides	Hypoxidaceae
Curcuma pseudomontana	Zingiberaceae
Dendrobium barbatulum	Orchidaceae
Dendrophthoe falcata	Loranthaceae
Dicliptera foetida	Acanthaceae
Elephantopus scaber	Asteraceae
Eranthemum roseum	Acanthaceae
Haplanthodes tentaculatus	Acanthaceae
Lea indica	Vitaceae
Pogostemon paniculatus	Lamiaceae
Rungia repens	Acanthaceae
Sida rhombifolia	Malvaceae
Smithsonia straminea	Orchidaceae
Stachyphrynium spicatum	Marantaceae
Urena lobata	Malvaceae

Species	Family
Ampelocissus latifolia	Vitaceae
Atalantia scandens	Rutaceae
Calycopteris floribunda	Combretaceae
Celtis timorensis	Cannabaceae
Cissus latifolia	Vitaceae
Clerodendrum serratum	Verbenaceae
Combretum latifolium	Combretaceae
Dalbergia horrida	Fabaceae
Dioscorea bulbifera	Dioscoreaceae
Diploclisia glaucescens	Menispermaceae
Ipomoea triloba	Convolvulaceae
Solena amplexicaulis	Cucurbitaceae
Symphorema involucratum	Lamiaceae
Ziziphus rugosa	Rhamnaceae

Table 2: Climbers

Species Name	Family
Breynia retusa	Phyllanthaceae
Capparis zeylanica	Capparaceae
Carissa carandas	Apocynaceae
Costus speciosus	Costaceae
Grewia abutilifolia	Tiliaceae
Ixora coccinia	Rubiaceae

Table 3: Shrubs

Table 1: Herbs

Species Name	Family
Artocarpus heterophyllus	Moraceae
Bridelia retusa	Phyllanthaceae
Careya arborea	Lecythidaceae
Caryota urens	Arecaceae
Casearia graveolens	Salicaceae
Cassia fistula	Fabaceae
Catunaregum spinosa	Rubiaceae
Dillenia Pentagyna	Dilleniaceae
Excoecaria insignis	Euphorbiaceae
Ficus hispida	Moraceae
Flacourtia indica	Salicaceae
Flacourtia montana	Salicaceae
Garcinia indica	Clusiaceae
Garuga pinnata	Burseraceae
Grewia tiliifolia	Tiliaceae
Holigarna wightii	Anacardiaceae
Xantolis tomentosa	Sapotaceae
Zanthoxylum rhetsa	Rutaceae
Tectona grandis	Verbenaceae

Species Name	Family
Ixora brachiata	Rubiaceae
Lagerstroemia microcarpa	Lythraceae
Lanea coromandelica	Anacardiaceae
Macaranga peltata	Euphorbiaceae
Mammea suriga	Calophyllaceae
Mangifera indica	Anacardiaceae
Memecylon umbellatum	Melastomataceae
Mimusops elengi	Sapotaceae
Pterocarpus marsupium	Dipterocarpaceae
Radermachera xylocarpa	Bignoniaceae
Saraca asoca	Caesalpiniaceae
Schleichera oleosa	Sapindaceae
Spondias pinnata	Anacardiaceae
Sterculia guttata	Sterculiaceae
Syzigium cumini	Myrtaceae
Tabernaemontana alternifolia	Apocynaceae

Table 4: Trees

Cultural Significance of the sites:

1. **Malan Sacred Grove:** The sacred grove is dedicated to a masculine deity Bhanoba. The deity is believed to be protecting the village. Small rituals are performed there by families in the village.
2. **Chikhli Sacred Grove:** It is dedicated to feminine deities like Zolai, Vaghai, which are belived to be protecting the villagers. It is also believed that worshipping these goddesses helps in curing skin diseases. This sacred grove also has tombs of the ancestors of the families and priests in the village. Some old cremation grounds are also observed in the sacred grove.
3. **Patpanhale:** It is dedicated to the feminine deities Manai and Mahalaxmi. The deities are believed to protect the village lands, and to look after the well being of the villages.

Presence of Endemic and IUCN listed plants:

1. ***Garcinia indica*-** Commonly used in the food preparations in coastal areas of India, the tree species is endemic to Western Ghats. Although found in abundance because of its cultivation for commercial purposes, the species is limited to the areas of Western Ghats.

2. ***Saraca asoca-*** Listed as a vulnerable species, ***Saraca asoca*** was represented by very few individuals in the areas of Sacred groves of Malan. The presence of this highly medicinal and vulnerable species makes the sacred grove important from the point of view of conservation.
3. ***Curculigo orchioides-*** Commonly known as Kali musli, the species is of great medicinal importance and has been declared a threatened species.
4. ***Smithsonia straminea-*** Belonging to orchidaceae family, the species has been recorded as Endgangered by IUCN criteria (2000). Its first report from Dapoli Taluka of Maharashtra made by Datar and Ghate (2012) also showed its northernmost distribution. From this point of view, the record of this species from Patpanhale Sacred Grove of Guhagar Taluka becomes important, as this is the only record so far in the Guhagar Taluka of Maharashtra.



Smithsonia straminea



Lepidagathis lutea

5. ***Lepidagathis lutea*** – A herb endemic to the Western Ghats. Found on rocks and gravelly soils. It was found on an exposed rock in the periphery of the sacred grove at Malan.

Presence of plants specific to the sacred groves:

Mammea suriga was found to be abundant in all the sites. The occurrence of this tree in private lands has become very rare. In the studies done by Gawde et al (2018), in Dapoli Tahsil of Ratnagiri and Sathish et al (2020) in Sacred forests of Karnataka, it was observed that the species was mainly located in the area of sacred groves and was not recorded from the areas around it. Similar observations have been recorded about *Ixora brachiata*. The same findings resulted from this study.

The tree felling to sell wood, or cultivation results in the loss of the previously established plant diversity and an increase in the number of introduced species or introduced varieties. The original diversity then thrives in small patches of sacred forests protected by the community in the name of deities. The presence of species like *Mammea suriga*, *Ixora brachiate*, in the region of sacred forests is a very good example of it.

Signs of mammals:

The sacred groves, although of small sizes showed signs of existence of wild mammals in the areas around. The exposed rocks along the periphery of the Malan Sacred Grove showed leopard droppings at 13 different points.



Leopard dropping

Porcupine droppings were recorded at 2 places in the Sacred Groves of Malan and Patpanhale.



Porcupine dropping

Discussions:

All three sacred groves are small in size. Out of these, sacred groves at Malan and Patpanhale do not have their boundaries demarcated. However, the boundary of the sacred grove at Chikhli has been protected by the Gram Panchayat and the So
cial Forestry Department. The social forestry department has also tried to protect the sacred grove by fencing.

Despite being small, the plant data collected from surveys and evidence of the existence of mammals show that these sacred groves are significant.

The presence of endemic and IUCN-listed plant species, along with the existence of mammals in these sacred groves, is likely to attract amateur wildlife enthusiasts, researchers, as well as tourists who enjoy exploring nature.

If responsible and eco-friendly tourism is developed around these sacred groves, it could generate revenue for the village. Visiting researchers and tourists could interact with the locals, fostering awareness among the community about the significance of these natural and cultural treasures. This, in turn, could help prevent deforestation for activities like temple redevelopment. People would understand the importance of preserving these sacred groves in their current state.

These sacred groves are under constant threat. The sacred grove at Patpanhale has been fragmented due to the construction of a large road for high-tension cables. At Chikhli, while conservation work has been carried out by Social Forestry, the construction of walking pathways and placement of artificial animals have caused disturbances to the grove. The most critical measure to protect sacred groves is minimizing human intervention. These naturally evolved sacred groves are extremely important as ecological habitats.

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"Efficient One-Pot Oxidation of Benzoin to Benzil Followed by Rearrangement to a Benzilic Acid Derivative"

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Abstract

The synthesis of benzil from benzoin involves the the oxidation of benzoin, a secondary alcohol, to benzil, a diketone. This transformation is typically achieved by treating benzoin with an oxidizing agent such as nitric acid. The reaction proceeds via the information of an intermediate, leading to the formation of benzil, a yellow crystalline compound with a melting point of 95-97 °C. Subsequently, benzilic acid can be synthesized from benzil through a base induced rearrangement known as the benzilic acid rearrangement.in this process, benzil is treated with a strong base like potassium hydroxide in an alcoholic medium, leading to the formation of a carboxylate anion intermediate. Upon acidification, benzilic acid precipitates as a white crystalline solid with a melting point of 150-152 °C.

Keywords: *Benzoin, Oxidation, Benzil, Acidification, Benzilic Acid.*

Introduction:

The process to achieve benzil from benzoin comprises an oxidative reaction in which the secondary alcohol benzion is oxidized to produce the diketone benzil. This reaction is a famous illustration of how a hydroxyl group joined to a benzene ring may oxidize to generate a carbonyl group. Usually, an oxidizing agent like nitric acid (HNO3), bleach (sodium hypochloride, NaOCl), or even another weak oxidant is used for the conservation. The hydroxyl group of the benzoin is converted to a carbonyl group by the addition of oxygen, but the resultant benzil keeps the aromatic ring and forms a diketone structure. In order to avoid over-oxidation or adverse effects, the reaction usually has to be carefully controlled. Benzil is a yellow crystalline compound that is used as a precursor for additional chemical transformations and is significant in the research of organic processes.

The benzilic acid rearrangement is a well-known oraganic reaction that produces benzilic acid from benzil. This process involves the conversion of the diketone benzil into the hydroxy acid benzilic acid via a strong base reaction. Usually, an alcohol, most often ethanol or methanol, facilitates the reaction, which is carried out in the presence of a base like potassium hydroxide (KOH) or sodium hydroxide (NaOH). One of the carbonyl groups in benzil is deprotonated by the base to generate an alkoxide ion, which starts the rearrangement pathway. A new chiral centre is formed and the diketone structure is rearranged into a hydroxy acid as a result of this intermediate's subsequent nucleophilic assault on the nearby carbonyl group. Through acidification and recrystallization, the end product, benzilic acid, a white crystalline chemical, may be separated.

Since it shows that diketone may undergo structural rearrangements under simple circumstances, the benzilic acid rearrangement is an important process in organic chemistry. The resultant benzilic acid serves as a reagent in analytical chemistry and is crucial for the synthesis of several other chemical molecules. This change is a prime illustration of how working with functional groups may result in the creation of new, practical chemical structures.

Material and methodology:

Materials

- Benzion
- Conc. HNO3
- Cold water
- Benzil
- KOH
- Water
- Alcohol
- Conc. HCL

Apparatus-

- Conical flask
- Water bath
- Glass stirring rod
- Suction pump
- Filter papers
- Spatula
- Funnel
- Watch glass
- Tripot stand
- Beaker
- Porcrlain dish

Methodology:

1. **Synthesis of Benzil form Benzoin:**

Take a 4gm of benzoin and 20ml of conc. HNO3 in dry conical flask. Heat it on boiling water bath with occasional stirring until the evolution of oxides of nitrogen has stopped. (about 90min). pour the reaction the reaction mixture in 20ml of cold water and stir well. The oil crystallizes and yellow solid obtained. Filter the crude product at the suction pump, wash thoroughly with cold water to remove HNO3 and dry. Note the yield of crude benzil. Purify the small portion of the product and take its melting point.





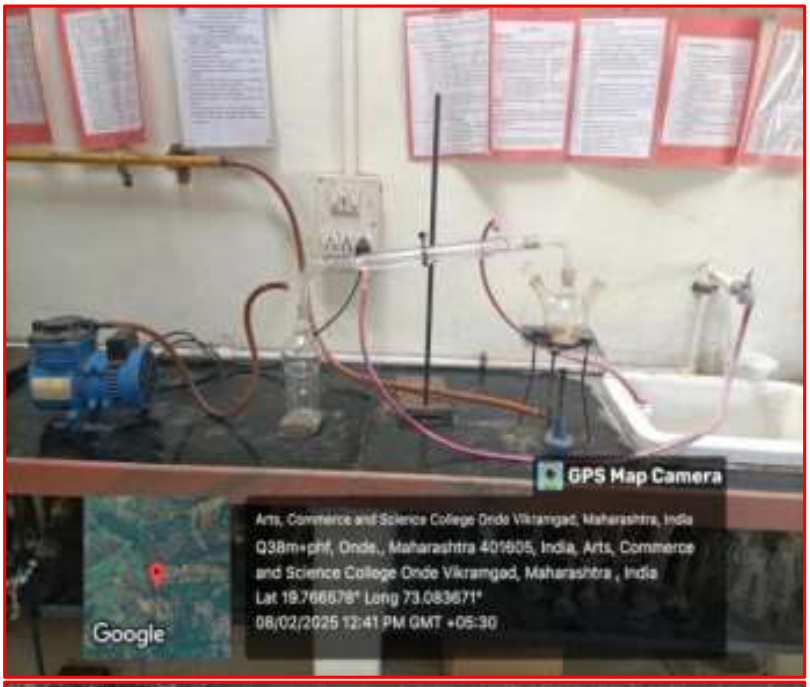


2. Synthesis of Benzilic Acid from Benzil:

Reflux the mixture of 2gm of Benzil, 2gm of KOH in 10ml of water and 5ml of alcohol on the water bath 10-15min. Pour the contents of the flask into a porcelain dish and allow it cool. The potassium salt of benzilic acid crystallize out. Filter with crystals at the pump and wash with ice cold alcohol. Dissolve the potassium salt in about 10ml water and acidify with Conc. HCL get precipitate. Wash the precipitate and recrystallize with hot water. Note yield of the pure benzilic acid.


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Result and Discussion:

Calculation:

1. Synthesis of Benzil form Benzoin:

Theoretical yield -

212.24 g of Benzion gives 216.23g of Benzil.

Therefore, 4g of benzoin = 216.23 x 4/212.24

= 3.96g of Benzil.

Observation-

Observed yield = 2.3g

Melting point = 93°C

Percentage yield-

Observed yield / Theoretical yield x 100

= 2.30/3.96x100

=58.08%

- Yield of Benzil:

The yielded 2.30g of Benzil, corresponding to 58.08% based on theoretical calculations.

- Physical properties:

The oil crystallizes yellow solid. Melting point is a 93°C.

Applications-

- Intermediate in organic synthesis.
- Synthesis of metal complexes.
- Uses in analytical chemistry.
- Dye and pigment manufacturing.

2. Synthesis of Benzilic Acid from Benzil:

Theoretical yield -

210g of Benzil gives 288g of Benzilic Acid

Therefore, 2g of Benzil = 288/210 x 2

= 2.18g.

Observation-

Observed yield = 1.4g

Melting point = 152°C

Percentage yield-

Observed yield / Theoretical yield x 100

= 1.4/2.18x100

= 64.23%

- Yield of Benzilic Acid:

The yielded 1.4g Benzilic Acid, corresponding to 64.23% based on theoretical calculations.

- Physical properties:

The crystallize brown solid. Melting point is a 152°C

Application-

- Synthesis of pharmaceuticals.
- Incapacitating agent.
- Hallucinogenic drug synthesis.
- Organic synthesis.
- Benzilic Acid rearrangement.
- Determination of Zirconium.

Conclusion:

Benzil, a diketone compound is commonly synthesized through the oxidation of benzoin. This transformation involves the conversion of benzoin, which the derived from benzaldehyde the benzoin condensation, into benzil using oxidizing agent such as copper salt, nitric acid or other oxidants. Benzilic acid is synthesized form benzil through a base induced rearrangement known as the benzilic acid rearrangement.

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Green and Sustainable Chemistry: New Frontiers for a Greener Planet

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Abstract:

The escalating environmental challenges of the 21st century ranging from climate change and resource depletion to pollution and hazardous waste have highlighted the urgent need for a shift towards more sustainable scientific practices. Green and Sustainable Chemistry emerges as a transformative discipline that not only addresses these concerns but also redefines the role of chemistry in achieving global sustainability goals. This chapter explores the principles, innovations, and applications of Green Chemistry, emphasizing its role in minimizing environmental impact while maximizing efficiency and safety in chemical processes. By integrating concepts such as atom economy, renewable feedstocks, energy efficiency, and non-toxic reagents, green chemistry provides a roadmap for sustainable industrial development and cleaner technologies. The chapter also delves into the interdisciplinary connections between chemistry, environmental science, and humanities, highlighting how ethical and societal considerations are crucial in shaping a sustainable future. Recent advancements, case studies, and emerging trends are presented to illustrate the growing impact of green chemistry in areas such as pharmaceuticals, materials science, agriculture, and education. Ultimately, this chapter advocates for a paradigm shift from traditional practices to sustainable innovations marking new frontiers in chemistry for a greener, more resilient planet

Keywords: *Green Chemistry, Environmental Science, Humanities, Sustainable Development*

Contents:

I. Introduction:

The 21st century has brought forth unprecedented environmental challenges, ranging from climate change and resource depletion to widespread pollution and biodiversity loss. In response, the scientific community has been called upon to rethink traditional practices and prioritize sustainability at every level of research and industry. Among these transformative approaches, green and sustainable chemistry has emerged as a key discipline with the potential to mitigate environmental harm while supporting technological and societal advancement.

Green chemistry, first formally defined by Paul Anastas and John Warner in the late 1990s, focuses on the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances [1]. Its twelve guiding principles emphasize energy efficiency, the use of renewable feedstocks, catalysis over stoichiometric reagents, and the reduction of waste collectively paving the way for cleaner, safer, and more efficient chemical processes [2].

Sustainable chemistry, while overlapping with green chemistry, encompasses a broader perspective. It incorporates the entire lifecycle of chemical products, including

resource extraction, production, usage, and end-of-life management. The aim is to ensure that chemical innovations not only avoid harm but actively contribute to environmental and societal well-being [3]. This holistic approach aligns with the United Nations Sustainable Development Goals (UN SDGs), particularly those related to clean water, clean energy, responsible consumption, and climate action [4].

Recent advances in green and sustainable chemistry have included the development of biodegradable materials, non-toxic solvents, heterogeneous catalysts, and photocatalytic systems for environmental remediation. Researchers are also exploring waste valorization transforming industrial or agricultural waste into value-added products as a means of closing the loop in chemical manufacturing [5].

This chapter seeks to highlight the emerging frontiers of green and sustainable chemistry. Through an interdisciplinary lens, it will explore innovative chemical strategies that not only address pressing environmental issues but also promote a more circular and resilient economy. Ultimately, this work underscores the urgent need for sustainable innovation in chemistry as a cornerstone for achieving a greener planet.

2. Principles and Evolution of Green and Sustainable Chemistry

Green and sustainable chemistry have emerged as crucial fields in addressing the environmental impact of chemical processes and products. These disciplines emphasize innovation that minimizes harm to human health and the environment while ensuring the efficient use of natural resources. Their evolution reflects a broader shift in scientific thinking from focusing solely on performance and cost to integrating ecological and social responsibility.

2.1 The Twelve Principles of Green Chemistry

The foundation of green chemistry lies in the Twelve Principles proposed by Paul Anastas and John Warner in 1998 [6]. These principles guide chemists in designing chemical products and processes that reduce or eliminate the use and generation of hazardous substances (Fig.1). They include:

1. ***Prevention:*** *It is better to prevent waste than to treat or clean up waste after it has been created.*
2. ***Atom Economy:*** *Synthetic methods should maximize the incorporation of all materials used in the process into the final product.*
3. ***Less Hazardous Chemical Syntheses:*** *Wherever practicable, synthetic methods should be used and generated with little or no toxicity to human health and the environment.*
4. ***Designing Safer Chemicals:*** *Chemical products should be designed to achieve their desired function while minimizing toxicity.*
5. ***Safer Solvents and Auxiliaries:*** *Use of auxiliary substances (e.g., solvents, separation agents) should be made unnecessary wherever possible and innocuous when used.*
6. ***Design for Energy Efficiency:*** *Energy requirements of chemical processes should be recognized for their environmental and economic impacts and minimized.*
7. ***Use of Renewable Feedstocks:*** *A raw material or feedstock should be renewable rather than depleting wherever technically and economically practicable.*
8. ***Reduce Derivatives:*** *Unnecessary derivatization (blocking groups, protection/deprotection, temporary modification) should be minimized or avoided.*
9. ***Catalysis:*** *Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.*

10. ***Design for Degradation:*** *Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment.*
11. ***Real-time Analysis for Pollution Prevention:*** *Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control.*
12. ***Inherently Safer Chemistry for Accident Prevention:*** *Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents.*



13.

14. Fig. 1. Principles of Green Chemistry proposed by Anastas and Warner

These principles collectively redefine how chemists approach synthesis and product design, steering away from the traditional focus on yield and toward environmental performance and safety.

2.2 Evolution Toward Sustainability

While green chemistry focuses on pollution prevention and safety at the molecular level, sustainable chemistry takes a broader system-level view. It integrates economic viability, ecological balance, and social equity into chemical innovation. This evolution aligns chemistry with the United Nations Sustainable Development Goals (SDGs), especially those related to clean water and sanitation (SDG 6), affordable and clean energy (SDG 7), responsible consumption and production (SDG 12), and climate action (SDG 13) [7].

Sustainable chemistry emphasizes:

- *Lifecycle thinking, assessing environmental impacts from cradle to grave.*
- *Circular economic principles, such as reuse, recycling, and regeneration.*
- *Cross-sector collaboration, combining chemistry with engineering, policy, and education.*

This expanded perspective reflects the growing awareness that sustainability challenges require interdisciplinary solutions, where chemists play a key role not only in minimizing harm but also in creating new value chains through clean technology, green materials, and waste valorization.

2.3 From Concept to Practice

The translation of green and sustainable chemistry from concept to practice has been supported by:

- *Government initiatives, like the U.S. Environmental Protection Agency's (EPA) Green Chemistry Program.*
- *Industrial adoption, where companies are integrating green metrics into process development.*
- *Academic engagement, with green chemistry curricula being introduced into universities worldwide.*

The field continues to evolve with the integration of emerging technologies such as artificial intelligence (AI), machine learning, and process intensification, which promise to enhance the design and scalability of sustainable chemical systems.

3. Innovations in Green Synthesis and Catalysis

Green chemistry has redefined traditional synthetic methodologies by prioritizing not only efficiency and selectivity but also environmental safety, energy conservation, and waste minimization. Among the most influential innovations are the use of environmentally benign solvents and the development of advanced catalytic systems. These innovations are essential for the sustainable transformation of raw materials into valuable chemicals, pharmaceuticals, and materials.

3.1 Green Solvents and Reaction Media

Solvents constitute a significant portion of the total mass used in chemical processes, especially in pharmaceutical and fine chemical industries. Traditional organic solvents such as dichloromethane, benzene, and toluene are widely used for their solvating power but are also associated with health hazards, flammability, toxicity, and environmental persistence. They contribute significantly to volatile organic compound (VOC) emissions, which are regulated under various environmental protection acts [8].

To address these issues, green solvents have emerged as a cornerstone of sustainable synthesis. These solvents are designed or selected based on their low toxicity, biodegradability, renewability, and minimal environmental impact. Prominent classes include:

- ***Supercritical Carbon Dioxide ($scCO_2$):*** *Used extensively as a replacement for organic solvents, $scCO_2$ is a non-toxic, non-flammable, and recyclable medium. It exhibits unique properties above its critical point (31.1°C and 73.8 bar), such as tunable density and viscosity, making it suitable for extractions, hydrogenation, and polymerizations.*
- ***Ionic Liquids (ILs):*** *These are salts that are liquid at temperatures below 100°C and are known for their negligible vapor pressure, thermal stability, and ability to dissolve both polar and non-polar compounds. They offer versatility in catalytic reactions and electrochemistry, though concerns about their long-term toxicity and biodegradability remain.*
- ***Deep Eutectic Solvents (DESs):*** *These are mixtures of hydrogen bond donors and acceptors that form a eutectic with a melting point lower than that of the individual components. They are inexpensive, biodegradable, and can often be synthesized from renewable resources like chloride and urea or sugars, making them highly attractive alternatives.*
- ***Bio-based Solvents:*** *Examples include ethyl lactate, limonene, and 2-methyltetrahydrofuran, which are derived from biomass and exhibit favorable safety profiles. These solvents are gaining popularity due to increasing regulatory pressure and demand for bio-renewable options.*

The implementation of green solvents not only improves the environmental footprint of chemical processes but also often enhances reaction selectivity, product purity, and ease of downstream processing. They also support the move toward continuous-flow chemistry, where solvent recycling and process intensification can be more easily managed.

3.2 Catalysis: From Homogeneous to Heterogeneous

Catalysis lies at the heart of green chemistry, offering pathways to improve reaction efficiency, reduce energy input, eliminate stoichiometric reagents, and minimize waste. The use of catalysts aligns directly with the 9th principle of green chemistry, which favors catalytic over stoichiometric transformations [9]. Catalysis can be broadly categorized into homogeneous, heterogeneous, biocatalytic, and photocatalytic systems each offering unique advantages for sustainable chemical synthesis:

Homogeneous Catalysis

Homogeneous catalysts, typically transition metal complexes, operate in the same phase as the reactants and offer excellent activity, selectivity, and tunability. They are widely used in fine chemical and pharmaceutical manufacturing. However, their recovery and recyclability remain challenges, as do concerns about metal contamination in final products.

Heterogeneous Catalysis

Heterogeneous catalysts, such as metal oxides, zeolites, and supported nanoparticles, are typically in a solid phase and can be easily separated and reused. These catalysts are critical in large-scale industrial processes, including hydrotreating, oxidation, and polymerization.

Green developments include the use of bio-waste derived catalysts, earth-abundant metals (like Fe, Cu, and Mn), and metal-free catalysts such as doped carbon materials.

Biocatalysis

Enzymes and whole-cell systems are increasingly used in organic synthesis due to their high specificity, mild reaction conditions, and environmental friendliness. Biocatalysis is revolutionizing asymmetric synthesis, particularly in pharmaceutical manufacturing. Enzyme engineering and immobilization techniques have significantly broadened their industrial applicability [10].

Nanocatalysis and Hybrid Systems

Nanocatalysts offer a bridge between homogeneous and heterogeneous systems, combining high surface area, tunable properties, and ease of recovery. Supported metal nanoparticles, magnetic nanocatalysts, and metal-organic frameworks (MOFs) are being explored for various sustainable transformations.

Photocatalysis and Electrocatalysis

Driven by sunlight or electric current, these catalytic systems are central to green energy and environmental applications, such as water splitting, CO_2 reduction, and pollutant degradation. Semiconductors like TiO_2, ZnO, and graphitic carbon nitride are widely researched for their catalytic potential under visible light [11].

These innovations in catalysis not only enhance the efficacy and safety of chemical transformations but also reduce reliance on hazardous reagents, enable renewable energy integration, and promote sustainable industrial practices. The synergy between green solvents and advanced catalysts represents a powerful strategy for sustainable synthesis in both academic and industrial settings.

4. Renewable Feedstocks and Biomass Utilization

The transition from fossil-based raw materials to renewable feedstocks represents a fundamental strategy in advancing the goals of green and sustainable chemistry. Traditional petrochemical resources are not only finite but also contribute significantly to environmental pollution and greenhouse gas emissions. In contrast, renewable feedstocks derived from biological sources offer a cleaner, more sustainable alternative that aligns with the principles of circular economy and climate responsibility (Fig. 2). Biomass such as agricultural residues (e.g., corn stover, wheat straw), forestry byproducts (e.g., sawdust, bark), and food and municipal organic waste is abundant, renewable, and capable of being converted into a broad array of valuable products including platform chemicals, biodegradable polymers, and specialty materials [12].

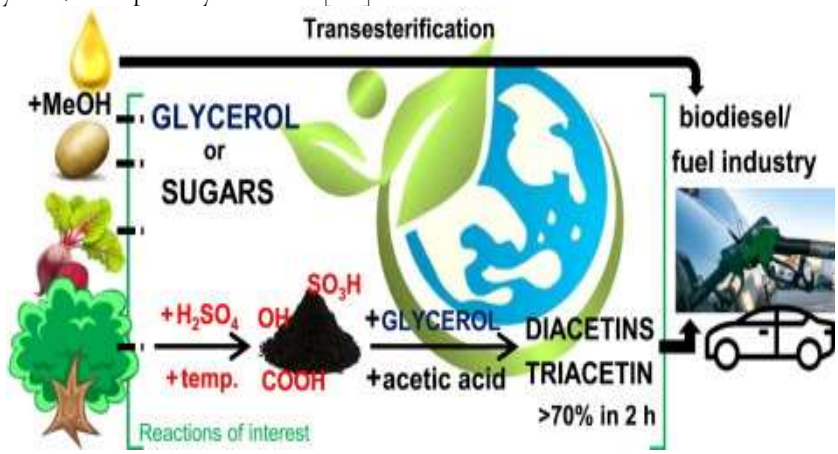


Fig. 2 Biomass Utilization (Transesterification)

Among the various forms of biomass, lignocellulosic biomass has emerged as a particularly promising resource due to its widespread availability, low cost, and non-competition with food supply chains. This biomass primarily consists of three major components: cellulose, hemicellulose, and lignin. Each of these components can serve as a feedstock for different types of chemical transformations. Cellulose and hemicellulose can be enzymatically hydrolyzed into simple sugars, which are then fermented by microbes to produce bio-based chemicals such as ethanol, lactic acid, succinic acid, and 5-hydroxymethylfurfural (HMF). Lignin, though more chemically complex, is rich in aromatic content

and holds potential for conversion into phenolic compounds, adhesives, and sustainable materials, although its industrial utilization remains a significant technical challenge [13].

Additionally, the concept of platform chemicals molecules derived from biomass that can be used to synthesize a wide range of downstream products has become central to the green chemistry agenda. Chemicals like HMF, levulinic acid, glycerol, and furfural not only replace fossil-derived equivalents but also open new pathways for material innovation. These developments highlight the role of renewable feedstocks not just as substitutes but as enablers of entirely new chemical processes and products with improved environmental profiles.

Despite these advancements, several barriers remain, including high initial processing costs, variability in biomass composition, logistical challenges in feedstock collection and transport, and the need for robust, scalable conversion technologies. Overcoming these challenges will require continued interdisciplinary research, supportive policy frameworks, and investments in sustainable infrastructure. Nevertheless, the shift toward renewable feedstock is an indispensable component of the global effort to create a more sustainable and resilient chemical industry.

5. Waste Minimization and Valorization Strategies

One of the foundational principles of green and sustainable chemistry is the prevention of waste generation rather than the management of waste after its formation. This approach, encapsulated in the maxim "prevention is better than cure," aims to reduce the environmental burden of chemical processes while improving resource efficiency. Waste minimization involves designing synthetic routes and industrial processes that maximize material utilization, minimize hazardous by-products, and enhance atom economy. When waste is inevitably produced, valorization strategies seek to transform these byproducts into useful materials, fuels, or chemicals, thereby closing the loop on resource cycles and moving towards a truly circular economy (Fig. 3).



Fig. 3 Summary of organic waste valorisation into polymeric matrices or nanoparticles towards circular bionanocomposites. Certain figures are reproduced from Flaticon with permission.

In the industrial context, concepts from industrial ecology, such as *waste-to-wealth*, *industrial symbiosis*, and *zero-waste manufacturing*, are gaining prominence. These frameworks encourage industries to view waste streams not as liabilities but as untapped resources. A classic example of this is carbon dioxide (CO_2) capture and utilization (CCU). Traditionally regarded as a greenhouse gas and waste product of combustion and fermentation processes, CO_2 is now being chemically converted into value-added products such as methanol, urea, cyclic carbonates, and polycarbonates. Methanol serves as a clean fuel and a key building block in the chemical industry. Technologies such as electrochemical

reduction of CO_2 using renewable electricity are paving the way for low-carbon production systems [14].

Organic and food waste, which constitutes a large portion of municipal solid waste, also offers vast potential for valorization. Through processes such as anaerobic digestion, fermentation, and pyrolysis, food waste can be converted into biogas, biochar, organic acids, and even bioplastics like polyhydroxyalkanoates (PHAs).

These waste valorization strategies not only address environmental challenges such as landfill overflows, pollution, and greenhouse gas emissions but also offer significant economic benefits by creating new revenue streams, reducing raw material costs, and enhancing supply chain resilience. However, successful implementation of waste valorization requires overcoming several challenges, including the heterogeneous nature of waste, the need for cost-effective separation and purification technologies, and the development of policy incentives and market mechanisms that support industrial adoption.

6. Green Materials and Environmental Applications

Green materials are integral to the vision of sustainable chemistry, offering innovative alternatives to traditional substances that are often non-renewable, toxic, or environmentally persistent [15]. Among these, biodegradable polymers and materials for environmental remediation stand out as essential tools for reducing ecological damage and promoting circularity. These green materials not only replace hazardous counterparts but also support eco-friendly design, waste reduction, and restoration of polluted ecosystems.

6.1 Biodegradable Polymers

Biodegradable polymers are designed to break down naturally by the action of microorganisms, enzymes, or environmental factors such as moisture and sunlight. Their use addresses one of the most pressing environmental concerns: plastic pollution. Their environmental friendliness, combined with economic viability, makes starch-based polymers a key component in reducing dependency on petroleum-based plastics and promoting sustainable material use.

6.2 Environmental Remediation

Green chemistry is also revolutionizing how we clean up environmental pollution. The focus is on creating safe, efficient, and low-impact materials for removing toxins from soil, air, and water systems [16].

The integration of green remediation technologies significantly enhances environmental sustainability by harnessing renewable energy sources such as sunlight and utilizing natural or waste-derived materials. This approach minimizes dependence on traditional clean-up methods that are often energy-intensive and involve hazardous chemicals, thereby reducing secondary pollution and carbon emissions. Moreover, by converting agricultural and industrial waste into functional materials such as bio-adsorbents or catalytic agents these strategies not only address pollution but also contribute to waste valorization. Collectively, such innovations help restore ecological balance, promote circular economy practices, and advance the broader goal of sustainable environmental management.

7. Education, Policy, and Industry Engagement

Achieving a truly sustainable chemical future hinges not only on scientific and technological breakthroughs but also on the collective effort of education systems, policy frameworks, and industry stakeholders. As green chemistry evolves from a niche discipline into a global necessity, there is an urgent need to integrate its principles into all levels of education to cultivate a new generation of environmentally conscious scientists, engineers, and decision-makers. Educational reform plays a pivotal role in embedding sustainability into the mindset of future professionals. Initiatives such as the UNESCO Green Chemistry Education Network and the International Union of Pure and Applied Chemistry (IUPAC) have been instrumental in promoting curriculum development, teacher training, and resource sharing to advance green chemistry education worldwide [17]. At the university level, interdisciplinary programs that blend chemistry with environmental science, engineering, and economics are being encouraged, while school level programs are beginning to introduce fundamental concepts such as pollution prevention, renewable resources, and safe laboratory practices. Laboratory instruction

is also evolving to adopt microscale and safer experiments, reducing chemical waste and exposure risks for students.

Beyond the classroom, government policies and regulatory bodies serve as catalysts for the widespread adoption of green chemistry in the commercial and industrial sectors. Policies like REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) in the European Union and the Safer Choice Program by the U.S. Environmental Protection Agency (EPA) are designed to promote the use of safer chemicals and processes. REACH imposes strict guidelines on chemical safety, pushing industries to replace hazardous substances with environmentally benign alternatives wherever possible. Similarly, the EPA's Safer Choice Program helps consumers and businesses identify products that meet high standards for human and environmental health, thereby incentivizing manufacturers to innovate sustainably. In many countries, extended producer responsibility (EPR) policies are also being introduced, requiring manufacturers to take accountability for the end-of-life management of their products, especially in sectors such as electronics, packaging, and chemicals.

Industry engagement is another cornerstone of the green chemistry movement. Companies are increasingly recognizing that sustainable practices not only reduce environmental impact but also create competitive advantages, enhance brand reputation, and open new markets. Industry-academia collaborations, green certification schemes, and investment in clean technologies are all examples of how the private sector is embracing sustainability. Green chemistry metrics, such as atom economy, life cycle analysis (LCA), and process mass intensity (PMI), are being adopted to evaluate and improve the sustainability of industrial operations. Moreover, global initiatives such as the United Nations Sustainable Development Goals (SDGs) and the Global Green Chemistry Initiative (GGCI) are fostering multi-sector partnerships aimed at aligning chemistry with broader socio-economic and environmental objectives.

Ultimately, the transition to sustainable chemistry is a multidisciplinary and multi-stakeholder endeavor. Integrating education, regulatory policies, and industrial innovation creates a synergistic pathway toward systemic change. Continuous support from policymakers, educators, and business leaders is essential to accelerate the adoption of green chemistry and to ensure that scientific progress translates into tangible environmental and societal benefits.

8. Future Perspectives and Challenges

Despite the notable advances in green and sustainable chemistry, several critical challenges must still be addressed to ensure its widespread implementation and impact. One of the foremost hurdles is the economic viability of green technologies. Many sustainable processes and materials, while environmentally beneficial, remain cost-prohibitive when compared to conventional alternatives. High initial capital investments, limited scalability, and lack of established supply chains often deter industries from adopting greener practices. Bridging this economic gap requires continued investment in research and development, government incentives, and market-driven demand for eco-friendly solutions.

Another persistent challenge lies in the limited and region-specific availability of renewable feedstocks. Biomass resources, for example, may be abundant in agricultural regions but scarce in arid or densely urbanized areas, leading to logistical constraints and uneven access to sustainable raw materials. To address this, strategies such as decentralized production systems, feedstock diversification, and valorization of local waste streams must be prioritized.

Furthermore, the complexity of sustainability issues calls for interdisciplinary collaboration across chemistry, chemical engineering, environmental science, economics, and even social sciences. Designing green processes not only involves technical optimization but also requires an understanding of regulatory frameworks, consumer behavior, and socio-economic impacts. The integration of life cycle assessment (LCA), systems thinking, and sustainability metrics into chemical education and industrial decision-making is crucial for fostering a holistic and effective approach to green innovation.

Looking ahead, the future of green chemistry will likely be shaped by emerging technologies and novel methodologies. The application of artificial intelligence (AI) and machine learning (ML) in process design is poised to revolutionize how chemists develop and optimize reactions, enabling predictive modeling of reaction pathways, toxicity screening, and real-time optimization of green metrics. Additionally, integrated biorefineries which combine chemical, biological, and thermal processes to convert biomass into fuels, chemicals, and materials are expected to play a pivotal role in

replacing fossil-based infrastructure. These systems promote circularity and resource efficiency while aligning with carbon neutrality goals.

Another promising direction is the advancement of net-zero chemical manufacturing, where carbon emissions are minimized or offset through carbon capture, utilization, renewable energy integration, and waste valorization. Such innovations represent not only technological milestones but also align with global climate targets, including the Paris Agreement and the United Nations Sustainable Development Goals (SDGs).

9.Conclusion

Green and sustainable chemistry represents not only a transformative scientific evolution but also a profound ethical responsibility to safeguard the planet for current and future generations. In an era marked by environmental degradation, resource scarcity, and climate change, the role of chemistry must transcend traditional boundaries to become a driving force for sustainable development. By embracing the twelve principles of green chemistry, researchers and industries are reshaping how chemicals are designed, synthesized, utilized, and disposed of with a focus on minimizing toxicity, maximizing efficiency, and promoting renewability.

Innovations in synthetic methodologies, catalytic systems, renewable feedstocks, and green materials have significantly advanced the goal of building a circular and low-carbon economy. Concurrently, the development of waste valorization strategies, biodegradable alternatives to conventional plastics, and environmentally friendly remediation technologies demonstrate the versatility and societal value of sustainable chemical solutions. However, true progress also requires systemic change, supported by robust educational frameworks, policy interventions, and industry engagement.

Looking ahead, the integration of emerging technologies such as artificial intelligence, biotechnology, and renewable energy systems with green chemistry will further enhance our ability to address global challenges. Yet, overcoming barriers related to scalability, economics, and interdisciplinary coordination remains essential. Only through continued collaboration across scientific disciplines, industries, and policymakers can the vision of a sustainable, equitable, and innovation-driven future be fully realized.

In essence, green chemistry is not just a field of science, it is a pathway toward harmony between human progress and environmental stewardship. Its principles and practices serve as guiding lights in our collective journey toward a more resilient, resource-efficient, and greener planet.

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Differential Equation of Generalized Hermite Polynomials

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Abstract

Generating function play vital role in the investigation of various useful properties of the sequence which they generate. The Generalized Hermite polynomials $H_{m,n}(x)$ [3] is defined. In present paper we have obtained a differential equation of Generalized Hermite polynomials. Particular Case is also obtained.

Keywords: *Generalized Hermite Polynomials, differential equations.*

1. Introduction

Dattoli [1] has defined generalized Hermite Polynomials as

$$exp(mxt - t^m) = \sum_{n=0}^{\infty} \frac{H_{m,n}(x)\, t^n}{n!} \qquad (1.1)$$

Dattoli , Srivastava, Djordjević [1,3,4] studied the generalized Hermite Polynomials and derived some generating relations.

The explicit form of (1.1) is

$$H_{m,n}(x) = \sum_{k=0}^{\left[\frac{m}{n}\right]} \frac{(-1)^n\, n!\, (mx)^{n-mk}}{k!\, (n-mk)!} \qquad (1.2)$$

2. Differential equations

Differentiating (1.1) w. r. to x, we get,

$$mt\, exp(mxt - t^m) = \sum_{n=0}^{\infty} \frac{H'_{m,n}(x)\, t^n}{n!}$$

$$mt \sum_{n=0}^{\infty} \frac{H_{m,n}(x)\, t^n}{n!} = \sum_{n=0}^{\infty} \frac{H'_{m,n}(x)\, t^n}{n!}$$

$$\sum_{n=0}^{\infty} \frac{m\, H_{m,n}(x)\, t^{n+1}}{n!} = \sum_{n=0}^{\infty} \frac{H'_{m,n}(x)\, t^n}{n!}$$

Replacing n by $n-1$ in the left hand side,

$$\sum_{n=0}^{\infty} \frac{m\, H_{m,n-1}(x)\, t^n}{(n-1)!} = \sum_{n=0}^{\infty} \frac{H'_{m,n}(x)\, t^n}{n!}$$

$$\sum_{n=0}^{\infty} \frac{mn\, H_{m,n-1}(x)\, t^n}{n!} = \sum_{n=0}^{\infty} \frac{H'_{m,n}(x)\, t^n}{n!}$$

Comparing the coefficients of $\frac{t^n}{n!}$ we get,

$$mn\, H_{m,n-1}(x) = H'_{m,n}(x)$$

$$H'_{m,n}(x) = mn\, H_{m,n-1}(x) \tag{2.1}$$

Differentiating w.r. to x, we get

$$H''_{m,n}(x) = mn\, m(n-1)\, H_{m,n-2}(x)$$

$$\frac{d^2}{dx^2}[H_{m,n}(x)] = mn\, m(n-1)\, H_{m,n-2}(x)$$

$$\frac{d^2}{dx^2}[H_{m,n}(x)] = m^2\, n(n-1)\, H_{m,n-2}(x)$$

Again differentiating w.r. to x,

$$\frac{d^3}{dx^3}[H_{m,n}(x)] = m^3\, n(n-1)(n-2)\, H_{m,n-3}(x)$$

In general

$$\frac{d^r}{dx^r}[H_{m,n}(x)] = m^r\, n(n-1)(n-2)\ldots(n-r+1)\, H_{m,n-r}(x)$$

$$\frac{d^r}{dx^r}[H_{m,n}(x)] = m^r\, n(n-1)(n-2)\ldots(n-r+1)\, \frac{(n-r)!}{(n-r)!} H_{m,n-r}(x)$$

$$\frac{d^r}{dx^r}[H_{m,n}(x)] = \frac{m^r\, n!}{(n-r)!} H_{m,n-r}(x) \tag{2.2}$$

Differentiating (1.1) w.r. to t we get,

$$(mx - mt^{m-1})\, exp(mxt - t^m) = \sum_{n=0}^{\infty} \frac{H_{m,n}(x)\, n\, t^{n-1}}{n!}$$

$$(mx - mt^{m-1}) \sum_{n=0}^{\infty} \frac{H_{m,n}(x)\, t^n}{n!} = \sum_{n=0}^{\infty} \frac{H_{m,n}(x)\, n\, t^{n-1}}{n!}$$

$$\sum_{n=0}^{\infty} \frac{mx\, H_{m,n}(x)\, t^n}{n!} - \sum_{n=0}^{\infty} \frac{m\, H_{m,n}(x)\, t^{n+m-1}}{n!} = \sum_{n=0}^{\infty} \frac{H_{m,n}(x)\, n\, t^{n-1}}{n!}$$

$$\sum_{n=1}^{\infty} \frac{mx\, H_{m,n-1}(x)\, t^{n-1}}{(n-1)!} - \sum_{n=m}^{\infty} \frac{m\, H_{m,n-m}(x)\, t^{n-1}}{(n-m)!} = \sum_{n=1}^{\infty} \frac{H_{m,n}(x)\ t^{n-1}}{(n-1)!}$$

$$\sum_{n=1}^{\infty} \frac{mxH_{m,n-1}(x)t^{n-1}}{(n-1)!}$$

$$- \sum_{n=m}^{\infty} \frac{m(n-1)(n-2)(n-3)\ldots[n-(m-1)]H_{m,n-m}(x)t^{n-1}}{(n-1)(n-2)(n-3)\ldots[n-(m-1)]\,(n-m)!}$$

$$= \sum_{n=1}^{\infty} \frac{H_{m,n}(x)\ t^{n-1}}{(n-1)!}$$

$$\sum_{n=1}^{\infty} \frac{mxH_{m,n-1}(x)t^{n-1}}{(n-1)!}$$

$$-\sum_{n=m}^{\infty} \frac{m(n-1)(n-2)(n-3)\dots[n-(m-1)]H_{m,n-m}(x)t^{n-1}}{(n-1)!}$$

$$=\sum_{n=1}^{\infty} \frac{H_{m,n}(x)\ t^{n-1}}{(n-1)!}$$

Comparing the coefficients of $\frac{t^{n-1}}{(n-1)!}$ we get,

$$mxH_{m,n-1}(x) - m(n-1)(n-2)(n-3)\dots[n-(m-1)]H_{m,n-m}(x) = H_{m,n}(x)$$

from (2.1), we can write

$$\frac{mxH'_{m,n}(x)}{m\,n} - \frac{m(n-1)(n-2)(n-3)\dots[n-(m-1)]}{m^m\,n!} D^m[H_{m,n}(x)] = H_{m,n}(x)$$

$$\frac{xH'_{m,n}(x)}{n} - \frac{m(n-1)!}{m^m\,n!} D^m[H_{m,n}(x)] = H_{m,n}(x)$$

$$\frac{xH'_{m,n}(x)}{n} - \frac{1}{n\,m^{m-1}} D^m[H_{m,n}(x)] = H_{m,n}(x)$$

$$xH'_{m,n}(x) - \frac{1}{m^{m-1}} D^m[H_{m,n}(x)] = n\,H_{m,n}(x)$$

$$\frac{1}{m^{m-1}} D^m[H_{m,n}(x)] = xH'_{m,n}(x) - n\,H_{m,n}(x)$$

$$D^m[H_{m,n}(x)] = m^{m-1}xH'_{m,n}(x) - nm^{m-1}\,H_{m,n}(x)$$

$$D^m[H_{m,n}(x)] - m^{m-1}x\,D[H_{m,n}(x)] + nm^{m-1}\,H_{m,n}(x) = 0 \qquad (2.3)$$

where, $D = \frac{d}{dx}$.

3. Particular Case

For $m = 2$ in equation (2.3), we derive the differential equation of the Hermite polynomials.

$$D^2[H_n(x)] - 2x\,D[H_n(x)] + 2n\,H_n(x) = 0.$$

$$\frac{d^2}{dx^2}[H_n(x)] - 2x\,\frac{d}{dx}D[H_n(x)] + 2n\,H_n(x) = 0.$$

$$H''_n(x) - 2x\,H'_n(x) + 2n\,H_n(x) = 0.$$

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Integrating Energy and Environmental Law for Sustainable Energy Transition in India

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Abstract

India's rapid economic growth and energy demands have positioned it at the connection of global climate action and sustainable development debates. This paper examines the environmental and legal implications of India's coal-dominated energy sector and its ambitious renewable energy transition, arguing that fragmented legislation and weak enforcement undermine climate goals. Through doctrinal analysis of key statutes including the Environment Protection Act (1986), Electricity Act (2003), and Forest Rights Act (2006), the study reveals systemic gaps in India's legal framework. Despite progress under the Energy Conservation Act (2001) and Paris Agreement NDCs, challenges persist: 54% of thermal plants operate in water-stressed regions, renewable projects face land-use conflictsbypass environmental safeguards. This study emphasizes the urgency of integrating environmental justice into energy governance to secure India's socio-ecological future.

Keywords: *Energy policy, Environmental law, Climate Change, Sustainable Development, Legal Fragmentation, India.*

I. Introduction

Energy is a fundamental physical concept that underpins human civilization, essential not only for basic needs like clean water, shelter, sanitation, and healthcare, but also for the broader goals of social welfare and economic development. As humanity faces unprecedented challenges in the 21st century, the intricate relationship between energy consumption, environmental sustainability, and human development has become increasingly apparent.

The world stands at a critical juncture in its energy journey. While conventional fossil fuels have historically powered human progress, their continued use has led to severe environmental degradation through greenhouse gas emissions and climate change. The World Energy Council projects that without significant changes in current practices, global energy demand will increase by 50-80% compared to 1990 levels, with annual consumption nearly doubling from 22 billion kWh to 53 billion kWh(1,2). This trajectory raises serious concerns about environmental sustainability, particularly as industrialized economies, representing just 25% of the world's population, consume approximately 75% of global energy resources(3). Within this global energy landscape, the building sector emerges as a significant contributor, consuming approximately 40% of total world annual energy needs for lighting, heating, cooling, and air-conditioning.

The global energy-environment nexus has emerged as a central concern in contemporary climate discourse, particularly in light of the Intergovernmental Panel on Climate Change (IPCC) warnings about the unsustainable trajectory of fossil fuel consumption(4). Simultaneously, international mandates such as Sustainable Development Goal 7 (SDG 7) urge nations to ensure access to affordable, reliable, sustainable, and modern energy for all. In this context, India presents a compelling case study of the tensions and trade-offs involved in balancing economic development with environmental sustainability(5). As one of the world's fastest-growing

economies and the third-largest energy consumer, India relies heavily on coal, which constitutes 57% of its total energy mix and generates nearly 70% of its electricity. Yet, it also leads globally in renewable energy expansion, with a record addition of 40 GW of solar capacity in 2023 alone.
This dual trajectory reveals a fundamental contradiction: while India pursues ambitious green energy targets, it continues to depend on environmentally detrimental fossil fuel infrastructure. Legal conflicts further illustrate this tension most especially, the T.N. Godavarman Thirumulpad v. Union of India (1996) case, in which the Supreme Court restricted mining operations in forested areas, emphasizing the judiciary's role in safeguarding ecological interests even when they conflict with energy imperatives (6). Such judicial interventions reflect the fragmented and often contradictory nature of India's legal system, where environmental protection laws such as the Environment Protection Act (1986) operate in silos from energy governance statutes like the Electricity Act (2003).

This paper argues that India's energy transition must be guided by an integrated legal framework that harmonizes environmental safeguards with energy security mandates. The objective of the study is threefold: first, to critically analyze the environmental and legal impacts of India's coal-dominated energy sector; second, to evaluate the effectiveness and limitations of existing legislation governing the energy transition; and third, to propose legal reforms that facilitate a just, sustainable, and climate-resilient energy future. Through a combination of doctrinal legal analysis, policy review, and case law examination, the study seeks to contribute to the growing discourse on aligning India's energy ambitions with its ecological responsibilities.

2. Evolution of India's Electrical Energy Policy: Environmental Integration

India's energy planning trajectory since independence can be broadly categorized into five key phases, each shaped by socio-political contexts and shifting policy priorities. The first phase (1947–1970), immediately post-independence, focused primarily on ensuring supply adequacy in electricity and the growth of oil and gas sectors. Infrastructure development was considered the backbone of the national economy, and policy efforts aimed at supporting this vision(7,8). In the second phase, during the 1970s, global oil shocks triggered an energy access crisis, shifting focus toward energy conservation and reduced petroleum consumption. Key developments during this period included the nationalization of the coal sector—coking coal in 1972 and non-coking coal in 1973—and the establishment of Coal India Limited (1975) and the National Thermal Power Corporation (NTPC)(9). While regulatory measures were introduced in coal and petroleum sectors, the emphasis remained on fulfilling basic energy access rather than transitioning to sustainable energy sources.

The 1980s, or the third phase, marked a period of growing energy demand driven by the rise of the business class. Energy saving targets were introduced for the first time, and the Advisory Board on Energy was established in 1983 to guide the development of an integrated national energy policy. The decade saw efforts to diversify supply sources and included the establishment of the Nuclear Power Corporation of India Limited in 1987. All energy departments, excluding atomic energy, were brought under a unified Ministry of Energy, streamlining governance. The fourth phase, the 1990s, was characterized by economic liberalization, which led to significant structural reforms in the energy sector. These included deregulation, privatization, and foreign investment incentives. The Energy Conservation Bill was drafted, and the Bureau of Energy Efficiency (BEE) was set up to address system inefficiencies and promote sustainability. The Ministry of Non-Conventional Energy Sources (MNES), later renamed the Ministry of New and Renewable Energy (MNRE), was established in 1992 to focus on renewable energy development.
Despite these reforms, the electricity sector remained fiscally strained until the 1990s, with significant losses due to high transmission and distribution inefficiencies and low plant load factors. Amendments to the Electricity Supply Act in 1991 enabled private sector participation through long-term power purchase agreements, but political interference in state-run electricity

boards (SEBs) persisted. The Central Electricity Regulatory Commission (CERC) was established in 1998 under the Regulatory Commission Act to enhance regulatory consistency. The unbundling of SEBs into separate generation, transmission, and distribution entities was a landmark reform, complemented by the introduction of availability-based tariffs in 2000, which enforced grid discipline(10).

The fifth and ongoing phase, beginning in the 2000s, aligns India's energy planning with climate change mitigation. Programs like the Accelerated Power Development and Reforms Program (APDRP) and its successor, Restructured-APDRP, aimed to attract private investment and reduce aggregate technical and commercial (AT&C) losses. The Electricity Act of 2003 introduced a market-oriented framework promoting competition, accountability, rural electrification, and renewable energy(11). Key policy instruments following this act included the National Electricity Policy (2005), National Tariff Policy (2006), and Integrated Energy Policy (2006), which facilitated power market reforms and the establishment of national power exchanges(12).

Sustainability came into sharp focus with the launch of the National Action Plan on Climate Change (NAPCC) in 2008, comprising eight national missions including those promoting solar energy and energy efficiency(13). Complementary initiatives included the Energy Conservation Act (2001, amended in 2010), the Perform, Achieve, and Trade (PAT) scheme (2012)(14), and the National Mission for Enhanced Energy Efficiency (NMEEE). These efforts helped reduce energy intensity over the last decade. The "One Nation One Grid" initiative, finalized in 2014, synchronized India's power systems nationally. CERC continues to evolve grid regulations to tighten frequency ranges and improve reliability. Notably, the open access policy has enhanced energy security by enabling large industrial consumers to procure power directly from cost-effective sources(15).

3. Environmental Impacts of India's Electrical Energy Sector:

3.1 Coal Dominance

India's electricity sector remains heavily reliant on coal, which accounts for a substantial share of both energy production and environmental degradation. Thermal power plants are a major source of air pollution, contributing nearly 60% of the total PM2.5 in industrial zones, as reported by the Central Pollution Control Board (CPCB, 2023)(16). Despite the Ministry of Environment, Forest and Climate Change issuing stringent emission norms under S.O. 3305(E) in December 2015 mandated retrofitting technologies like flue gas desulfurization (FGD), as of 2023, only 8% of plants installed FGD systems. Deadline extended to 2026 (MoEFCC Notification, 2022)(17). A significant number of plants have repeatedly missed deadlines for implementing pollution control measures, citing cost and logistical constraints, thereby undermining the policy's effectiveness. Additionally, coal-based power plants impose considerable stress on water resources. According to NITI Aayog's 2022 report, 54% of thermal plants operate in water-stressed regions, while 87% of coal mines face water scarcity(18). Many of these facilities continue to extract groundwater without the necessary clearances, often violating the Water (Prevention and Control of Pollution) Act, 1974. This exacerbates local water insecurity, particularly in arid states like Rajasthan and Maharashtra, where communities face competition over dwindling water reserves.

3.2 Renewables' Hidden Costs

While renewable energy is often championed as a sustainable alternative, its environmental and social trade-offs are increasingly evident. Large-scale solar parks, particularly in ecologically sensitive and tribal-dominated areas such as Rajasthan, have triggered land-use conflicts. Several projects face ongoing litigation under the Forest Rights Act (2006), as they are accused of encroaching on community forest lands without obtaining free, prior, and informed consent from indigenous populations. These conflicts highlight the gap between green energy ambitions and just energy transitions. Moreover, renewable technologies like solar photovoltaics

(PV) pose long-term environmental risks through the generation of electronic waste (e-waste). India's E-Waste Management Rules (2016) do not yet include a comprehensive framework for managing the end-of-life disposal of solar panels. With solar infrastructure expected to surge under initiatives like the National Solar Mission, this regulatory gap could result in a significant waste burden over the coming decades. The lack of clear guidelines for recycling, dismantling, or safe landfilling of decommissioned panels not only poses risks to soil and groundwater but also undermines the overall sustainability narrative of India's energy transition.

4. Legal Framework Analysis

India's energy governance is fractured across competing statutes, creating a regulatory landscape where environmental protection and energy security often collide. The Environment Protection Act (EPA), 1986 empowers the central government to set emission standards (Section 3), but delegation of enforcement to under-resourced State Pollution Control Boards (SPCBs) has led to systemic non-compliance(19). The Electricity Act, 2003, while progressive in promoting renewables through Section 3(1), suffers from weak deterrence. Its penalty clause (Section 142) caps fines at ₹1 lakh (~$1,200) for violations like missing Renewable Purchase Obligations (RPOs)—a sum dwarfed by the average ₹50 crore cost of compliance for discoms. This loophole enabled Andhra Pradesh to retroactively slash solar tariffs in 2019, violating Section 63's competitive bidding mandate yet facing no legal repercussions (ReNew Power v. APERC, 2020). Whereas, the Energy Conservation Act, 2001 has delivered measurable outcomes. Its Perform, Achieve, and Trade (PAT) scheme reduced energy intensity by 13% in energy-intensive sectors like cement and aluminum (2012–2023). However, it excludes small industries, which account for 70% of industrial energy use (BEE, 2023), limiting its transformative potential.

5. India's Climate Commitments and Legal Alignment

India's Nationally Determined Contributions (NDCs) under the Paris Agreement have driven significant legal and policy changes, but inconsistencies persist between ambition and implementation. The push to meet solar energy targets has been supported through mechanisms like Renewable Purchase Obligations (RPOs), mandated under the Electricity Act (2003). However, enforcement remains a major concern. While RPOs under the Electricity Act aim for 40% non-fossil capacity by 2030, 12 states missed 2022 targets (CEEW, 2023). Penalties averaged ₹5 lakh/state is less than 0.1% of annual discom losses, rendering them ineffective deterrents. The Energy Conservation (Amendment) Act, 2022 introduced a carbon credit market, aligning with Article 6 of the Paris Agreement. However, its exclusion of the coal sector—responsible for 70% of India's emissions—risks tokenism. Meanwhile, global pressures like the EU's Carbon Border Adjustment Mechanism (CBAM), which threatens ₹45,000 crore in steel exports (TERI, 2023), are driving reforms(20). Amendments to the Companies Act, 2013 now mandate ESG disclosures (Section 134), linking corporate governance to climate accountability.

Yet critical gaps remain:

- The Draft Offshore Wind Policy (2023) bypasses mandatory EIAs under the Coastal Regulation Zone Notification (2019), endangering marine ecosystems.
- The Forest (Conservation) Amendment Act, 2023 exempts solar projects from forest clearances, risking tribal land rights under the Forest Rights Act, 2006.

6. Case Studies: Legal Perspectives on Energy vs. Environment

The evolving legal discourse around India's energy transition is best understood through key case studies that reveal the tensions between energy development and environmental justice. The Hasdeo Arand case (2022) in Chhattisgarh is emblematic of this conflict. Despite significant tribal opposition and ecological concerns, the High Court permitted coal mining in one of central India's most pristine forest regions, raising questions about the limits of constitutional protections for indigenous rights under the Panchayats (Extension to Scheduled Areas) Act (PESA) and the Forest Rights Act (2006). In contrast, the Aranya case (2019), adjudicated by the National Green

Tribunal (NGT), upheld biodiversity conservation by halting encroachments into a protected forest zone, illustrating a more precautionary legal approach.

Similarly, land acquisition for renewable energy infrastructure has provoked litigation and legal reform. In Farmers' Union v. Rajasthan Government (2021), a coalition of landowners challenged the acquisition of land for a large solar park under the Right to Fair Compensation and Transparency in Land Acquisition, Rehabilitation and Resettlement (LARR) Act (2013). The litigation prompted policy adjustments around compensation and resettlement, underscoring the need for just transitions even within the renewable energy space. Meanwhile, India's nascent offshore wind energy policy, introduced in draft form in 2023, has attracted scrutiny for failing to incorporate mandatory Environmental Impact Assessments (EIAs) under the Coastal Regulation Zone (CRZ) Notification(19). This omission raises concerns about the policy's compatibility with existing coastal and marine protection laws, especially in the context of fishing communities whose traditional rights remain unaddressed.

7. Recommendations for Integrated Legal Reform

To enable a truly sustainable energy transition, India's fragmented legal regime requires consolidation through a Unified Energy-Environment Code. This would involve integrating key provisions from the Electricity Act (2003), Environment Protection Act (1986), and Indian Forest Act (1927) into a comprehensive Sustainable Energy Transition Act, thereby eliminating regulatory overlaps and ensuring climate-sensitive development across sectors. Further, the National Green Tribunal (NGT), which has been instrumental in environmental adjudication, should see its mandate expanded to review and assess the climate resilience of large-scale energy infrastructure projects. This would align environmental jurisprudence with emerging climate science.

At the state level, legislative innovation is essential to operationalize national commitments. States could adopt model laws mandating rooftop solar installations in new developments, inspired by Kerala's 2022 solar policy that made rooftop systems mandatory for certain building typologies. Additionally, the authority of State Pollution Control Boards (SPCBs) should be reinforced, particularly in regulating power distribution companies (DISCOMs), which often bypass pollution norms and renewable mandates due to weak enforcement mechanisms. A dedicated Just Transition Law should also be enacted to ensure that coal-dependent regions are not left behind. Such a law could institutionalize financial flows from the Coal Cess (₹400 per ton), channeling them into worker retraining, livelihood diversification, and ecological restoration projects under the Compensatory Afforestation Fund Act.

Moreover, India's regulatory framework for managing the environmental consequences of clean energy must evolve. The E-Waste Management Rules (2016) need to be amended to include end-of-life recycling targets for solar photovoltaic panels and related equipment. With the projected surge in solar installations, proactive e-waste regulation is vital to prevent a new ecological crisis from emerging within the green energy sector.

8. Conclusion

India's energy future lies at the intersection of economic ambition and ecological integrity, and the legal system must evolve to reflect this reality. Judicial precedents such as the Vedanta Case (2020) demonstrate the courts' growing emphasis on sustainability and corporate accountability, yet legislative responses have remained piecemeal and reactive. To overcome this inertia, India needs a forward-looking, integrated legal strategy that prioritizes long-term climate goals without compromising developmental equity. A "green federalism" approach, wherein state-level innovations, like Gujarat's pioneering hybrid wind-solar policy, are harmonized with national climate objectives can serve as a legal and institutional blueprint. This model not only allows for decentralized experimentation but also ensures alignment with India's international obligations. Ultimately, rewriting the legal architecture to support a just, inclusive, and climate-resilient energy

transition is not merely a regulatory necessity but a moral imperative for securing the country's socio-environmental future.

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1, 5-Benzothiazepines in Medicinal Chemistry: Structural Diversity, Biological Targets and Drug Discovery

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Abstract:

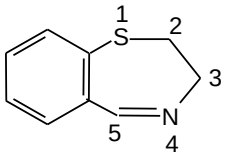
1, 5-Benzothiazepines represent a pivotal class of heterocyclic compounds exhibiting remarkable structural diversity and broad-spectrum biological activities. This comprehensive review highlights recent advances in the synthesis, functionalization, and pharmacological profiling of 1, 5-benzothiazepine derivatives. Emphasis is placed on their interaction with various biological targets, including calcium channels, kinases, and enzymes implicated in cancer, inflammation, and neurological disorders. The structural modifications influencing bioactivity are systematically discussed, offering insights into structure-activity relationships (SAR) that underpin their therapeutic potential.

By integrating medicinal chemistry perspectives with recent drug discovery efforts, this review underscores the promise of 1, 5-benzothiazepines as versatile scaffolds in the development of novel pharmaceutical agents.

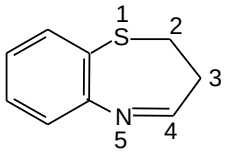
Keywords: *1, 5-Benzothiazepines, structural diversity, biological activities, drug discovery.*

Introduction:

1,5-Benzothiazepine is one of the three possible benzo-condensed derivatives, viz., 1,4-, 4,1- and 1,5-benzothiazepines of the 1,4-thiazepine.[1] 1,5-Benzothiazepine is a seven membered ring heterocyclic compound containing sulphur and nitrogen as hetero atoms. Benzene ring fused with thiazepine is known as benzothiazepine. Recently the successful exploitation of 1,5-benzothiazepine type of compounds such as diltiazem, thiazesim, chloro-diazepoxide and diazepams as potential CNS, cardiovascular and psychopharmacological agents has been reported. Owing to their well-known bioactivities, 1,5-benzothiazepines have been intensely studied



1,4-Benzothiazepine



1,5-Benzothiazepine

The parent 1,5-benzothiazepine itself has not hitherto been described in the literature. However, its derivatives belong to the most frequently studied benzothiazepines. This may be due to their easy availability and the wide range of their bioactivities.

Antibacterial[2-4] and antifungal[2] properties of 2,4-diaryl, 2,3-dihydro-1,5-benzothiazepines have been reported.

Several 4,6-Bis (2'-substituted-2',3'-dihydro-1,5-benzothiazepin-4'-yl) resorcinol have been found to be potential antifeedants.[5]

Some new tricyclic derivatives with structural analogy to TIBO were prepared starting from properly substituted 1,5-benzothiazepine. All synthesised compounds were submitted to screening for *invitro* anti-HIV-1 activity. Only two compounds showed moderate activity.[6]

Synthesis and biological evaluation of 5*H*-indolo [3,2-*b*] [1,5] benzothiazepine derivatives, designed as conformationally constrained analogues of the human immuno deficiency virus type-I (HIV-I) reverse transcriptase inhibitor, was carried out by Silvestri *et al.*[7]

Benzothiazepines such as *Diltiazem*[8] [(a)] or *Thiazesim*[9] are constantly used as antidepressant, coronary vasodilator and antiangina agents. Synthesis and biological activity of natriuretic metabolite of diltiazem and its derivatives have been reported.[8 (b)]

Some new thieno and pyrazolo [2,1] benzothiazepine derivatives[10] have been synthesised which showed better antidepressant activity than the ref. drugs imipramine and tianeptine.

A. Levai[11] has reviewed the syntheses of four known groups of optically active 1,5-benzothiazepines. The references included show the most important biological activities e.g., CNS agent, cardiotonic agent, histamine H_2 antagonist, anti-ulcer agent, etc.

Bioassay screening of 10-substituted-2-chloro-6*a*, 7-dihydro-6*H*-7-(4-substituted phenyl)-6-phenyl-[1] benzopyrano[3,4-*c*] [1,5] benzothiazepines show mild analgesic and anti-convulsant activity.[12]

W. James *et al.*[13] have summarized the reports of new compounds with anticonvulsant activity, that include benzothiazepines as antiepileptic drugs. Recently 1,5-benzothiazepine derivatives[14] are reported to be anti-convulsant agents.

Krapcho and Yale[15] reported therapeutic activities like CNS depressant, ataractic agents and antispasmodics in 1,5-benzothiazepine derivatives.

The antihypertensive[16] property of 1,5-benzothiazepine derivatives have been reported recently. Earlier, Kawakami Masaru *et. al.* [17] have tested hypotensive effects in normotensive and hypertensive rats using a new 1,5-benzothiazepine derivative and reported as a useful hypertensive agent. The hypotensive and antimyocardial-stunning effects of a new 1,5-benzothiazepine anti-hypertensive agent[18] were investigated in dogs.

2,3-Dihydro-1,5-benzothiazepin-4-(5*H*)-ones substituted with an alkyl, alkoxy, alkylthio, hydroxy or amino group on the fused benzene ring of 1,5-benzothiazepine skeleton were synthesized and their vasodialating, antihypertensive and platelet aggregation-inhibitory activities were investigated.[19]

Benzothiazepines useful as intermediates for antihypertensives were patented[20] by Takeda Mikio *et al.*

Recent research has expanded the therapeutic potential of Benzothiazepines derivatives, particularly in oncology. A study synthesized novel BTZ compounds using polyethylene glycol-400 (PEG-400)-mediated pathways, achieving yields over 95% in under an hour. In vitro evaluations revealed that compound 2c exhibited potent cytotoxic activity against liver cancer cells (Hep G-2) with an IC_{50} of 3.29 μM, outperforming the standard drug methotrexate. These findings underscore the promise of BTZ derivatives as anticancer agents, warranting further exploration and development[21].

Notably, BTZ derivatives have shown promise in inhibiting α-glucosidase, an enzyme implicated in diabetes mellitus, highlighting their potential as antidiabetic agents[22].

• Methods of Synthesis of 1, 5-Benzothiazepines and Their Derivatives

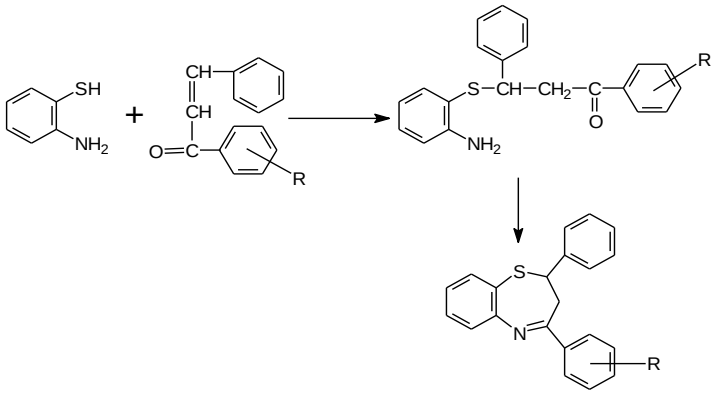
Synthesis and chemical transformations of 2,3-dihydro-1,5-benzothiazepines have been intensely studied by several research groups and as a result, numerous new 1,5-benzothiazepine derivatives have been described in the literature.

• From α-β-Unsaturated Carbonyl Compounds

1. Chalcones and *o*-Aminothiophenol

The synthesis of 1,5-benzothiazepines have been performed conveniently by the reaction of **α-β-**unsaturated ketones with 2-aminothiophenol (ATP). First Ried and Marx[23] then Stephens and Field[24] reported their synthesis from chalcones as chalcone and a slight excess of *o*-ATP were dissolved in boiling methanol. Then piperidine was added, followed by addition of glacial acetic acid. The reaction was reported to take place through formation of an intermediate propiophenone.

This two-step reaction sequence, viz., first nucleophilic addition of the mercapto group to the β-carbon atom of the unsaturated ketone followed by condensation of the amino and carbonyl groups to form the seven-membered hetero ring have been explained by A. Levai.[25] Also, the influence of substitution pattern of aromatic rings of the chalcone on these reactions have been investigated.[26]



Modifications in the known reaction conditions or development of new procedure have given newer insight into the formation of 1,5-benzothiazepines.

A mixture of 2-ATP and benzalacetophenone (chalcone) in *o*-xylene was refluxed for 3hr, to get 2-(substituted phenyl)-4-phenyl-1,5-benzothiazepines.[27] Earlier Jadhav and Ingle[28] reported the synthesis of 2,4-diaryl-2,3-dihydro-1,5-benzothiazepines. Different 4-(*p*-chlorophenyl) -2-(*p*-methoxyphenyl)-8-substituted-2,3-dihydro-1,5-benzothiazepines have been synthesized by U.C. Pant *et. al.*[29]

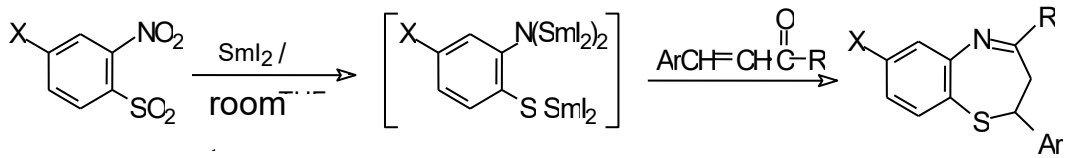
2, 4-Diaryl–2,3-dihydro-1,5-benzothiazepines have been prepared in satisfactory yields by reaction of chalcones with 2-ATP in anhydrous toluene.[30] U.C. Pant and A. Bhatia[31] prepared 2-(4-Chlorophenyl)-4-(4-methoxyphenyl)-8-substituted–2, 5-dihydro-1,5-benzothiazepines by treating 5-substituted-2-aminobenzenethiol with 4-chloro-4'-methoxybenzalacetophenones in pyridine.

Recently single step syntheses of 2-(4-chlorophenyl)-4-(4-chlorophenyl)-2, 5-dihydro-8-substituted-1,5-benzothiazepines[32] have been achieved by the reaction of 5-substituted–2-aminobenzenethiols with dichloro benzalacetophenone, in ethanol containing dry hydrogen chloride gas.

Simple and convenient procedures have been developed for the synthesis of 2,4-diaryl-2,3-dihydro-1,5-benzothiazepines by the reaction of 2'-hydroxychalcones with 2-ATP either in hot ethanol in presence of piperidine or in hot toluene in presence of trifluoroacetic acid. [33]

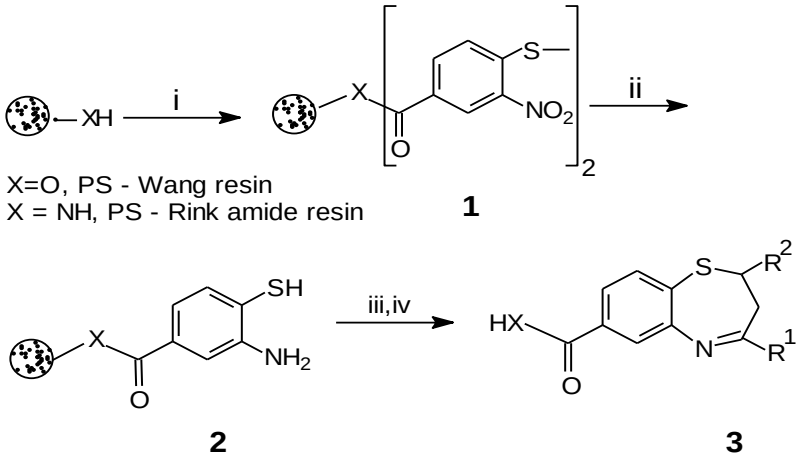
From Chalcones and Nitro disulfides

A new route to 2, 3-dihydro-1,5-benzothiazepines from nitro disulfides and α-β unsaturated ketones (chalcones) by SmI_2 has been reported.[34]



3. Solid Phase Combinatorial Synthesis

Recently, a solid phase combinatorial approach[35] was envisaged for the synthesis of 2, 3-dihydro-[1, 5]-benzothiazepine derivatives. For this purpose, bis-(2-nitro-4-carboxyphenyl) disulfide was loaded on Wang resin and Rink amide resin. The nitrogroup was reduced to its amine with concomitant cleavage of the disulfide bond using $SnCl_2$-$2H_2O$ to afford **2**. Nucleophilic attack on an α-β-unsaturated ketone, followed by TFA cleavage from the resin, gave 2, 3-dihydro-[1,5]-benzothiazepine **3**.



Reagents:

(i) bis-(2-nitro-4-carboxyphenyl) disulfide, HOBt, DIC, DMF, rt, 12h.

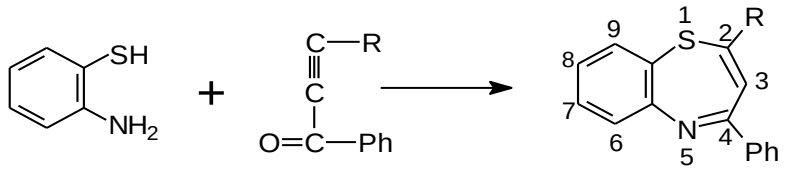
(ii) $SnCl_2$-$2H_2O$, NaOAc, DMF, rt, 4h.

(iii) R^1-CO-CH=CH-R^2 (Chalcone),EtOH,1% AcOH,80°C,12h.

(iv) 20% TFA, 1h.

4. From Alkynones and *o*-Amino thiophenol

2-Aminothiophenol was allowed to react with alkynones[36] in a mixture of hot methanol and acetic acid to obtain 2, 4-disubstituted 1,5-benzothiazepines.



1,5-Benzothiazepine derivatives are very important and useful compounds in organic and pharmaceutical chemistry.

Synthesis of benzothiazepines has been intensely studied and numerous procedures are described in the literature. Although this reaction has been investigated by several research groups, and a number of 1,5-benzothiazepine derivatives have been reported,

The substituted1,5-benzothiazepines can conveniently be synthesised by the reaction of 2-aminothiophenol with α,β-unsaturated ketones like chalcones. This microwave irradiation method is attributed to have following features:

1) Smooth reaction condition.
2) Reaction time is very short just in 2-3 minutes.
3) Hydroxychalcones always gave the product in better yields.
4) No side products are formed.
5) Product is isolated easily.

However, the combination of solvents, strong acid and long reaction time period makes this method environmentally hazardous. Thus, a simple, general and efficient procedure for the synthesis of this important heterocyclic system is adopted.

The application of microwave irradiation (MWI) to organic synthesis has been the focus of considerable attention in recent years and is becoming an increasingly popular technology. The salient features of the microwave approach are rapid reaction rates, cleaner reaction conditions and enhancements in chemical yields.

Under the framework of 'Green Chemistry' we have followed an environmentally benign synthesis of benzothiazepines. Further attractions of this method are that it allows reactions in open vessels (thus avoiding the risk of high pressure development) and synthesis on preparative scales. Here in we report a facile microwave synthesis of 1, 5-benzothiazepines from 2-aminothiophenol and various chalcones in the presence of catalytic amount of glacial acetic acid using DMF as a reaction mediator.

Conclusion:

1 ,5-Benzothiazepine the main seven-membered heterocyclic ring system reported for their cardiac and psychotherapeutic activities, also were highlighted as important biologically active scaffolds. The eagerness to identify novel drugs for the treatment of diseases, has fuelled the development of new molecular scaffolds. The 1,5-benzothiazepine framework is a versatile pharmacophore whose derivatives demonstrated remarkable biological activities such as anti-HIV, anti-tuberculosis, anti-cancer, angiotensin converting enzyme inhibitor, anti-bacterial, anti-fungal, etc. So, it is concluded that the 1,5-benzothiazepine is one of the most important pharmacophores

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Nanomaterials for Sustainable Energy Applications: Recent Advances and Future Perspectives

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Abstract:

Nanomaterials are revolutionizing the field of sustainable energy by offering unique properties such as high surface area, tunable bandgaps, and enhanced catalytic activity. This chapter reviews recent advancements in nanomaterial-based technologies across solar energy conversion, energy storage systems, hydrogen production, and fuel cells. The multifunctional roles of nanostructured materials such as metal oxides, perovskites, carbon-based nanomaterials, and emerging 2D materials are discussed. Furthermore, the challenges hindering commercialization and the future research pathways for nanomaterials in sustainable energy are explored. Emphasis is placed on green synthesis routes and the scalability of these materials for real-world energy applications.

Keywords: *Nanomaterials; Sustainable Energy; Solar Cells; Energy Storage; Hydrogen Production; Fuel Cells; Photocatalysis; Green Synthesis; Perovskites; 2D Materials*

1. Introduction

The increasing global energy demand, coupled with the pressing need to reduce greenhouse gas emissions, has intensified the search for sustainable and renewable energy solutions. Among emerging technologies, nanomaterials have proven to be highly promising in revolutionizing energy systems by enabling higher performance, miniaturization, and resource efficiency. Defined by at least one dimension in the nanometer range, nanomaterials possess unique surface, optical, and electronic characteristics that differ significantly from their bulk counterparts, making them ideal for diverse energy applications.

In energy conversion systems such as solar cells, nanomaterials can enhance light absorption, charge separation, and transport. In storage technologies like batteries and supercapacitors, they offer high surface area and tailored porosity for improved ion diffusion and electrochemical activity. Additionally, in hydrogen production and fuel cell systems, nanostructured catalysts significantly boost reaction rates and fuel utilization efficiency.

As global research in nanoscience expands, it becomes imperative to consolidate recent findings, identify existing challenges, and propose forward-thinking strategies to bridge the gap between lab-scale innovations and commercial-scale deployment. This chapter aims to provide a comprehensive overview of the current state-of-the-art and future perspectives in nanomaterials for sustainable energy applications.

2. Recent Advances in Nanomaterials for Energy Applications

2.1 Nanomaterials in Solar Energy Conversion

Nanomaterials have played a transformative role in enhancing solar cell efficiency. Silicon-based photovoltaics, although dominant, face limitations in cost and energy payback time. Nanostructured materials like quantum dots, perovskites, and plasmonic nanoparticles have shown promising results in overcoming these barriers.

a. Perovskite Solar Cells (PSCs) :

Perovskite solar cells (PSCs) have reached power conversion efficiencies (PCEs) exceeding 25%, and the use of nanocrystalline TiO_2 or ZnO as electron transport layers (ETLs) has played a crucial role in enhancing charge extraction. Wenzhong Shen & Et al (2024) have demonstrated a simple low-temperature bilayered ETL by adding $SnCl_2$ to the colloidal TiO_2 nanocrystals for efficient planar PSCs. The TiO_2@SnO_2 bilayered ETL was recognized for the better electron extraction and hole blocking ability than TiO_2, owing to that Sn doping of TiO_2 raises the Fermi level and a stronger built-in electric field drives the flow of electrons from TiO_2 to SnO_2.[1a]
These materials, particularly ZnO, are beneficial due to their high transparency, suitable energy band structure, and good electron mobility, leading to improved device performance and stability. ZnO is a promising ETL for planar PSCs due to its ability to simplify device architecture and enable low-temperature processing, making it suitable for cost-effective and flexible devices. Its key properties—mobility, energy levels, defect states, and stability—are crucial to device performance. This section briefly covers ZnO deposition methods and recent advances in its application in PSCs, along with optimization strategies like doping and surface modification to overcome challenges such as energy mismatch and low electron mobility.[1b]

b. Quantum Dots (QDs):

QDs such as PbS and CdSe have tunable bandgaps and exhibit multiple exciton generation (MEG), potentially exceeding the Shockley–Queisser limit. Quantum Dots (QDs) like PbS and CdSe have tunable bandgaps and exhibit Multiple Exciton Generation (MEG), which can potentially exceed the Shockley–Queisser limit. This means that they can generate more than one electron-hole pair when absorbing a single high-energy photon, potentially increasing the efficiency of solar cells.[2a-b]

Colloidal quantum dots (QDs) are promising for next-gen solar cells, with PbS QDs leading due to their air stability. PbSe QDs offer better performance via multiple exciton generation but suffer from poor stability. This work introduces a direct cation exchange method to create air-stable PbSe QDs with chloride and cadmium passivation. These QDs retain their optical properties for over 30 days and enable high-efficiency solar cells (over 6% PCE) without extra protection—a record for PbSe QD devices.[2c]

c. Plasmonic Nanoparticles:

Particles whose electron density can couple with electromagnetic radiation of wavelengths that are far larger than the particle due to the nature of the dielectric-metal interface between the medium and the particles called as Plasmonic nanoparticles. Plasmonic NPs like those made of gold (Au) or silver (Ag), which enhance light trapping and absorption due to the phenomenon of localized surface plasmon resonance (LSPR). LSPR occurs when light interacts with the collective electrons on the surface of these nanoparticles, causing them to oscillate and generate a strong electromagnetic field. This enhanced field leads to increased light absorption and scattering, effectively trapping and enhancing the absorption of light.[3a]

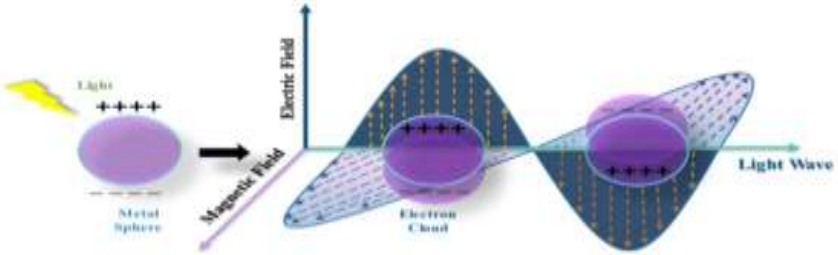


Figure : The electrons in a metal can careen like a jelly, pulled back by the attraction of the positive metal ions that they leave behind.[3 b & C]

Localized surface plasmons (LSPs) are the non-propagating excitations of the conducting electrons coupled with EM field. The curved surface of the spherical nanoparticle applies a

restoring force, which produces resonance in the electrons. This is called a localized surface plasmon resonance.

d. Carbon-based Nanomaterials:

Carbon nanostructures such as graphene, graphene oxide (GO), and carbon nanotubes (CNTs) are increasingly being integrated into solar cells for their exceptional conductivity and transparency. Graphene serves as a transparent electrode or interfacial layer to improve charge extraction and reduce recombination. CNTs can form percolating networks that facilitate hole transport in hybrid and perovskite solar cells, enhancing both mechanical flexibility and stability. Reduced graphene oxide (rGO) layers are used to improve energy band alignment and interface quality in perovskite solar cells.[4a &b]

e. Dye-Sensitized Solar Cells (DSSCs):

Nanostructured materials enhance light harvesting and electron transport in DSSCs. TiO_2 nanotubes and mesoporous TiO_2 provide large surface areas for dye loading and effective pathways for electron transport. Incorporating ZnO nanorods and SnO_2 nanospheres can reduce electron recombination and enhance open-circuit voltage. Doping nanomaterials (e.g., Nb-doped TiO_2) improves electrical conductivity and reduces interfacial resistance.[5]

2.2 Nanomaterials in Energy Storage Systems

Energy storage is vital for balancing intermittent renewable energy sources. Nanomaterials improve electrochemical performance in batteries and supercapacitors by offering faster ion transport and higher electrode/electrolyte interface area.

a. **Lithium-ion Batteries (LIBs):** Nanostructured anode materials like Si nanoparticles, TiO_2 nanotubes, and graphene composites increase specific capacity and cycle life. Additionally, lithium iron phosphate ($LiFePO_4$) nanoparticles and layered transition metal oxides (e.g., NMC—nickel manganese cobalt oxide) in nanostructured forms are used for enhanced cathode performance.[6]

b. **Sodium-ion Batteries (SIBs):** Due to sodium's abundance, nanostructured $NaFePO_4$ and hard carbon nanosheets are being explored as alternatives. Other nanomaterials like SnS_2 nanosheets and Prussian blue analogues (PBAs) are being researched for improved capacity and rate capability.[7]

c. **Supercapacitors:** Carbon nanotubes (CNTs), graphene, and metal-organic frameworks (MOFs) enhance capacitance and energy density. Additionally, pseudocapacitive materials such as MnO_2 nanoparticles, conductive polymers (e.g., polyaniline and polypyrrole in nanostructured forms), and transition metal dichalcogenides (TMDs) like MoS_2 are being incorporated to improve energy storage.[8]

d. **Lithium-sulfur (Li-S) Batteries:** Sulfur nanocomposites and conductive carbon-based nanostructures (e.g., graphene-sulfur hybrids) help suppress polysulfide shuttle effects and improve conductivity.[9]

e. **Solid-State Batteries:** Nanostructured solid electrolytes such as garnet-type $Li_7La_3Zr_2O_{12}$ (LLZO) nanoparticles and sulfide-based nanomaterials enhance ionic conductivity and interface stability.[10]

f. **Flow Batteries:** In redox flow systems, nanostructured carbon felt electrodes with functionalized surfaces or embedded metal nanoparticles increase electrochemical activity and reduce overpotentials.[11]

2.3 Nanomaterials for Hydrogen Production

Hydrogen is a clean energy carrier, and photocatalytic water splitting using nanomaterials is a sustainable production route.

a. **Photocatalysts**: TiO_2, g-C_3N_4, ZnO, and $BiVO_4$ nanostructures exhibit efficient light absorption and electron-hole separation.[12]

b. **Co-catalysts**: Noble metal nanoparticles (Pt, Pd) are commonly used to increase hydrogen evolution rates.[13]

c. **2D Materials**: MXenes and transition metal dichalcogenides (TMDs) are being investigated for their catalytic activity and conductivity.[14]

2.4 Nanomaterials in Fuel Cells:

a. **Enhanced Electrocatalytic Surface Area**: Nanomaterials provide a high surface-to-volume ratio, which increases the number of active sites for electrochemical reactions in fuel cells, thereby boosting their performance.[15]

b. **Nanostructured Membranes for PEMFCs**: Incorporating inorganic nanomaterials such as silica or zirconia into Nafion membranes improves thermal stability and water retention, enhancing PEMFC durability under dry conditions.[16]

c. **Core-Shell Nanoparticles**: Pt-based core–shell nanoparticles (e.g., Pd@Pt, Au@Pt) reduce Pt loading while maintaining high catalytic activity, addressing cost and resource concerns in PEMFCs.[17]

d. **Perovskite Nanomaterials in SOFCs: Nanostructured perovskites (e.g., $La_{1-x}Sr_xCoO_3$) are used as** cathode materials to enhance oxygen ion conductivity and stability at intermediate temperatures.[18]

e. **Durability and Degradation Resistance**: Nanomaterials such as TiO_2 or SiC are used to reinforce catalyst supports, enhancing resistance to corrosion and carbon degradation during long-term operation.[19]

3. Challenges and Future Perspectives

Despite the remarkable advances in the field of nanomaterials, particularly in their synthesis, characterization, and application, several key challenges must be addressed to fully realize their potential in commercial and large-scale applications. The following points outline the most pressing issues, along with considerations for future developments:

I. **Scalability:** While many nanomaterials have demonstrated excellent properties at the laboratory scale, translating these techniques to industrial-scale production remains a significant hurdle. Laboratory synthesis methods often involve complex procedures, precise control over reaction conditions, and high-purity reagents, which are difficult and expensive to replicate on a larger scale. Moreover, batch-to-batch consistency becomes harder to maintain, and the development of continuous, scalable, and economically viable manufacturing processes is essential for commercialization.

II. **Stability:** Nanomaterials often exhibit high surface area and reactivity, which, although beneficial for applications like catalysis or energy storage, can also lead to instability under operational conditions. Issues such as particle aggregation, oxidation, sintering, and phase transformations can degrade performance over time. For example, metal nanoparticles may oxidize or coalesce at elevated temperatures, leading to a loss in catalytic activity. Addressing these issues requires the development of robust stabilization strategies, such as surface passivation, core-shell structures, or embedding nanomaterials in protective matrices.

III. **Toxicity and Environmental Impact:** The increased use of nanomaterials raises important questions regarding their impact on human health and the environment. Nanoparticles can interact with biological systems in unforeseen ways, potentially leading to cytotoxicity, genotoxicity, or bioaccumulation. Additionally, improper disposal or release of nanomaterials into ecosystems may disrupt microbial activity or aquatic life. Therefore, comprehensive risk assessments, development of green synthesis routes, and strict regulatory frameworks are crucial to ensure the safe handling, usage, and disposal of nanomaterials.

IV. **Cost-effectiveness:** Many high-performance nanomaterials rely on rare or expensive elements such as platinum (Pt), palladium (Pd), or rare earth elements, which significantly increases the cost of production. This economic constraint limits their widespread adoption, particularly in cost-sensitive industries. Future research should focus on developing low-cost alternatives, such as earth-abundant materials or efficient recycling strategies, as well as optimizing synthesis processes to minimize material waste and energy consumption.

4. Future Research Directions

To advance the practical implementation and broaden the impact of nanomaterials, future research must focus on innovative, sustainable, and interdisciplinary approaches. The following directions highlight promising pathways that address existing limitations while aligning with global priorities in green technology, resource efficiency, and smart materials design:

I. **Development of Green Synthesis Routes:**

The shift toward environmentally sustainable nanomaterial synthesis is both a scientific and ethical imperative. Future research should emphasize the development of **green synthesis techniques** that minimize hazardous reagents, reduce energy consumption, and promote biodegradability. In particular, **plant-based extracts** and other **biotemplates** offer naturally occurring compounds that can act as reducing and stabilizing agents, enabling the eco-friendly production of nanoparticles. Additionally, **low-temperature synthesis methods** present a viable alternative to traditional high-energy techniques, offering better control over nanostructure formation while reducing the overall environmental footprint. These methods not only support sustainability goals but also open up new applications in biomedical, food, and agricultural sectors due to their inherently biocompatible nature.

II. **Engineering of Heterostructures and Core–Shell Architectures:** Structural innovation at the nanoscale continues to be a cornerstone of material advancement. Future research will increasingly focus on heterostructures and core–shell architectures, which combine multiple materials or phases to exploit synergistic properties not attainable in single-component systems. Such engineered nanostructures can exhibit enhanced charge separation, magnetic coupling, or catalytic activity, depending on their composition and interface design. For instance, in energy applications, these architectures can improve electron transport and structural integrity, leading to higher efficiency and longer operational lifetimes. Continued exploration of interface chemistry, lattice matching, and morphology control will be crucial for optimizing these complex systems.

III. **Integration of Artificial Intelligence (AI) and Machine Learning (ML):** The application of **AI and ML** is rapidly transforming the landscape of materials research. These tools enable high-throughput screening, property prediction, and process optimization by uncovering patterns in large, multidimensional datasets. In the context of nanomaterials, ML algorithms can predict optimal synthesis conditions, forecast long-term stability, and even propose novel material combinations with targeted functionalities. Future research should focus on creating robust, data-rich models, incorporating real-time feedback from experiments, and integrating AI into automated laboratories. This data-driven approach will significantly accelerate the discovery-to-deployment cycle of next-generation nanomaterials.

V. **Emphasis on Circular Economy and Recyclability:**

Sustainable nanomaterials research must also account for end-of-life considerations. Embracing the principles of the circular economy, future work should prioritize the design of nanomaterials that are easily recyclable, reusable, or biodegradable. This includes developing energy devices—such as batteries, fuel cells, and supercapacitors—that incorporate non-toxic, abundant materials and can be efficiently disassembled and recovered. Integrating life-cycle assessments (LCA) into the early

stages of material design will help identify environmental bottlenecks and inform greener innovation pathways. Additionally, scalable methods for the recovery and reuse of nanomaterials will play a critical role in minimizing waste and conserving finite resources.

5. Conclusion

Nanomaterials have unlocked new paradigms in sustainable energy technologies by delivering breakthroughs in efficiency, durability, and functionality. From solar energy harvesting to next-generation storage and clean fuel generation, their contributions are both significant and transformative. However, realizing their full potential requires overcoming key barriers, including material stability under operational conditions, cost of rare elements, environmental safety, and the scalability of synthesis methods.

Future advancements will increasingly rely on multidisciplinary strategies—employing green chemistry for eco-friendly production, leveraging AI for accelerated materials discovery, and designing recyclable architectures for circular economy compatibility. As the global transition toward decarbonization intensifies, nanomaterials are poised to play an indispensable role in creating a resilient, sustainable, and low-carbon energy future.

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Role Of Nanomaterials In Biomedicine

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Abstract:

The design and development of nanomaterials have become a primary focus of research due to their potential applications in the biomedical field. Factors such as size, shape, surface charge, and microstructure are critical considerations in the production of nanoparticles (NPs), as they directly influence the performance of these materials. These characteristics are also highly dependent on the methods used for their synthesis. This chapter aims to provide a comprehensive analysis of recent advancements in nanomaterials for biomedical engineering, with a specific focus on material selection. The current article describes key applications of nanomaterials in diagnosis as biosensors and in bioimaging. Their role in therapeutic interventions and drug delivery systems are comprehensively detailed. Challenges such as ensuring delivery efficiency and minimizing potential toxicity are also addressed. Ultimately, fostering collaboration between researchers and industry experts is essential to advance the development and clinical application of these materials, unlocking the full promise of nanomedicine in modern healthcare.

Keywords: *Nanomaterials, biosensors, bioimaging, therapeutic action, drug delivery*

Introduction:

Nanotechnology is an exciting and constantly evolving field which holds promise for varied applications that have a pivotal influence in advancing key human solutions and interventions. Nanotechnology focuses on design and creation of nanomaterials; materials having dimensions ranging between 1 to 100nm by two approaches namely top down and bottom up approach. The first approach or the top down approach works by downsizing bulk materials to the desired size. The second approach or the bottom up approach works by scaling up and creating larger structures of desired size from basic units. Thus nanotechnology helps to create nanoparticles which are having dimensions that range between 1 to 100 nm. The small size range in which these particles exist, results in their greater surface area in comparison to their volume ratio and hence they possess remarkable surface properties. Nanotechnology has not only made it possible to create nanomaterials of desired dimensions but also it is possible to control their structures thereby controlling their properties. Hence they find applications in numerous fields such as biological applications, environmental applications, biomedical applications, analytical applications, applications as nanosensors, applications in nanoelectronics and many more. Also, they show promise for applications in newer areas such as packaging materials in food applications and nanocarriers of bioactive compounds.

In particular, metallic nanoparticles and carbon nanomaterials have been widely used in electrochemical sensing of biomolecules due to their increased surface area and good electrical

conductivity. Numerous biomedical applications of metallic nanoparticles are well reported as they are biocompatible and have good electrical conductivity. However it is found that metallic nanoparticles synthesised by the top-down approach have a tendency to agglomerate due to which they cannot be used for biomedical applications. The bottom-up approach method in general and chemical reduction method in particular is commonly used method to synthesise metallic nanoparticles. The flexibility, simplicity, low cost and production of homogenous particles makes this method highly advantageous. In the recent past, less toxic biological method of nanoparticle synthesis which is relatively economical, environment friendly and sustainable is gaining preference. Carbon nanomaterials are interesting nanomaterials which are fundamentally carbon-based and at least one dimension is reported to be smaller than 100 nm. They exist in different structures and morphologies which include graphene oxide, fullerenes, carbon nanotubes, carbon nanorods, carbon nanofibres, carbon thin films/sheets or carbon nanoparticles/ quantum dots. Carbon nanomaterials possess unique structural, electrical and thermal which makes them well-suited for biomedical applications.

Biomedical Applications Of Nanomaterials:

Background:

The recent decades have seen a significant growth in applications of nanomaterials in biomedicine and have potential for changing various aspects of health management. Nanotechnology has the capability to modify the properties of such nanomaterials by designing their structures and their characteristics at nanoscale thus making them potential candidates for use in the identification, treatment and regrowth of dysfunctional biological systems. Nanomedicine is an emerging term which refines therapeutic identification, treatment and protection of diseases at the human cellular level. Their primary focus is on the nanomaterial's interaction with the biological subject. The role of nanomaterials in biosensors is very interesting as it allows the utilization of many new transduction innovations with enhanced selectivity and specificity for in vivo studies of various substances.

Nanomaterials are increasingly favoured due to their due to their ease of modification and control and they play a crucial role in early diagnostics, therapy, drug delivery and treatment.

The biomedical applications of nanomaterials can be broadly divided into three areas:

1. Diagnosis
2. Remedy/Therapy
3. Drug delivery

The biomedical applications of nanomaterials are dependent primarily on their bioactivity and biocompatibility properties. Bioimaging and biosensors are included under diagnostic role of nanomaterials. Some remedy/therapy applications include use of nanomaterials as anti-bacterial agents, anti-cancer agents and for wound healing or tissue engineering. Drug delivery with nanomaterials includes medicine or gene delivery to the targeted site.

I.Nanomaterials as diagnostic tools for Biomedical Applications:

Biosensors:

A biosensor is basically an analytical instrument which can analyse biological samples. It functions by converting a chemical, biological or biochemical response into an electrical signal. A biosensor is made of three basic parts; namely a bioelement, the transducer and the electronic unit.

Biosensors have gained importance over the years due to their successful use for cancer diagnosis. Nanomaterials particularly metal nanoparticles have demonstrated exceptional sensitivity in tumour cell detection. Metal nanoparticles can easily attach to recognition molecules, i.e. antibodies on biomolecular surfaces for effective identification. Metal nanoparticles have readily tuneable and strong optical characteristics that can be used in optical imaging. Different types of sensors such as electrical, electrochemical, colorimetric, fluorescent and bio-barcode assay sensors can be developed based on their typical properties. Au nanoclusters showing red fluorescence were prepared using microwave by Tian et al. The study demonstrated that cancerous cells, like HepG2, could trigger fluorescent signals in Au nanoclusters, while normal cells showed no such effect. The results of MTT assay positively indicated that they had potential to be used for the initial detection of cancer cells. AuNPs and graphene oxide system prepared by Saeed et al showed good sensitivity for early breast cancer detection. Biconjugated Au nanorod have shown increased sensitivity in tumour detection in comparison to traditional biosensing technique (SPR). MOF made of AgNPs and modified La(III) acted as a "turn-off" fluorescent biosensor with excellent sensitivity as a miRNA-155 biomarker. Graphene-functionalized silver nanoparticles (GF/AgNPs) have demonstrated promising effectiveness in lung cancer detection. The integration of AuNPs with carbon nanotubes (MWCNT) offers significant potential as a biosensor for human cancer detection owing to their enhanced sensitivity. Carbon based material development has gained popularity as they are biocompatible and have huge void spaces. As a result, it is possible to incorporate functional nanomaterials into their core. Nitrogen doped graphene quantum dots showed promising and fast results with good detection levels as a sensor of a newly emerging cancer biomarker i.e. hydrogen peroxide. Nanohybrids consisting of ZnO nanorods – AuNPs exhibited a sensitive response to ovarian cancer .

Detection of pathogens, microbes and infections caused such as urinary tract infection have been carried out using electrochemical biosensors. Hafnium oxide based biosensor has been found effective in detecting any infection caused in the human body post insertion of an implant.

The electrochemical biosensors have revolutionised glucose level testing and monitoring of diabetic patients as they account for almost 80% of biosensors used worldwide in home settings. Commercially available glucose monitoring sensors can be replaced by nanomaterial based biosensors such as carbon nanotube based materials, graphene based nanomaterials or carbon quantum dots. These nanomaterial-based electrochemical biosensors have shown the way for development of noninvasive glucose detection methods by testing of saliva, tears, urine or other serum samples where the level of glucose falls in the micromolar range. Electrochemical biosensors utilizing carbon nanotubes have shown significant potential for effective glucose detection. For example, glucose biosensor having nanoelectrode arrays made of vertically placed carbon nanotubes (single walled) has been created. Glucose biosensors can face interference from ascorbic acid and uric acid which naturally occur in the body. This problem was effectively addressed by a novel palladium nanoparticle modified carbon nanotube used in combination with anion repelling Nafion which also exhibited good sensitivity. Thus hybrid sensors made up of carbon nanotubes and metal nanoparticles were developed and their performance in glucose detection has been very promising. Cobalt nanoparticles modified carbon nanotubes developed by Yang et al showed high sensitivity and low detection limits for glucose sensing. Au/Pd co-deposited carbon nanotubes

(single walled) has shown excellent glucose detection limit and sensing range. This biosensor on modification wherein Pt nanospheres were used gave better sensitivity. These advanced hybrid sensors can accurately measure blood glucose levels for both diabetic and healthy patients. Glucose detection with use of graphene based biosensors has produced equally promising results as compared to carbon nanotube based biosensors. Graphene based biosensors created by Kang et al was able to monitor glucose levels with good detection limit and sensitivity. Other similar graphene based biosensors such as polymer polypyrrole graphene biosensor was developed and tested for glucose detection with good results. Further graphene metal hybrid biosensor made up of graphite nanoplatlets and Pt nanoparticles showed high glucose sensitivity with low detection limit. Also multi-layered graphene sheets with Pt were developed and tested for glucose levels with great success.

Carbon quantum dots or CQDs are gaining attention to be developed as electrochemical biosensors for detection of glucose and other biomolecules such as dopamine, hemoglobin, cholesterol, ascorbic acid. They can be used in H_2O_2 detection and reduction owing to their remarkable electrocatalytic properties. Hemoglobin detection using CQDs combined with polymers was used by Barati et al and Kour et al and the sensitivity and selectivity results were excellent. Also H_2O_2 detection using CQD nano-composites (PtNPs-CDs/IL-GO) have been reported by Chen et al with excellent results in terms of selectivity.

An electrochemical biosensor for glucose identification was developed by Dave et al. This graphene based CQD biosensor was discovered to be biocompatible and made greater enzyme absorption on the electrodes possible. Thus it demonstrated promise for application as an electrochemical biosensor.

Bioimaging:

Bioimaging also called as biomedical imaging is a non-invasive technique to visualize biological events in real time. The advancement of nanotechnology has resulted in increased use of nanomaterials which include nanorods, nanoshells, nanosphere, nanoparticles and quantum dots for bioimaging and cancer therapy. Their main advantage being that they are cost effective, non–invasive, show high sensitivity and are suitable for extended monitoring. Fluorescent nanoparticles generally consist of multiple fluorophore molecules, which contribute to their enhanced photoluminescent emission. Encapsulating them in the particle enhances stability, minimizes photobleaching, and lowers toxicity.

Some functionalized nanomaterials which acted as fluorescent probes have potential for contrast agent applications. A conjugate of fluorescent Au nanoparticles with diatriozoic acid and nucleolin served as a contrast agent to identify the $CL1{-}5$CL1−5 tumour location.

CQDs offer high photostability, good biocompatibility, simple synthetic routes, flexible designability, multicolor emission, crimson/near-infrared emission and two/multiphoton luminescence, positioning them as next-generation fluorescent probes for both in vitro and in vivo bioimaging. Hence quantum dots have been widely investigated for bioimaging applications over the last few decades. In many applications as reported by Zheng and co-workers traditional quantum dots are applied instead of organic dyes and fluorescent molecules as they are highly fluorescent, stable and resistant against metabolic degradation. The recent discovery that CQDs can be utilized for photoluminescence emission in the near infrared spectral range is highly promising for in vivo nanotechnology, as this spectral window offers greater tissue transparency

within the body. Yang et al synthesized CQDs by oxidising carbon soot using nitric acid and passivating them with PEG1500. These quantum dots had size smaller than 10nm and this proved to be advantageous as they could function as probes in tiny biological structures. When compared for bioimaging and cytotoxicity commercial semiconductor CdSe/ZnS quantum dots demonstrated more biocompatiblity and luminescence with a quantum yield (QY) of 20%, outperforming CdSe/ZnS QDs. Surface passivation enables CQDs to modify their optical characteristics, enhancing their suitability for bioimaging applications. Also, CQDs synthesized hydrothermally method have been applied for in vitro and in vivo optical bioimaging studies. Shereema and co-workers synthesized CQDs from maltose using microwave technique through microwave treatment, resulting in passivated CQDs. These passivated CQDs successfully entered cells, emitting green fluorescence, and importantly, the cells maintained high viability even after 24 hours of incubation. CQDs with sizes smaller than 10 nm were synthesized hydrothermally by Xue and co-workers using varying molar ratios of alkali lignin, citric acid and ethylenediamine. At a concentration of 0.62 mg/ml, these CQDs exhibited 90% cell viability when incubated with HeLa cells for 24 hours. A significant number of CQDs were absorbed by the cells via endocytosis, emitting fluorescence primarily in the cytoplasm, with weaker emissions observed in the nucleus. Upon excitation at different wavelengths, they displayed red, green and blue fluorescence. Given their low toxicity, excellent biocompatibility and intrinsic capability for multicolor fluorescence emission, these CQDs present promising potential for bioimaging and biolabeling applications. Huang and co-workers successfully prepared CQDs having a size range from 2 to 6nm. Xylose, glucose and urea were used for the synthesis; xylose and glucose being biorefinery by-products and urea helping in the passivation. These CQDS showed approximately 13% quantum yield when excited at 365 nm wavelength. These CQDs exhibited stable fluorescence characteristics when subjected to temperatures of 4 to 60^{o}C as well as photobleaching. On incubation with L929 fibroblasts, the CQDs maintained cell viability more than 90% up to a concentration of 400 mg/ml. The in vivo studies were done by inoculating tumour cells in a mouse and CQDs were intravenously injected via the tail vein. Imaging at different time points (0 to 24 hours) revealed the distribution and behavior of CQDs, and after euthanizing the mouse, organ images were captured. Both in vitro and in vivo imaging experiments demonstrated the low toxicity, antioxidant properties, and impressive bioimaging performance of the CQDs.

Graphene based quantum dots such as mesoporous silica nanoparticles conjugated with graphene QDs is useful in fluorescent bioimaging for real-time tracking of the doxorubicin (DOX) delivery system. Quantum dots provide superior optical properties over organic dyes, but their potential toxicity limits their broader use. Topical administration can help mitigate this toxicity. In a study of in vivo endoscopic imaging for human bladder cancer, quantum dots conjugated with anti-CD47 were topically administered. The procedure was successful, and no signs of acute toxicity were observed up to 7 days after the treatment.

Polymer dots can be used in multiplexed molecular imaging and utilizes semiconducting polymers with strong fluorescence. Studies have reported extremely enhanced (ten fold) brightness of polymer dots over commercial fluorescent dyes. Quantum dots such as those containing CdSe and CdTe, InP and InAs, PbTe, PbSe behave as fluorescent semiconductor nanoparticles. They are ideal for bioimaging applications as their narrow and symmetric emission band (~30 nm); dependent on sizes and compositions of nanoparticles can be readily altered.

Biomolecule conjugated quantum dots are useful for targeted imaging. Lead sulfide quantum dots, with emission peaks at 1100 nm, are effective for cerebral venous thrombosis imaging using near-infrared fluorescence. In a study involving septic mice, these quantum dots proved to be a valuable tool for assessing the pathological condition of their cerebral blood vessels. Indium arsenide quantum dots that emit in the short wavelength infrared region are useful for multicolor imaging as they provide high resolution, are easily modifiable, provide deep tissue penetration and enable fast image acquisition in small-animal models. They were able to quantify metabolic turnover rates of lipoproteins across multiple organs simultaneously and generate detailed 3D quantitative flow maps of the mouse brain vasculature.

2.Biomedical Applications of nanomaterials in therapy/treatment:

The term biomedical applications include use of nanomaterials for therapeutic applications as well as regenerative medicine.

Antibacterial applications:

Gold nanoparticles developed in high yield from banana peels by SI et al were found to be useful in biomedical applications as antibacterial agents against E. coli bacteria. Iron nanoparticles, naturally synthesised from extracts of spinach and banana leaves showed good potency against Bacillus subtilis and Escherichia coli bacteria. The bactericidal potency of these particles was found to be similar. These nanoparticles were able to penetrate microbial membranes, causing electrolyte leakage, which ultimately led to cell death. Tyagi and co-workers predicted the possible action mechanism involved the nanomaterials increasing the bacterial cell membrane permeability, preventing denaturation of bacterial protein and DNA replication by release of silver ions.

The innovative application of nZnOs as antimicrobial agents has sparked significant research interest in integrating them into medical instruments, leveraging their desirable properties. Additionally, their ability to absorb UV light enhances their antibacterial activity by increasing conductivity, which facilitates their interaction with bacteria. Also they exhibit stability at high temperatures and their positive charge enables effective interaction with the negatively charged surfaces of bacteria, promoting their entry and exerting bactericidal effects. Further they are cost-effective and less toxic than silver as toxicity of silver nanoparticles leads to cell lysis and growth inhibition in various microorganisms but at the same time pose potential risks to human health. As a result, nZnOs have been developed as a safer and more efficient alternative in antimicrobial applications.

Anticancer applications:

Deaths caused by cancer are increasing at an alarming rate globally, with cancer being recognized as the second most common cause of death, accounting for millions of fatalities each year. Addressing cancer requires early detection and effective treatment. Traditional medical treatments have limitations due to their broad action range and significant toxicity to the entire body. However, advanced nanomaterials are offering promising solutions to challenges such as tumor microenvironment, tumor hypoxia, poor stability, low penetration, nonspecific targeting, fast drug clearance and improving drug efficiency. In recent decades, carbon nanomaterials, including fullerenes, carbon nanotubes and carbon dots have gained considerable interest from researchers across various scientific fields, particularly biomedicine, as they possess distinctive physical and chemical characteristics and are biocompatible. As a result, these carbon-based

materials have recently shown great promise as novel platforms for delivering anticancer drugs, owing to their stability and effectiveness.

Biologically prepared silver nanoparticles from leaf extract of Artemisia turcomanica were tested against gastric cancer cell line anticancer activity and induction of apoptosis. The results indicated that the biologically prepared silver nanoparticles effectively induced apoptosis and exhibited cytotoxic and anticancer effects against gastric cancer cells in a dose- and time-dependent manner. These biologically synthesized nanoparticles may demonstrate stronger anticancer properties compared to commercially available silver nanoparticles. Mousavi and co-workers demonstrated that silver nanoparticles disrupt signalling pathways and inhibiting cell growth by interacting with membrane proteins. By fusing with or being internalized through endocytosis, the nanoparticles enter cells and interfere with the mitochondria's electron transport chain. Sivamaruthi and co-workers prepared bimetallic nanoparticles composed of silver and palladium from aqueous fruit extract of T. chebula. These nanoparticles demonstrated good potential against lung cancer cells (A549). Sivamaruthi and co-workers explained the anticancer potential exhibited by these bimetallic nanoparticles composed of silver and palladium. They were found to cause DNA damage by stimulating generation of reactive oxygen metabolites caused by dysfunction in the respiratory chain. This, in turn, activates the apoptotic cascade, leading to cell death.

Virmani and co-workers synthesised gold nanoparticles biologically using tulsi extract as well as chemically by chemical reduction method. Both these nanoparticles were tested against normal (HEK293) and cancerous (HeLa, A549, H1299 and MCF-7) cell lines. The biologically prepared gold nanoparticles reported higher cytotoxicity against cancerous cells than chemically prepared gold nanoparticles as demonstrated by both cell proliferation and IC50 assays. Further, biologically prepared gold nanoparticles reported low or negligible cytotoxicity against HEK293 cells. Bao et al synthesized CQDs hydrothermally utilizing nitrogen and sulphur containing organic carbon source. These NIR CDs were used for thermal-based treatment and imaging in a mouse model. The study revealed that these NIR CDs exhibited 59% efficiency of photothermal conversion and can quickly heat up when exposed to laser irradiation of 808 nm, effectively killing tumor cells. Recent studies have demonstrated the effectiveness of keratin-coated gold nanoparticles in targeting and destroying brain cancer cells through photothermal therapy. The photothermal therapy triggered by gold nanoparticles in a system designed for immunotherapy marks a significant advancement in the fight against malignant solid tumors. This innovative approach has been thoroughly explored, progressing from in vivo studies to clinical trial applications in patients with solid tumors. While these systems show great potential in nanomedicine, they still carry risks, including incorrect cell targeting, unanticipated side effects and unintended immune responses. Therefore, combining hyperthermia with chemotherapy or cancer immunotherapy has shown enhanced benefits in the treatment of cancer patients.

Regenerative Medicine:

There has been a steady increase in patients needing organ or tissue transplantation. Nanomedicine is an evolving area of research which can provide these solutions. Nanomaterials serve as a platform for cell growth and cell proliferation and can deliver drug and biological molecules, enabling the delivery of medicines and biological molecules. This approach facilitates the regeneration of new tissue or organs, replacing damaged body parts in a controlled

environment. Synthetically engineered biodegradable nanoplatforms such as polyglycolic acid, poly(L-lactic acid), polycaprolactone, polyphosphazenes, poly(D,L-lactide-co-glycolide) etc., are utilized to direct cell growth which serves as a guided regeneration method.

Damaged nerve generation or nerve tissue recovery at the injury sites remains one of the most significant challenges in regenerative medicine. Various types of nanomaterials have been developed and are being studied for their potential to prevent or heal nerve damage. Metallic nanoparticles, magnetic nanoparticles, silica nanoparticles and quantum dots are among the inorganic nanomaterials being explored for nerve regeneration in damaged tissues. Some unique organic nanomaterials have been explored for their potential applications in regeneration of neural tissue. Natural nanomaterials such as polymeric nanoparticles, dendrimers, liposomes, micelles, nanofibres and nanomaterials (carbon based) are also being explored for similar applications. All these nanomaterials, with their suitable physicochemical properties, have shown promise for applications in regeneration of neural tissue. These materials have demonstrated positive outcomes, aiding in cell attachment and cell expansion, enhancing neuronal cell separation, and promoting neuron recovery. Additionally, nanomaterials can replicate the surface characteristics of damaged tissues. Nanomaterials exhibit unparalleled cytocompatibility, synergistic, optical, electrical, mechanical and other distinctive properties when compared to traditional materials. These remarkable properties possessed by nanomaterials have significantly advanced tissue development beyond what is currently achievable. Consequently, nanomaterials have proven valuable in the regeneration of various tissues, including ligament, vascular, bladder and bone tissue.

Further, wound treatments with regenerative medicine approach are gaining increasing popularity. Nanotechnology has garnered significant attention from scientists in this field. Additionally, there has been a strong focus on incorporating some inorganic agents, such as zinc, copper and silver, into these therapeutic devices as antibacterial agents. Nanoparticles containing antibiotics or antibacterial agents have proven to be highly effective in wound treatment. Polymeric nanomaterial prepared with nanofibers, which have bioactive molecules, and antibacterial agents, represent a type of polymer nanomaterial. These nanofibers have shown remarkable results when used as materials for skin regeneration or as wound healing patches.
Unblemished polymeric nanofibres or composite nanofibres with unique morphologies and multidimensional congregations going from one-dimensional (1D) to three-dimensional (3D) can be acquired from electrospinning. Basically, these nanofibres have a greater surface-area-to-volume ratio, tuneable porosity and simple surface functionalisation, which present various opportunities for applications, especially in the biomedical field.

Electrospinning is widely used as a method for manufacturing nanofibers due to its straightforward process, cost-effectiveness and versatility and has been recognized worldwide by material researchers. This technique allows for the production of pure composite or polymeric nanofibers with special morphologies and dimensions, ranging from 1D to 3D configurations. They can be used for numerous biomedical applications due to their high surface-area-to-volume ratio, tunable porosity, and ease of surface functionalization. Due to the ongoing advancements in nanomaterials prepared by electrospinning method, they are being tested for biomedical applications, such as wound dressings, patches for rapid hemostasis , antibacterial mats and skin regeneration scaffolds.

3.Drug delivery:

Sustained and targeted drug delivery is crucial for enhancing medication effectiveness and achieving better outcomes over a longer duration. Nanoparticles when used as drug carriers are proving effective for both the applications. An in vivo study conducted on diabetic rodents showed that subcutaneously administered insulin-loaded polymeric nanoparticles, ranging in size from 85 to 185 nm, had a longer-lasting hypoglycemic effect compared to free insulin. Targeted drug delivery to the liver can be achievable by modifying the dimensions and surface characteristics of the nanoparticles to match that of the perforations of the veins in the liver (106–175 nm). Permeable veins with pore sizes between 380-780nm characterise various tumours. Nanoparticles ranging from 100 to 300 nm in size can pass through these pores and accumulate in tumors as they possess high permeability and retention effect. Additionally, by attaching ligands, nanoparticles can efficiently target almost any type of cell that has specific cell receptors.

Recently, a variety of nanoparticle-based therapeutic platforms, such as liposomes, nanoparticles, and polymeric micelles, have been developed to enhance targeted drug delivery to tumors while minimizing exposure to normal tissues and reducing unwanted side effects. For instance, NC-6004, a polymeric micellar nanoparticle conjugated with cisplatin (CDDP), has demonstrated improved anti-tumour efficacy and reduced nephrotoxicity and neurotoxicity in gastric cancer treatment.

Nanocarriers are particularly beneficial for extending drug circulation time within the body, as they tend to persist longer in circulation compared to larger particles, which are usually cleared more rapidly. Larger particles often accumulate in organs like the spleen and liver, rather than in the targeted regions. In contrast, smaller nanoparticles have a greater likelihood of being absorbed by various cells, including those at the target site. Nanoparticles derived from biological sources are particularly well-suited for drug delivery due to their biocompatibility, biodegradability, and ability to mimic natural biological processes. Gold nanoparticles, for example, are highly effective in delivering large biomolecules. Their versatile functional properties and tunable size make them an excellent platform for the identification and targeted distribution of biomolecules. Pokharkar, Sastry,et al demonstrated the capability of gold nanoparticles which are functionalized to effectively transport insulin.

Metallic nanoparticles synthesized from natural sources are increasingly being explored for theranostic applications and drug delivery. This approach is gaining significant attention in the field of green nanotechnology. Biogenic nanocarriers, in particular, have become a prominent research focus globally, as they offer an eco-friendly alternative to traditional synthetic methods. Numerous patents have been registered for studies on the biogenic synthesis of nanomaterials intended for biomedical applications, underscoring the growing interest and potential in this area of research.

Many novel nanoparticle-based drug formulations are under development and undergoing evaluation in both early and late-stage clinical trials, with some designed for active targeting or stimulus-responsive release. A range of nanoparticle formulations has been approved by the FDA and EMA for treating various cancers. For instance, pegylated liposomal doxorubicin and liposomal daunorubicin are available in the United States, while non-pegylated liposomal doxorubicin is approved in Europe. Nab-paclitaxel, using nanoparticle albumin-bound particles, is approved by both the FDA and EMA. To enhance the selectivity of chemotherapeutic drugs, various proteins and small peptides are often conjugated to the surfaces of nanoparticle. One

example of targeting ligands used in chemotherapy drug delivery is serum glycoprotein. Additionally, the antimalarial drug chloroquine has been shown to reduce the immunological clearance of nanoparticle by resident macrophages in the liver, promoting increased tumour accumulation of the nanodrug.

Conclusion:

Till date, some biomedical applications of biomaterials have been accepted, such as plastic surgery, joint substitutions, heart valves, restorative applications and drug delivery devices. The introduction of new innovations in areas like plastic surgery, nerve regeneration, and wound healing is expected to further drive the growth of this market. The cardiovascular biomaterials market dominates other biomaterial sectors due to the high prevalence of cardiovascular diseases, while the orthopedic biomaterials market ranks as the second largest in the biomaterials industry.
Currently, a disparity exists between the rapid advancements in nanomaterial innovation and their practical implementation in biomedical applications. While most members of the commercial network understand the potential of nanotechnology and are capable of launching and managing marketable products, they have a limited understanding of the scientific principles and the complex internal processes that govern the functionality of these products. On the other hand, those involved in scientific research recognize nanomedicine as an extension of nanotechnology, but they often lack the business expertise necessary to bring a product to market. Therefore, their collaborative interaction is essential to successfully drive nanomedicine-based innovations into a commercial success.

Several key principles must be applied when scaling up the nanomaterial production for the biomedical field, with Quality by Design (QbD) being one of the most critical. For instance, it is well-established that the properties of nanomaterials, such as minimal side effects influence patient satisfaction. In this context, QbD plays a vital role in eliminating undesirable side effects from nanomaterials before they reach the market. Successful collaboration between industry professionals and scientists is essential, and a productive team should begin with clearly defined, measurable objectives for the product that are approved by healthcare regulatory bodies.

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Customer Acquisition And Retention Strategies In Nationalized Banks: An Analytical Study

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Abstract:

Given the fierce competition in modern banking in India, nationalized banks face the challenging task of attracting new customers and retaining existing ones. This thesis is a research paper where the researcher looks at the different strategies that have been employed by nationalized banks so as to increase the number of customers they acquire and retain amid competition with the private sector banks and online financial sites. It uses both secondary and primary data, such as the surveys of customers, the reports of financial institutions, and interviews with banking specialists. Some of the major aspects covered are: the extent of government-led financial inclusion programs; digital banking innovations; customer service excellence; and personal customer relationship management. These results indicate that, though the nationalized banks still benefit by being trusted by the people and having expansive rural coverage, there are still loopholes in the field of digital outreach, customer experience, and redressal of grievances. The research finds that nationalized banks need a balanced strategy, combining technology, service excellence, and strategic communication to exploit their strengths and stay competitive, as well as have long-term customer loyalty. It is recommended that digital infrastructure can be improved, the interactions between the employees and customers can be done better, and data analytics can be used to administer relationships in specific areas.

Keywords: Customer Acquisition, Customer Retention, Nationalized Banks, Banking Strategies, Customer Relationship Management, Financial Inclusion

Introduction:

The Indian banking system has experienced a paradigm shift over the past decades through liberalization, technological changes, and the rise of expectations of customers in the system. Traditionally, the backbone of India's financial system was nationalized banks, but today, a complex and competitive environment is characterized by the fast emergence of private sector banks, fintech organizations, and digital-first financial services. In that regard, the concept of attracting new customers and, at the same time, retaining the old ones has come up as a strategic aspect affecting the nationalized banks. Customer acquisition, the term 'acquisition refers to acquiring new customers and promoting your products or services using targeted marketing, outreach initiatives, and value-added services. For nationalised banks, government-led financial inclusion initiatives such as the Pradhan Mantri Jan Dhan Yojana (PMJDY) and Direct Benefit Transfer (DBT) schemes have played a pivotal role in expanding their customer base, particularly in rural and underserved regions. However, acquiring new customers alone is insufficient for ensuring sustainable growth. Therefore, retaining customers requires continuous delivery of services, individualized interaction, and modern banking experiences. Despite their wide-ranging distribution, trustworthiness, and affiliation with government-supported plans, nationalized banks encounter several difficulties in managing their relationships with customers. These involve

decrepit infrastructure, red tape, low innovation, and the adoption of digital tools at slower rates than in the private sector. Factors like convenience, speed, technology integration, and personalized experiences contribute to customer loyalty in the digital age, and all of those dimensions mean a strategic reconsideration of conventional banking operations. This research seeks to learn about the customer acquisition and retention strategies embraced by nationalized banks in India. It aims at assessing the effectiveness of these strategies, determining the gaps that exist, and further recommending effective recommendations that can be offered to ensure that the nationalized banks remain relevant and competitive in developing times when the financial environment is changing vigorously.

Objectives of the Study:

1) To identify key strategies used by nationalized banks for customer acquisition.
2) To examine the tools and programs designed for customer retention.
3) To evaluate the effectiveness of these strategies in today's competitive environment.
4) To recommend strategic improvements for better customer engagement and loyalty.

Review of Literature:

Some researchers have addressed the emerging customer acquisition and retention strategies adopted by nationalized banks in India. Kotler and Keller (2016) emphasize the value of long-term customer relationships, arguing that customer retention is more cost-effective than constant acquisition. Gupta and Dev (2012) found that public sector banks have effectively expanded their customer base through financial inclusion initiatives, though they lag in targeted marketing. Malhotra and Singh (2018) compared public and private sector banks and noted that, while nationalized banks have a wider reach and customer trust, they are slower to adopt modern CRM tools. Sharma and Goyal (2019) concluded that service quality, grievance redressal, and employee responsiveness are key factors driving customer loyalty in public sector banks. Kumar and Rajan (2020) highlighted the growing role of digital banking in customer acquisition, especially among youth, but noted challenges in personalization and consistent service. The RBI's Annual Report (2021) reaffirmed that nationalized banks have been instrumental in promoting financial inclusion but face high customer attrition due to bureaucratic inefficiencies. Singh and Kapoor (2022) observed that personal communication and relationship-building practices play a crucial role in customer retention in semi-urban and rural branches. Bhattacharya and Saha (2023) argue that nationalized banks can enhance retention through data-driven decision-making and AI-based customer insights. Supporting this, the KPMG Banking Report (2023) stressed that customer experience, seamless digital access, and loyalty programs are essential for sustaining competitiveness—areas where nationalized banks still need strategic improvements.

Research Methodology:

This study uses a mixed-methods approach to analyze customer acquisition and retention strategies at nationalized banks in India. It focuses on 250 account holders and 50 bank employees from five banks. Data was collected through questionnaires, interviews, and surveys. The study is limited to strategies implemented in the past five years, reflecting post-pandemic digital transformation and policy reforms. Limitations include sample size and geographical coverage. The study provides a balanced evaluation of nationalized banks' adaptation to customer-centric strategies in a competitive banking environment.

Customer Acquisition & Retention Strategies in Nationalized Banks:

Nationalized banks have made some good contributions to financial inclusion in India, and since their launch under the Jan Dhan scheme, more than 49 crore accounts have been opened until March 2023. Such banks are mainly sustained by government policies, a linkage system, and social welfare payouts. Nationalized banks have adopted digital initiatives to facilitate the smooth transaction of customer acquisition, with 65 per cent of the new customers aged below 35 years pursuing digital channels. Video KYC and e-document verification have helped banks such as

Canara Bank and Union Bank cut the time to open their accounts to less than a day (24 hours) compared to the average of 4 days.

The extended physical reach of nationalized banks has significantly aided their acquisition of new customers, especially in semi-urban and rural areas. In India, 68% of bank branches are owned by the public sector, which results in 56% of new savings accounts being opened in rural areas during the year 2022-23. Yet, they have a low rate of retaining customers, and on average, 72 percent of customers are retained in the public sector banks, rather than the mostly competitive 85 percent of the customer retention rate by the major banks in the private sector.

The major drivers of customer retention include confidence in government support, the distance to bank branches, and the availability of ATM facilities. Nonetheless, not all respondents were satisfied with their customer service; only 40 percent rated it as satisfactory, and 36 percent expressed happiness with the digital convenience. Customer complaints and service delivery are also at stake because of service lag and ATM hitches, and online services hitches that make up 43 per cent of total complaints made by customers against public sector banks. The complaints received in nationalized banks could only be addressed within 30 days by 60 percent of the companies, rather than 78 percent in the case of private banks.

The experience is topped by digital, with a big difference between nationalized and privately owned banks. The mobile banking applications of nationalized banks commonly rank 3.8/5 on Google Play and reach 4.5/5 on the other side of the coin, namely the private sector. Only 42% of customers reported monthly active use of nationalized banks' mobile apps, whereas private banks enjoy 67% monthly active user engagement.

Customer relationship management (CRM) and personalization are essential for customer retention, but nationalized banks are lagging in this area. The banks that adopted rigorous CRM programs, such as SBI Wealth and PNB One, experienced a 12 percent increase in client engagement compared to the banks that did not implement such programs.

Employee responses about the retention practices indicated that the major internal issues were the lack of training to work with digital tools and customer connections, the non-use of customer data analytics to focus on retention processes, and poor implementation of the loyalty or referral program. The solution to these gaps must find uses in taking advantage of technology, CRM integration, and employee training to encourage sustainable growth and loyalty in the new banking ecosystem.

Customer Acquisition Strategies in Nationalized Banks:

The acquisition of new customers has depended on different strategies relating to nationalized banks in India. These are: financial inclusion programs; rural outreach; digitalization; government orders and direct deposits; consumer confidence and heritage branding; advertising and marketing campaigns; and financial literacy. Nationalized banks have been at the forefront of executing flagship financial inclusion programs, such as the Pradhan Mantri Jan Dhan Yojana (PMJDY), which opened over 49 crore accounts nationwide. The repayment in FY 2022-23 was also 2.4 lakh crore, which was 58 per cent of Mudra loans. The nationalized banks have attracted and retained low-income and informal sector customers due to the enrollment of over 20 crore individuals in the Jan Suraksha Schemes.

The other strategy employed by the nationalized banks is rural penetration, which aims at increasing penetration into rural locations. They employ more than 130,000 Business Correspondents (BCs) and use mobile banking vans to service over 3,200 villages. 68 percent of the rural bank branches in India are nationalized banks, which guarantee high visibility and confidence among the rural customer segment. Digitalization is a new column of customer acquisition, and more than 65 percent of the new savings accounts are opened digitally using Aadhaar-powered e-KYC and mobile applications. By early 2024, nationalized banks were carrying

out over 1.6 billion UPI transactions per month, including a share of around 34 per cent of all UPI transactions by volume among the public sector banks, SBI.

Government mandates and direct transfers are key acquisition drivers, with nationalized banks being the primary conduits for Direct Benefit Transfers (DBT) and LPG subsidy deposits through banks (PAHAL Scheme). Confidence in government-owned institutions still plays an immense role in terms of opening new accounts, where 71 per cent of the Indian respondents had more confidence in government-owned banks than in the private sector banks as concerns their banks to store their savings and benefits. Finally, the preparation of promotional campaigns and financial literacy drives still attracts new customers. In FY 2023, the nationalized banks had organized more than 1.2 lakh financial literacy camps in the urban-rural areas, and through school-college partnerships and vocational training institutes, they managed to reach more than 50 lakh young people 2023.

Customer Retention Strategies in Nationalized Banks:

The nationalized banks are considering proper retention strategies that will guarantee long-term profitability and sustainability for them. These banks are deploying various approaches, including dedicated relationship managers (RMs) for high-net-worth clients, loyalty programs, credit score monitoring, complaint resolution mechanisms, personalised banking services, digital banking enhancements, periodic feedback collection and analysis, employee training and customer engagement, and employee recognition programs. Relationship Managers (RMs) are being deployed to serve high-net-worth individuals and priority customers, with studies showing that clients assigned an RM had a 12% higher retention rate than those without dedicated support. Reward point programs associated with the use of a debit card, regular monthly pay-ins, or loan payments are also being used to enforce the benefits of loyalty and credit engagement. Union Bank and SBI banks have embedded an interface for credit score monitoring through a mobile application, which promotes financial discipline and builds a more extended relationship with the customer.

Effective grievance redressal fosters customer trust and retention. The bank has the Integrated Ombudsman Scheme, which has simplified the process of complaint resolution by uniting different platforms into one. According to the RBI Ombudsman Annual Report 2023, out of the total number of complaints raised against thousands of banks, 43 per cent have been related to complaints against public sector banks, and 60 per cent of the complaints against the banks have been answered within the stipulated period of 30 days.

Liquidity level: The level of liquidity is increasing, with the Indian Bank, SBI, and the Bank of Baroda testing personalized bank services where loans are pre-approved according to the patterns and type of customer availing the service; discounted interest on savings accounts; and other benefits based on the customer's pattern of usage. A study by IBA (2023) noted that 32% of customers receiving personalized offers were more likely to stay with their current bank.

Digital banking enhancements are critical to retaining digitally savvy customers, with SBI's YONO app reaching 60 million downloads and over 15 million monthly active users in 2023. Enhanced security systems, such as biometric logins to the account, OTP-based authentication, and AI-driven methods of detecting fraud, have increased user confidence. Nationalized banks are also undertaking some periodic feedback gatherings and analysis to identify actionable information. The retention must be done through employee training and customer relationships, wherein more than 1.2 lakh employees of banks were trained by the RBI under the Financial Literacy and Customer Service Framework in FY 2022-23.

Key Findings

The study was able to draw several important conclusions regarding the strategic performance and customer behaviour of nationalized banks in India. Firstly, a majority of customers (72%) identified trust in the government as the primary reason for selecting

nationalized banks over private institutions. This points to the long-term trust and faith in publicly owned banking systems, especially among the rural and older groups of people. Secondly, although 65% of the respondents said they use digital banking services, including mobile apps and internet banking, many of them compared them as less convenient and slower than those offered by the private sector, which requires a better interface design and functionality. Also, 43 per cent of customers were unhappy with the speed and efficiency of grievance redressal, indicating that customer service is still an issue of concern. Notably, the study established that customers who get rare contacts via call, SMS, or emails had a higher retention rate, 30 per cent higher than those customers who have poor contact, which helps in emphasizing the importance of managing relationships. Additionally, interpersonal banking—particularly communication with branch managers—has been shown to significantly increase customer loyalty, especially among older citizens and those in rural areas, who are likely to prefer humanized and personalized banking over virtual-only contact.

Conclusion:

The research indicates that one of the most important ways a nationalized bank grows and gains a competitive boost is through customer acquisition and retention. These banks have been able to increase their customer base with the support of government schemes such as PMJDY, DBT, and Mudra loans, but the main problem is maintaining the customer base by developing more customer touchpoints and providing better services to customers. The government ownership factor will be a great motivator to acquire customers, and the emergence of the digital banking arena has changed how customers expect things to be. Nationalized banks have to make an effort to fill the usability gap between their platforms and their commercial rivals. The use of human interaction as a retention policy is practical, as in the case of relationship-based banking among the elderly and rural people. Customer loyalty can only be ensured by conducting periodic feedback, training the employees, and using online statistics. Nationalized banks need to find a golden middle between the institutional credibility, their outreach ability, technological drive, and customer focus so that they enhance customer faith and loyalty as well.

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Facile Synthesis of Zirconium Doped Zinc Oxide Nanoparticles by Microwave Assisted Technique

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Abstract:

Zirconium-doped Zinc Oxide (ZnO) nanoparticles were successfully synthesized using a microwave-assisted technique, which offers a rapid and energy-efficient method for producing nanomaterials. In this study, various molar concentrations of Zirconium (Zr) were incorporated into ZnO to investigate the effects on the structural and optical properties of the resulting nanoparticles. The synthesis process involved the use of Zinc Acetate and Zirconium Nitrate as precursors, with microwave irradiation facilitating the formation of nanoparticles at room temperatures. X-ray diffraction (XRD) analysis confirmed the successful incorporation of Zirconium into the ZnO lattice, resulting in the formation of a hexagonal wurtzite structure. Scanning Electron Microscopy (SEM) revealed the formation of spherical nanoparticles with sizes ranging from 50 to 100 nm. Energy-dispersive X-ray Spectroscopy (EDX) further validated the doping of Zirconium in the ZnO matrix. The optical properties were studied using UV-Vis spectroscopy, which indicated a redshift in the absorption spectrum with increasing Zirconium concentration, suggesting the modification of the electronic structure. This microwave-assisted synthesis route presents an efficient and scalable method for producing doped ZnO nanoparticles.

Keywords: *Zirconium-doped Zinc Oxide, nanoparticles, microwave-assisted synthesis, structural properties, optical properties, X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy-dispersive X-ray Spectroscopy (EDX), UV-Vis Spectroscopy*

Introduction:

Nanotechnology and nanoscience are the study and application of extremely small objects with dimensions ranging from one to one hundred micrometers. Nanotechnology is being used in fields such as chemistry, biology, physics, materials science and engineering [1]. Nanoparticle synthesis the term to refers the process of making nanoparticles by combing two or more ingredients into one [2, 3]. Nanoparticles exhibit unique physical, chemical and green features that are not found in bulk materials [4]. This unique physicochemical property, along with other specific features of metallic nanoparticles such as small size, high surface to volume ratio, surface charge and surface chemistry, provide a significant opportunity to design diagnostic agents for diagnostic purposes and targeted drug delivery systems, in addition to benefiting from the intrinsic pharmaceutical potential of these nanoparticles [5–7].

Rare earth metals, transition metals and noble metals have all been doped into ZnO to improve its lattice behaviour in an effort to get around this constraint [8–10]. Doping with transition metals may improve ZnO's photo catalytic efficiency since these metals contain vacant d-orbital subshells. Additionally, they have atomic radii that are parallel to those of Zinc (Zn), which results in doping of the ZnO lattice. As a result, it might result in improved thermal stability, electron-hole recombination being suppressed, particle size increasing and an increase in specific surface area, eventually enhancing photo catalytic performance [11–15]. The band gap of pure ZnO is around 3.2 eV, which means that it can only absorb ultraviolet (UV) light. However, when Zirconium is doped into ZnO, the band gap can be reduced, which allows the material to absorb visible light as well [16] Zirconium was chosen as a dopant due to its abundance, unoccupied d orbits that can trap excited electrons one at a time, preventing the recombination of the electron-hole pair and reducing ZnO's photo-corrosive properties.

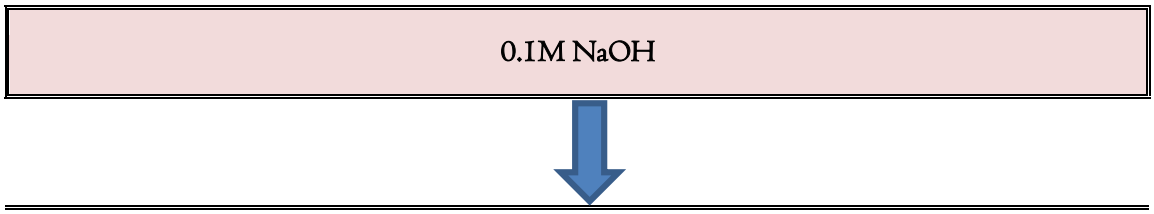
This study reports the synthesis of Zirconium doped ZnO nanoparticles using microwave-assisted technique. Microwave technology is a rather recent addition to the means of material processing and it provides an alternative strategy through which possibly new material characteristics could be achieved along with economic advantages like lower energy consumption and faster time-to-market for products. Clearly, the benefits of this approach are: penetration depth irradiation, electric field distribution control, rapid uniform heating, self-regulating reactions and selective volumetric heating. [17]. The Polyethylene Glycol 300 used as a capping agent to create biocompatible metal nanoparticles. Further, the prepared Zr/ZnO nanoparticles were examined for its optical properties.

Experimental

Materials and Method

All reagents used during the synthesis were of reagent-grade quality and solutions were prepared without further purification using double-distilled water. The Zirconium doped ZnO nanoparticles were synthesized by dissolving specific amounts of Zinc Acetate Dihydrate [$Zn(CH_3COO)_2 \cdot 2H_2O$] and Zirconium Nitrate Hexahydrate [$Zr(NO_3)_4 \cdot 6H_2O$] in double distilled water. This solution was vigorously stirred while adding 2–3 mL of Polyethylene Glycol 300. A custom-made device was designed to maintain agitation while drop wise adding 0.1 M NaOH at a rate of 1 ml/min (stirring nonstop), to promote complete precipitation. Sediment was further centrifuged and washed with distilled water to eliminate water-soluble impurities. This washing cycle was performed three times for maximum purity. The final clean sediment was then centrifuged with excess water and acetone before being microwave irradiated for 10 minutes at 800 W in on-off cycling mode. The specimen was allowed to cool to room temperature after cyclization and then dried under ambient conditions. The dry product was etched in a controlled furnace set to 200°C for 3 hours before characterization.

The schematic flow chart for preparation of Nanocrystalline Zr-ZnO is given in Fig.1.



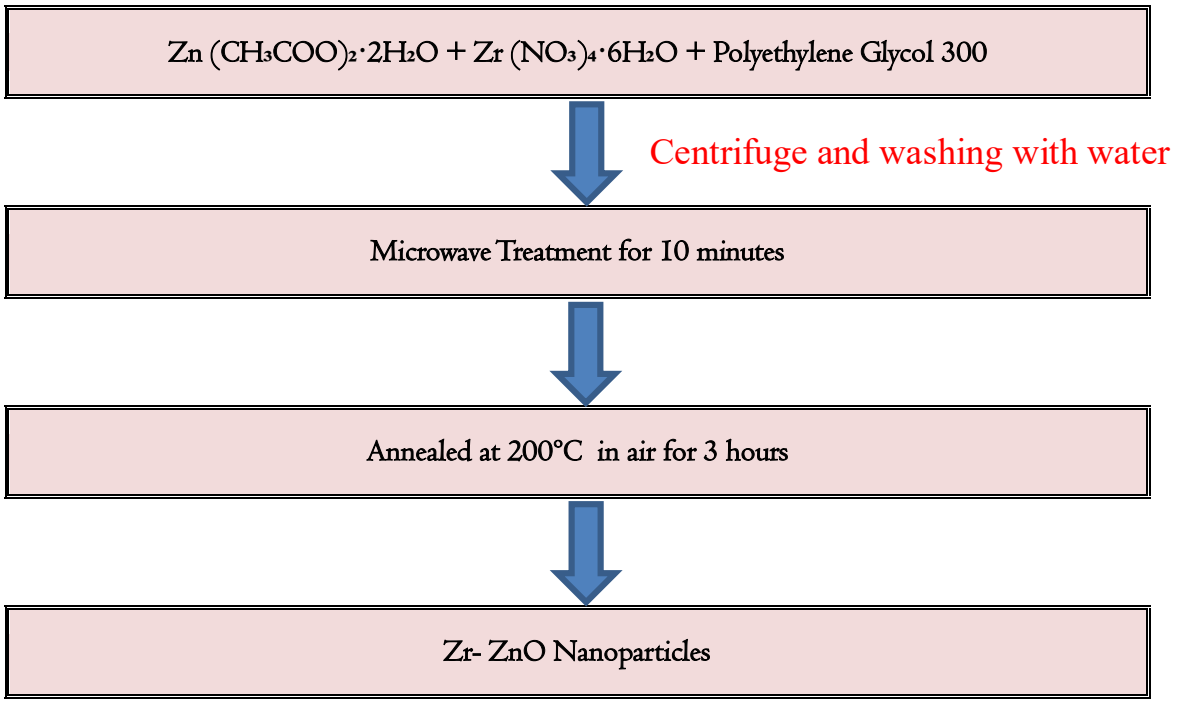


Fig. 1. Schematic flow chart for the preparation of nanocrystalline Zr-ZnO

Characterization of Zr/ZnO nanomaterials

X-ray Diffraction (XRD) study of the synthesized products was carried out by using Philips model PW-3710 X-ray Diffractometer with Cu-Kα = 1.5406 Å. Scanning Electron Microscopy (SEM) observation was performed with a JEOL JSM-6360 Scanning Electron Microscope. Energy Dispersive X-ray Spectrometer (EDS) was used for elemental analysis of these nanoparticles. To estimate the band gap, UV-Visible spectra of the products were obtained by using UV3600 Shimadzu UV-Visible Spectrophotometer. The FTIR spectra were recorded by using FTIR-8400, Shimadzu in the range of 4000 to 400 cm^{-1}.

Results and discussion

Fig. 2 (a-b) displays the XRD patterns of prepared pure ZnO with Zr/ZnO nanoparticles and the obtained results demonstrated that the prepared samples shows the characteristic hexagonal wurtzite structure which is concurred with standard JCPDS (card No.: 36–1451). Interestingly, when Zirconium doping content increased from 20 to 50% into nanoparticles, there is increment in intensity of plane in ZnO. The XRD planes of Zirconium doped ZnO nanoparticles have similar peaks and they are concurred with pure ZnO peaks. Based on achieved results, the lattice parameters also increase monotonically as the Zirconium content increases in nanoparticles. This could be due to the fact that Zr^{4+} has a larger ionic radius (0.84) than Zn^{2+} (0.74) to the fact that Zr^{4+} has a larger ionic radius (0.84) than Zn^{2+} (0.74) [18–19]. As more Zn^{2+} is replaced by Zr^{4+}, more lattice deformation and expansion of the ZnO crystal structure will be the result. However, the patterns of Zirconium doped ZnO nanoparticles are well correlated with pure ZnO. The average crystalline size (S) of prepared samples were obtained through Debey-Scherrer's Eq.

$$S = k\lambda/\beta\cos\theta$$

(Where 'k' is the Scherrer's constant (0.94), 'λ' is the wavelength (1.54 A°), 'β' is the FWHM (full width at half maxima) and 'θ' is the diffraction angle) and the findings revealed that the prepared Zr-ZnO nanoparticles exhibited lesser in size (30 nm) than pure ZnO (70 nm).

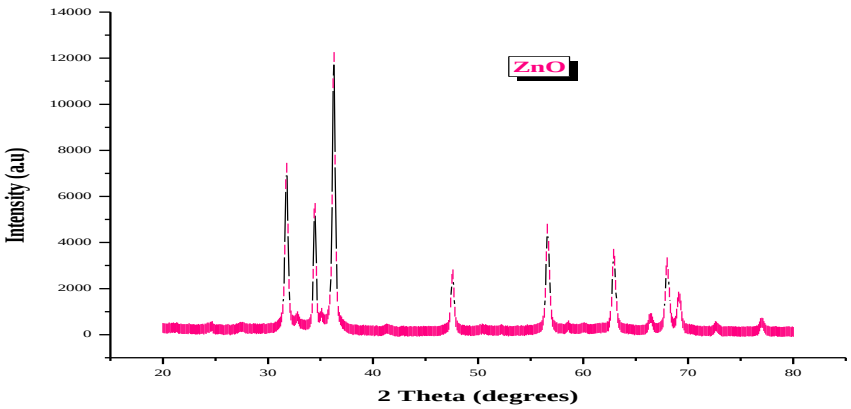


Fig. 2. (a) XRD pattern of ZnO

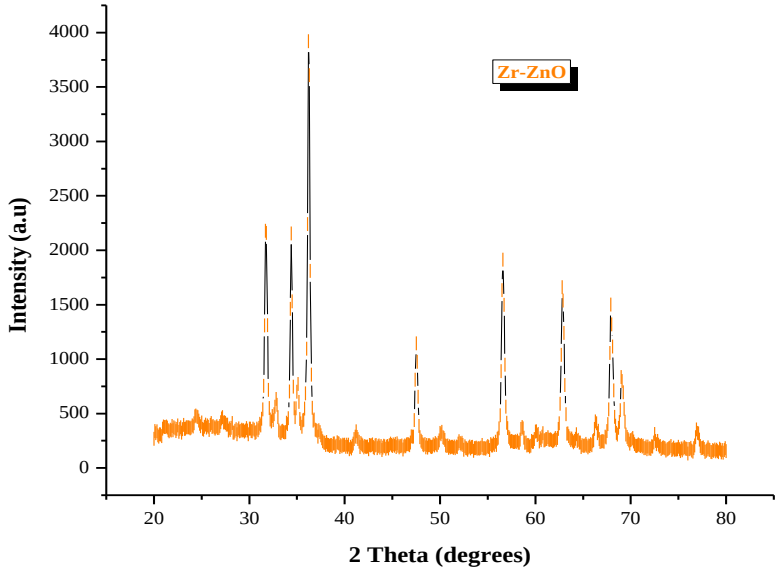


Fig. 2. (b) XRD pattern of Zr-ZnO

The morphology and size of prepared ZnO and Zr/ZnO nanoparticles were executed by SEM and EDS analysis. Fig. 3(a) describes about the pure ZnO SEM images which show the irregular shape with agglomeration. The successful doping of Zirconium into ZnO was demonstrated by the SEM image of tiny particles painted on the hexagonal surface of ZnO as presented in Fig. 3(b). Fig. 3(c) in ESI displays the EDX graph of prepared Zr-ZnO nanoparticles which confirms the formation of pure compound with the consistency of Zr (Zirconium), Zinc (Zn) and Oxygen (O) without any impurities. This EDX analysis is further evident from XRD patterns of prepared samples.



Fig. 3. (a) SEM image of ZnO

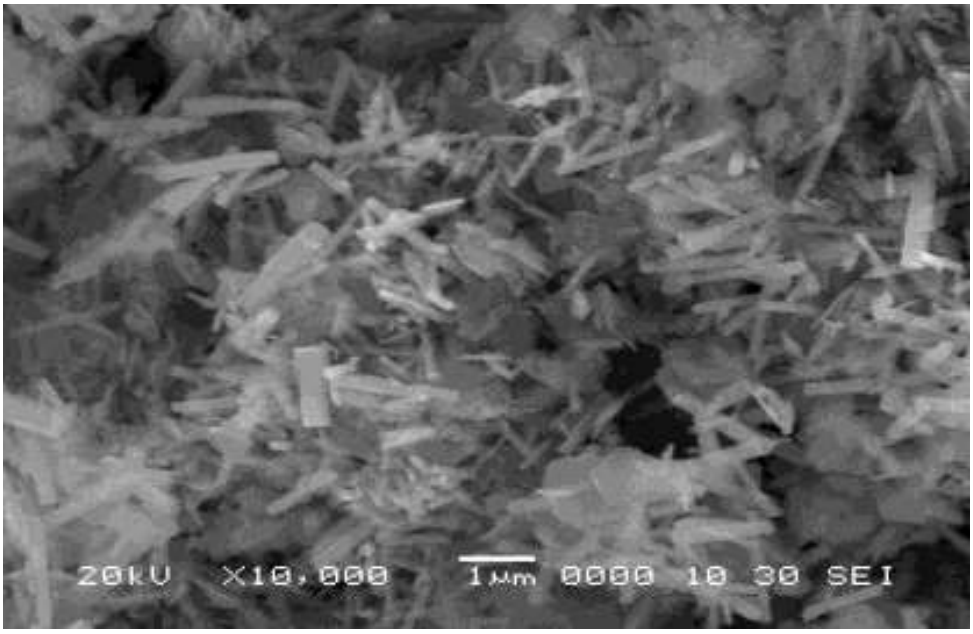


Fig. 3. (b) SEM image of Zr-ZnO

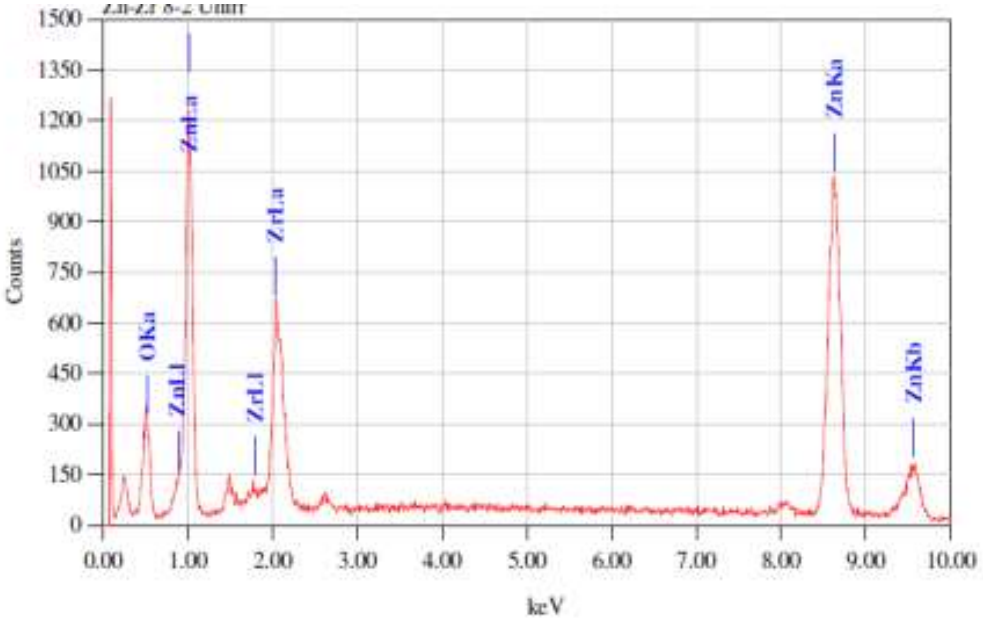


Fig. 3. (c) EDX graph of Zr-ZnO

Fig. 4 shows the FTIR spectra of prepared ZnO and Zirconium doped ZnO nanoparticles via combustion supported sol–gel approach. Information regarding the stretching vibrations of Zn-O is provided by the typical peaks located between 400 and 500 cm^{-1} [20]. The M-O peaks serve as the basis for the well-defined typical peak at around 500 cm^{-1}, which supports the development of ZnO and Zr(IV) doped ZnO nanoparticles [21–22]. The stretching vibrations (O-H) of water in the Zr-Zn-O or Zn-O lattice are responsible for the bandwidth around 3200–3600 cm^{-1} caused by the hydroxyl group (–OH) of water, which indicate the existence of water moieties adsorbed on the surface of the nanocatalyst [24]. There is no chemical interaction between metal-doped and un-doped ZnO as shown by the lack of substantial changes in the FTIR spectra observed when Zr(IV) was deposited on ZnO nanocatalyst in comparison to the undoped ZnO sample.

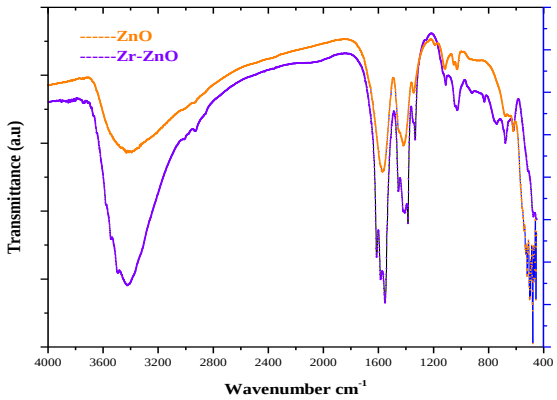


Fig. 4. FTIR spectra of ZnO/Zr-ZnO

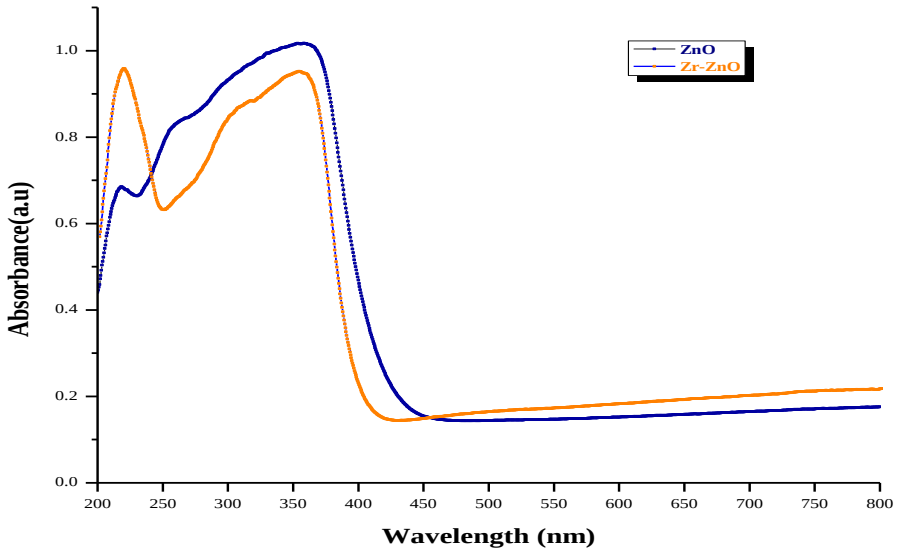


Fig. 5. UV-Visible spectra of ZnO/Zr-ZnO

Conclusion:

This study successfully illustrates the simple and effective microwave-assisted synthesis of Zirconium doped Zinc Oxide (Zr-ZnO) nanoparticles. The research shows the ease of this technique as it allows for the rapid and energy-efficient synthesis of nanoparticles with uniform incorporation of zirconium into the ZnO lattice structure. It was found that by adjusting the microwave power and the irradiation time, nanoparticles with advantageous structural, morphological and optical attributes were achieved. These were confirmed by XRD analysis which confirmed the crystalline nature of the synthesized nanoparticles and SEM imaging which provided evidence to their uniform and well dispersed morphology. In addition, the presence of enhanced optical behavior due to gargantuan doping was confirmed with UV-Visible Spectrophotometry as there was a shift in the absorption edge.

The synthesized Zr-ZnO nanoparticles can be used for large scale applications due to their cost effectiveness, ease of synthesis and improvement in materials performance. This microwave-assisted technique demonstrates potential for use in photocatalysis, solar energy conversion and in optoelectronic devices for advanced applications. Further research should be conducted to investigate the functional properties of the nanoparticles developed in specific fields of technology.

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"The Evolution of Shantanu Rao Kirloskar's Leadership: A Study on the Social, Economic, and Educational Impact of the Kirloskar Group of Companies"

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Abstract:

After the end of World War II, the Kirloskar Group grew rapidly under the leadership of S.L. Kirloskar. In 1946 he established Kirloskar Electric Company and Kirloskar Oil Engines Limited at Bangalore and Pune, respectively. He is credited with developing the manufacture of the diesel engine indigenously as an import substitute after India attained independence. The Kirloskar Group of Companies, recognized as one of India's leading conglomerates, has significantly influenced the country's industrial, economic, social, and educational domains. This paper analyzes the evolution of leadership under Shantanu Rao Kirloskar, emphasizing his strategic vision and its effects on the growth of the Kirloskar Group in these areas. It investigates how his leadership approach has shaped the company's contributions to society, particularly in education, job creation, and innovation. By conducting a thorough examination of both qualitative and quantitative data, the paper underscores the enduring legacy of Shantanu Rao Kirloskar in transforming India's industrial landscape.

This paper seeks to explore the evolution of leadership within the Kirloskar Group, particularly highlighting how Shantanu Rao Kirloskar's leadership has ushered the company into a new phase of growth. It will focus on advancements in social responsibility, economic development, and educational initiatives, while also assessing the implications of the company's progress for the future.

Keynote - *S.L. Kirloskar, Oil Engines Limited, Shantanu Rao Kirloskar,industrial landscape*

Introduction

S.L. Kirloskar was the son of Laxmanrao Kirloskar, who established the Kirloskar Group and the township of Kirloskarwadi. S. L. Kirloskar earned a Bachelor of Science degree in mechanical engineering from MIT in Cambridge, Massachusetts. He was among the first Indians to graduate from MIT. He also became a reserve officer in the US Army at the same time.1940 S.L. Kirloskar founded Mysore Kirloskar Ltd. to manufacture machine tools. Established in 1888 by Laxmanrao Kirloskar, the Kirloskar Group is a family-owned conglomerate based in Pune, India. Throughout its history, the company has diversified into various sectors, including manufacturing and engineering, under the guidance of multiple generations of the Kirloskar family, each playing a vital role in its expansion. The current leader, Shantanu Rao Kirloskar, has been pivotal in updating the group's vision and operational strategies.

Hypothesis

Primary Hypothesis:

The leadership of Shantanu Rao Kirloskar has played a crucial role in the ongoing growth of the Kirloskar Group, positively influencing its socio-economic contributions, advancing educational programs, and supporting sustainable industrial progress in India.

Secondary Hypothesis:

With Shantanu Rao Kirloskar at the helm, the Kirloskar Group has effectively woven corporate social responsibility (CSR) initiatives into its operations, promoting enduring social and economic advancement, especially in education and job creation.

Research Objectives

1.To investigate the leadership approach of Shantanu Rao Kirloskar and its influence on the expansion of the Kirloskar Group.

2.To explore the Kirloskar Group's impact on the Indian economy, focusing on job creation, innovation, and infrastructure development.

3.To review the educational programs spearheaded by the Kirloskar Group, especially in engineering and technical education.

4.To analyze the Kirloskar Group's commitment to social responsibility and sustainable practices.

Literature Review

This literature review will concentrate on the following areas:

1.The historical development of the Kirloskar Group, tracing its journey from inception to the current state.

2.An exploration of leadership theories, with an emphasis on transformational leadership and the dynamics of family-owned enterprises.

3.The economic influence of the Kirloskar Group on the industrialization of India.

4.The social and educational initiatives undertaken by the Kirloskar Group, particularly in the realms of rural development and skills enhancement.

5.An examination of corporate social responsibility (CSR) efforts by Indian conglomerates, with a particular emphasis on the Kirloskar Group.

Research Methodology

1. Data Collection:

1 Primary Data: Conducting interviews with essential stakeholders within the Kirloskar Group, including executives, staff members, and industry specialists. Utilizing surveys and questionnaires to assess the group's social influence on local communities and educational institutions.

2.Secondary Data: Gathering information from annual reports, company documentation, publicly accessible data from industry analyses, academic publications, news articles, and government documents regarding the Kirloskar Group's impact in India.

2. Qualitative Analysis:

Performing a case study examination of significant initiatives introduced by Shantanu Rao Kirloskar, such as the Kirloskar Institute of Advanced Management Studies (KIAMS) and various environmental projects.

Analyzing the leadership strategies implemented by Shantanu Rao Kirloskar.

3. Quantitative Analysis:

Conducting a statistical evaluation of the company's growth in revenue, market share, and job creation over the last ten years. Administering surveys to quantify the social impact of the Kirloskar Group's educational programs, such as the number of students who have benefited from scholarships or skill development initiatives.

4. Data Analysis Tools:

Employing descriptive statistical techniques to interpret survey results. Conducting a SWOT analysis of the Kirloskar Group under the leadership of Shantanu Rao Kirloskar.

Economic Growth:

This section will feature a graph depicting the Kirloskar Group's revenue growth, its entry into new markets, and the rise in job opportunities over the last ten years.

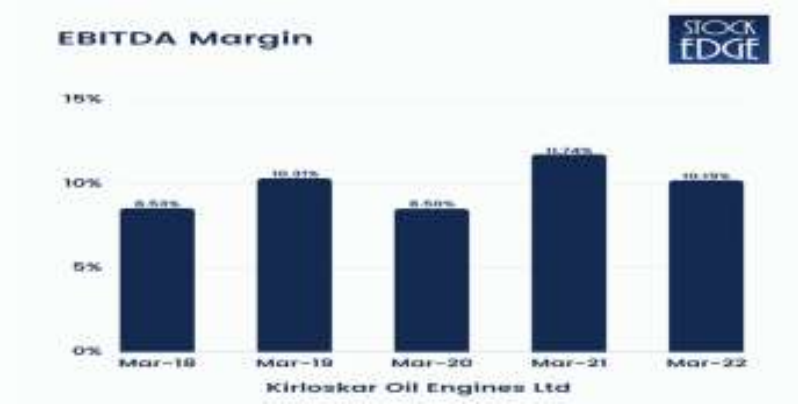
Social Impact:

A map will illustrate the areas in India where the Kirloskar Group has launched CSR initiatives, with a particular emphasis on rural and underserved populations.

Educational Impact:

A chart will present the number of students trained at Kirloskar institutions and the subsequent effects on employment in related industries, including the number of Kirloskar alumni employed by the company or in similar fields.

Charts & Maps



Revenue Growth of Kirloskar Group Over the Last Decade – Line graph.



Projected Income Statement: Kirloskar Oil Engines Limited

Finding -

I Leadership Style:

Shantanurao Laxmanrao Kirloskar, a prominent figure in Indian industrial history, played a pivotal role in shaping the Kirloskar Group into the engineering conglomerate it is today. Born into the Kirloskar family, his leadership and vision propelled the company beyond its initial focus on agricultural implements. He is widely recognized for his strategic foresight in

diversifying the group's interests and adopting modern manufacturing techniques. Kirloskar's commitment to innovation led to the introduction of a wide range of engineering products, significantly contributing to India's industrial growth.

His contributions extended beyond the realm of business. He was a strong advocate for technical education and skill development, recognizing the importance of a skilled workforce for a thriving industrial sector. He actively supported initiatives aimed at improving education and training opportunities for young people, believing that this was crucial for India's economic progress. Kirloskar's leadership style was characterized by a focus on quality, efficiency, and customer satisfaction. He instilled these values throughout the Kirloskar Group, fostering a culture of excellence that continues to define the company.

Socio-Economic Contributions:

Technological Advancement & Innovation

Shantanurao was a strong advocate for technological advancement and modernization within the Kirloskar Group. He invested heavily in research and development fostering a culture of innovation that led to the development of new products and technologies. This commitment to innovation helped the Kirloskar Group maintain a competitive edge in the global market.

Strategic Partnerships & Collaborations

Recognizing the importance of collaboration in a rapidly changing global landscape, Shantanurao forged strategic partnerships with leading international companies. These collaborations facilitated the transfer of technology and expertise, enabling the Kirloskar Group to enhance its capabilities and expand its product offerings.

Leadership & Succession Planning

As a visionary leader Shantanurao placed great emphasis on developing future leaders within the Kirloskar Group. He implemented robust training and development programs to nurture talent and ensure a smooth transition of leadership. His focus on succession planning helped ensure the long-term sustainability of the Kirloskar Group.

Financial Performance & Growth

Under Shantanurao's leadership the Kirloskar Group experienced significant financial growth and expansion. His strategic decisions and business acumen helped the company navigate economic challenges and capitalize on emerging opportunities. The Kirloskar Group became a leading industrial conglomerate in India, contributing significantly to the country's economic development.

Educational Initiatives /Sustainability and CSR:

The establishment of KIAMS and collaborations with educational institutions have been instrumental in developing technical skills and leadership capabilities among young professionals, making a significant impact on the Indian industrial landscape. mThe Kirloskar Group has woven sustainability into its fundamental business strategies, prioritizing eco-friendly technologies and social welfare initiatives in rural areas of India.

Kirloskar Pneumatic Company Limited

India’s leading name in Compressed Air, Air-conditioning & Refrigeration and Hydraulic Power Transmission Year of incorporation : 1958 No. of employees : 900

Product range

Air Compressors - Rotary Screw(Mobile/ Stationary) - Small (Garage) Compressors - Railway Brake Compressors/ Expressers Refrigeration & Air-Conditioning - Refrigeration Compressors - Air-Conditioning Compressors - Flake & Block Ice Plants - Transport Air-Conditioning - Specialized, Custom Built - Screw Compressor Packages - Turnkey Solutions

- Refrigeration & Air-Conditioning systems Gas Compressor Packages - Specialized Reciprocating Gas Compressor Packages for a wide range of Gases, Hydrocarbons Transmission - Locomotive Transmission Units - Hydraulic Marine GearBoxes - Industrial & Windmill GearBoxes - Torque Converters - Traction Gears and Pinions

Conclusion

Shantanu Rao Kirloskar's leadership has been instrumental in defining the future trajectory of the Kirloskar Group. His strategic foresight has broadened the company's global presence while fostering economic, social, and educational progress in India. Under his guidance, the Kirloskar Group has not only attained financial success but has also emphasized social responsibility and sustainable practices. The company's initiatives in education have significantly influenced technical education in India, positioning it as a key contributor to the nation's industrial development.

In summary, Shantanu Rao Kirloskar's leadership provides important lessons on how effective leadership can transform a family-owned business into a globally recognized and socially responsible organization.

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Synthesis of Eosin from Resorcinol via Fluorescein as an Intermediate

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Abstract:
This study outlines a synthetic pathway for the preparation of the synthetic dye eosin starting from resorcinol, utilizing fluorescein as an intermediate compound. Initially, resorcinol undergoes a condensation reaction with phthalic anhydride under acidic conditions to form fluorescein, a xanthene derivative. This intermediate undergoes further bromination or oxidation, leading to the formation of eosin. The process highlights the key steps of condensation, cyclization, and functional group manipulation, which are critical for achieving the characteristic red-pink color of eosin. The synthesis offers a practical route for producing eosin, a dye widely used in biological staining, textile applications, and analytical chemistry.

Keywords: *Synthetic dye, resorcinol, bromination, eosin etc*

I. Introduction:

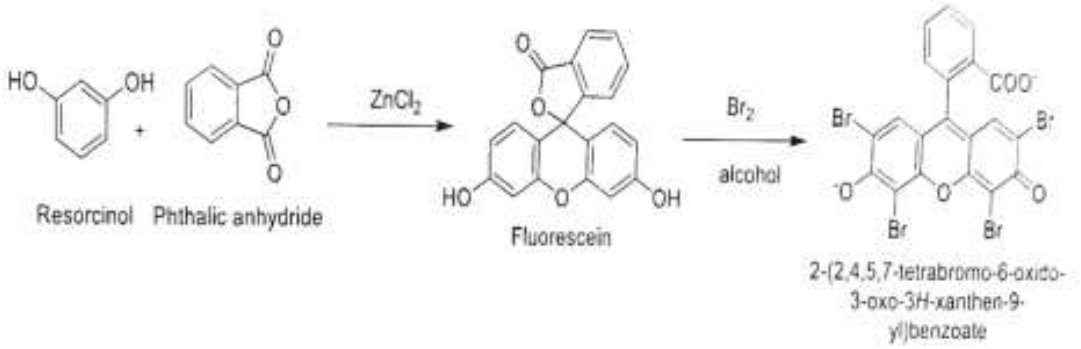
Eosin is a synthetic dye belonging to the xanthene class of compounds, known for its striking red-pink color. It has universal applications in biological staining, textile dyeing, and as a pH indicator. The synthesis of eosin is often carried out through various chemical transformations, with fluorescein being a key intermediate in its preparation.[1] Fluorescein itself is derived from aromatic compounds, and one of the most common precursors used in its synthesis is resorcinol (1, 3-dihydroxybenzene).[2]

Resorcinol, an important aromatic compound with two hydroxyl groups positioned on the benzene ring, serves as a versatile starting material for the synthesis of various organic dyes. In this synthesis, resorcinol reacts with phthalic anhydride under acidic conditions to form fluorescein, which, due to its conjugated aromatic structure, exhibits fluorescence and bright color. [3] This intermediate is then subjected to bromination to introduce the necessary functional groups, ultimately yielding eosin.

The transformation of resorcinol into eosin via fluorescein not only denotes the benefit of resorcinol in dye synthesis but also provides vision into the chemistry of xanthenes derivatives.[4] This approach offers an efficient and effective method for producing eosin, a dye that is widely utilized in various fields such as microscopy, medical diagnostics, and textile industries.[5]

Table: I Summary table for different methods for synthesis of eosin [8]

Method	Starting Material	Reagents	Product	Notes
Classical Bromination	Fluorescein	Br_2 or KBr + oxidant	Eosin Y	Common, efficient
Nitration + Bromination	Fluorescein	$HNO_3 + Br_2$	Eosin B	Yields nitro derivative
Green Method	Fluorescein	NBS, microwave	Eosin	Eco-friendly
Direct Two-Step	Resorcinol + Phthalic Anhydride	Acid catalyst → Br_2	Eosin Y	Useful for full synthesis



2. Material and Methodology:

Chemicals and materials: Resorcinol, Phthalic Anhydride $ZnCl_2$ (Anhydrous) fluorescein Water, ethanol, Br_2 etc.

Glassware and equipment: One round bottom flask (100 mL), pipettes, a Rubber Bulb, filter papers, one 100 mL beakers, a stem and a Buchner funnel, one Erlenmeyer flasks (100 mL), a glass rod, a graduated cylinder, a filtration flask, a spatula etc.

Reaction:

Procedure:

STEP-1 Synthesis of fluorescein from Resorcinol:

Take Phthalic anhydride (3.75 gm) and Resorcinol (5.5g) in RBF and heated to 180°C on oil bath freshly fused and powder zinc chloride(1.75 gm) is added in small portion during 30 to 40 minutes the mixture being stirred all the time with glass rode. At the end mass become so viscous that the stirring is not possible and allow RBF to cool down for 30 minutes

STEP-2 Synthesis of Eosin from Fluorescein:

3 ml Bromine is added drop wise with separating funnel during 15 to 20 minutes to a stirred suspension of fluorescein 4.15gm in 20 ml alcohol when half the reaction Br_2 has been added and the Fluorescein has been converted in to di Bromo Compound all solid material dissolved. Since, the bromo derivative is insoluble in alcohol. Further addition of Br_2 gives Tetra bromo derivative with separate out since it is sparingly soluble in alcohol. Mix allows standing for separated orange color eosin.





Fig: 1 Synthesis of fluorescein from Resorcinol




Fig: 2 Synthesis of Eosin from Fluorescein



Fig 3: Thin layer Chromatograph

3. Calculations:

Step 1: Synthesis of Fluorescein from Resorcinol

110.9 g Resorcinol react with Zinc Chloride to gives a 332.31 g of Fluorescein Therefore, 5.5 g of Fluorescein will give = X----------g of Resorcinol

X= (332.31 x 5.5)/110.9 = 16.48 g

Theoretical yield=16.48 g.

Practical yield=13.41 g

Percentage Practical Yield = Practical yield/Theoretical yield x100

13.41/16.48 x 100

=81.03%

Step 2: Synthesis of Eosin from Fluorescein

332.31 g Fluorescein react with Ethanol to gives a 691.85 g of Eosin Therefore, 5.2 g of Fluorescein will give = X--

X= (691.85 x 4.15)/332.31 = 8.64 g

Theoretical yield=8.64 g.

Practical yield=5.2 g

Percentage Practical Yield = Practical yield/Theoretical yield x100

5.2/8.64 x 100

=60.1%

4. Result and Discussion

Table .I: Physical data of reactants and product

Reagent	Melting point (°C)	Boiling/Melting point (°C)	%Practical yield	R_f Values
Fluorescein	315	314-316	81.3	0.73
Eosin	288	295	60.1	0.70

i. The yield of fluorescein is about 81.3% and the yield of product i.e. Eosin is 60.1% shows with this methodology we can achieved considerable better yield and the melting points shows the primary confirmation of formation of intermediate and product.

ii. The Rf value of reactant was 0.73 while that of product was 0.70. Reactant has an additional important aldehyde group which is not present Fluorescein acetone in that helps with hydrogen bonding with stationary phase. This way Eosin which is reactant here will form stronger interactions with stationary silica and hence take longer to move up the plates and so has lower Rf value. Eosin acetone with lesser interaction will be moving more rapidly through the plates.[6]

5. Conclusions:

The synthesis of eosin from resorcinol involves an intricate series of steps starting from bromination to form key intermediates, followed by coupling reactions that ultimately lead to the formation of the xanthene-based structure of eosin. The process requires careful control of reaction conditions, as well as effective purification steps to isolate the desired dye. Eosin's vibrant color, fluorescent properties, and versatility make it a valuable compound in a range of applications, particularly in biological staining and as a fluorescent dye for research and diagnostics.

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Correlation of Heavy Metal Content in Medicinal Plants and Soil Across Diverse Environmental Conditions

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Abstract

This study explores the relationship between the heavy metals (Chromium, Cadmium, and Lead) contamination levels in soil and medicinal plants (Neem, Tulsi) in Rural, Urban and Industrial environments. The objective of this research is to compare contamination level of three different environments and assess their potential prospect of bioaccumulation and to determine the level of heavy metals sampled. The assessment of the results from sample collection, preparation, and analysis using UV- visible spectrophotometry showed that urban environments had the highest level of heavy metal, followed by industry and rural environments. Overall, lead has maximum concentration in industry samples, while urban soil and rural plants had the highest concentrations of chromium and cadmium, respectively. The results also highlight the potential risk that heavy metals pose to the environment and human health, demonstrate the need for improved regulatory parameters and preventive measures to decrease exposure.

Keywords: *Medicinal plants, Heavy metal contamination, Tulsi (Ocimum sanctum), Neem (Azadirachta indica, health hazard, UV-Visible spectrophotometry.*

Introduction

- Importance of Tulsi and Neem

Tulsi (Ocimum sanctum) belongs to the Lamiaceae family and is a fragrant plant. With hairy stems and simple inverted green leaves that are unmistakably perfumed, it is an upright, much stretched sub bush that is 30 to 60 cm tall. Tulsi is the queen of natural plants and plays a vital role in our everyday lives. Tulsi is commonly referred as "Solution of Life" in Ayurveda and has lots of fundamental health benefits. In Indian Materia Medica tulsi leaves are described as remedy for pyrexia, bronchitis, and illness. In the preparation of Ayurvedic medications, tulsi leaves are often used. It is known to lengthen life expectancy. The plant's extracts are commonly used to treat a variety of ailments, including the common cold, irritation, intestinal illness, cardiac illness, migraines, stomach problems, kidney stones, heart problems, and more. Tulsi, an Indian basil, also aids in environmental cleanup. The tulsi plant is an excellent insect repellent that works wonders against flies, mosquitoes, and creepy crawlies. It is very important in the fight against malaria [1].
Neem (Azadirachta indica) are fast-growing, evergreen trees that belong to the Meliaceae family, also known as the mahogany family. They are well-known for their ability to withstand drought. The neem tree develops into a substantial shade tree with a thick, round canopy and can live for 150-200 years. Also, neem is famous for its solid unsavoury smell, its blossoms have a delectable nectar like aroma that can be smelled for miles. Its use dates to ancient India and its surrounding countries, where it has long been revered as one of the most adaptable plants in existence. Since every part of the neem tree is recognized to offer unique therapeutic benefits, it is still considered the "Village Dispensary" today. Neem plant has several benefits such as antioxidant property, anti-inflammatory effect, anti-viral property, hepatoprotective effect, etc [2].

- **Risk of Heavy Metal Contamination in Medicinal Plants**

Heavy metal contamination has been a concern in today's time especially if it in medicinal plants. The medicinal plants are consumed by humans and if it has heavy metals such as lead, cadmium, chromium, etc., it could be threat to someone's life.

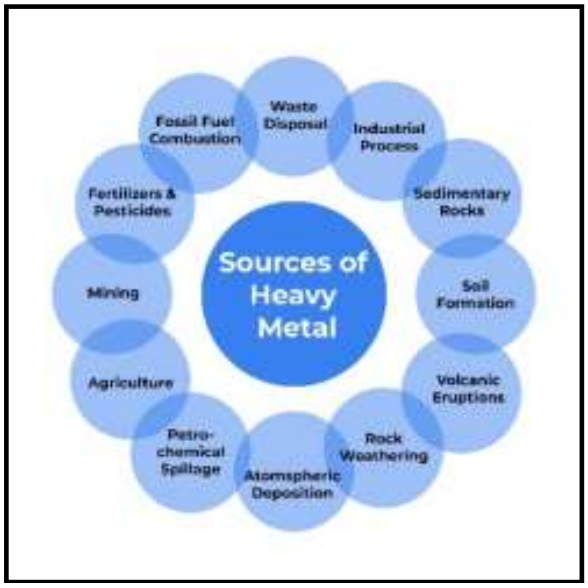


Fig. 1 Sources of Heavy Metal

1. Effect on Bones

Itai-Itai is a bone ailment that developed in Japan's Fuchu Toyama region following World War II. Affected individuals experience excruciating agony because of Itai-Itai, or "ouch-ouch," which appears as fractures and deformations in the long bones of the skeleton. Lead levels in the bone matrix rise during childhood and most of the adulthood because of exposure to lead from both environmental and occupational sources [3], [4].

2. Renal Effect

The primary condition brought on by acute cadmium exposure is kidney dysfunction. The type of cadmium that enters the kidney is called cadmium-metallothionein (CdMT). After passing through the glomerulus, Cd-MT is reabsorbed in the proximal tubules. Cadmium then builds up in the cells of the tubules. Cadmium levels in renal tubules cells rise during a person's lifetime. 2.4 µg of cadmium per gram of creatinine excretion in urine is associated with 4% renal tubular damage. Lead toxicity, renal cancer, renal dysfunction, the mechanism of lead nephrotoxicity, the role of the lead binding protein in renal cancer, and the negative effects of low-level ambient and long-term lead exposure on neurotoxicity were all documented. Three phases of lead-induced nephrotoxicity have been identified: acute or reversible nephropathy, followed by chronic nephropathy, and renal tubular cell neoplasia or adenocarcinoma as the last step [3], [4].

3. Effect on Respiratory System

The primary cause of inhalative cadmium poisoning is cigarette smoke. The human lungs absorb between 40 and 60 percent of the cadmium included in cigarette smoke. Typically, cadmium that has been inhaled as cadmium-cysteine complexes enters the bloodstream and causes lung edema, mucous membrane damage, and dyspnea. Animals have also been observed to suffer from chromium exposure, in addition to humans. Asthma, chronic rhinorrhea, nasal itching, discomfort, epistaxis, nasal mucosal atrophy, bronchitis, nasal septal perforation, and ulceration, pneumonoconiosis, pneumonia, and reduced pulmonary function are all brought on by prolonged exposure to Cr (VI)[3], [5].

4. Effect on Nervous System

Compared to the other organ systems in the human body, the nervous system is significantly impacted by lead toxicity. As the symptoms progress, coma, paralysis, or even death may result. One classifies lead as a neurotoxic. Pb has a half-life of 30 days in the blood and 2 to 3 years in the brain. The condition known as encephalopathy occurs when some areas of the human brain gradually deteriorate. Within a few weeks of exposure, the main symptoms of encephalopathy include headache, dullness, low attention span, memory loss, and hallucinations. Compared to adults, children are more prone to be impacted by lead exposure during their developmental stages. Children who have blood lead levels (BPb, a "biomarker" that measures the interactions between the biological system and an external environmental agent) below 10 μg/dL are shown to be significantly impacted, according to epidemiological research [4].

Chemical Behaviour in Plants and Soil

Cadmium (Cd)

The analogous chemicals Zn^{2+}, Co^{2+}, Fe^{2+}, Mg^{2+}, and Ni^{2+} are isotypic with the compounds of Cd. Cd can create complex ions ($CdOH^{+}$, $CdCl^{+}$) and organic chelates. Under conditions of high oxidation, it produces minerals such as cadmium oxide (CdO) and cadmium carbonate ($CdCO_3$), and during weathering, it accumulates in phosphate. The critical level of Cd was reported to be 10–20 mg/kg (DW), the reported phytotoxic level of Cd in plants ranged from 5–10 mg/kg. discovered that the rise in Cd2+ ions in the soil impeded the nitrification process and soil urease activity [6].

Chromium (Cr)

There are two oxidation states of Cr in soil: Cr (III) and Cr (VI). At pH 5.5, Cr (III), which is somewhat mobile in acidic environments, totally precipitates. Therefore, while Cr (VI) is extremely mobile in acidic and alkaline soils, the compounds of Cr (III) are quite stable in soils. In general, when soil pH rises, so do the adsorption strengths of the Cr (III) hydrolysis products that are adsorbed on the clay particles. The rise in the negative charge on the surface of clay particles is another factor contributing to Cr (III)'s high adsorption capacity [6].

Lead (Pb)

Soil contamination may be caused by the extraction and disposal of lead and its byproducts. In general, the chemical behaviour of lead in soil and the amount of organic matter in the soil are highly correlated. Consequently, it accumulates in soil that contains a lot of organic materials. A trace quantity of lead is soluble in soil and accessible to plants. This is because Pb binds well to soil colloids or organic materials. Furthermore, several biochemical parameters, including pH, cation-exchange capacity, microbial conditions, redox processes, and soil mineral composition, influence the behaviour of lead in soil, including its solubility, bioavailability, and mobility. Both the behaviour of the soil and the pace at which plants absorb lead may be impacted by these factors [6].

Experimental Procedure

1. Sample Collection (Plant and Soil)

Neem plant sample were collected from rural area in Wada, urban area near Badlapur road side and industrial area from Ambernath MIDC. Similarly, tulsi plant sample were collected from rural area in Wada and urban area from Badlapur residential site. Soil sample were collected of these very plants at a depth of 15 cm using sterilized augur. All these samples were stored zip lock bags with proper labelling to avoid contamination.

2. Sample Preparation

Plant and soil samples were first air dried and then followed oven drying to remove all the moisture content present in them. The samples were then treated in Wet Digestion procedure for further analysis process.

3. Stock and Standard Solution Preparation

Stock solutions of lead, chromium and cadmium were present for 1000 ppm in 1000 cm^3 using lead acetate, potassium dichromate and cadmium sulphate. Using this stock solution prepare 0.2, 0.4, 0.6, 0.8 & 1.0 ppm, these solutions are refer as 'Standard Solutions'.

Table 1 – Standard solutions of Chromium

Sr. No	Vol. of 100 ppm $K_2Cr_2O_7$	Vol. of H_2SO_4 (mL)	Vol. of 0.25% DPC (mL)	Conc. of Cr (VI)	Total Dilution (mL)	Absorbance (540 nm)
1.	0.2	10	2	0.2	100	0.140
2.	0.4	10	2	0.4	100	0.287
3.	0.6	10	2	0.6	100	0.439
4.	0.8	10	2	0.8	100	0.565
5.	1.0	10	2	1.0	100	0.680

Table 2 – Standard solutions of Cadmium

Sr. No	Vol. of 100 ppm $CdSO_4$	Vol. of pH 4 buffer (mL)	Vol. of 0.25% Dithizone (mL)	Conc. of Cd	Total Dilution (mL)	Absorbance (485 nm)
1.	0.2	5	5	0.2	100	0.253
2.	0.4	5	5	0.4	100	0.314
3.	0.6	5	5	0.6	100	0.447
4.	0.8	5	5	0.8	100	0.625
5.	1.0	5	5	1.0	100	0.992

Table 3 – Standard solutions of Lead

Sr. No	Vol. of 100 ppm $CdSO_4$	Vol. of pH 4 buffer (mL)	Vol. of 0.25% Dithizone (mL)	Conc. of Cd	Total Dilution (mL)	Absorbance (512 nm)
1.	0.2	5	5	0.2	100	0.243
2.	0.4	5	5	0.4	100	0.487
3.	0.6	5	5	0.6	100	0.647
4.	0.8	5	5	0.8	100	0.856
5.	1.0	5	5	1.0	100	1.235

4. Data Interpretation

The presence of heavy metals in different samples was studied using UV - Visible spectrophotometer (make – Labman) model number- LMSPUV1000B.

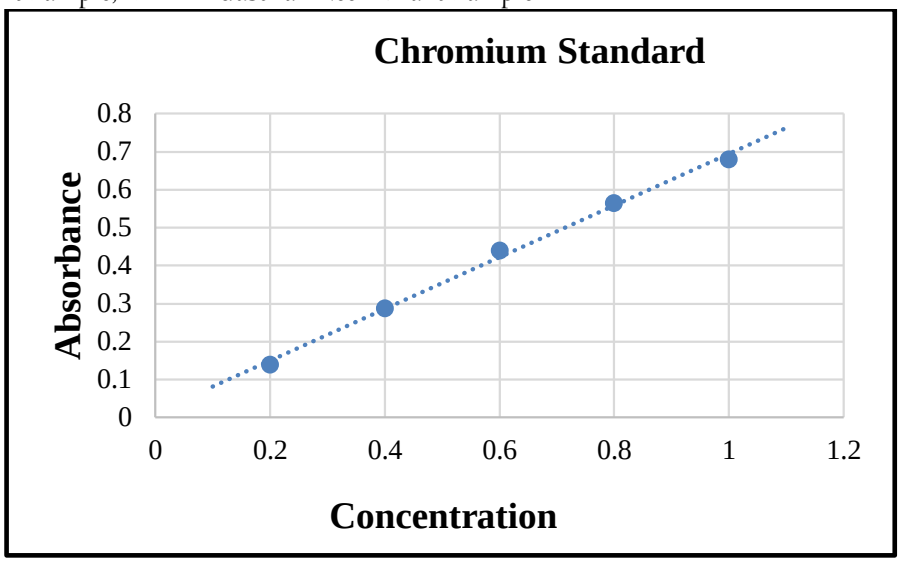
4.1 Chromium

Table 4 – Absorbance for Chromium

Sr. No	*Sample	Vol. of H_2SO_4 (mL)	Vol. of 0.25% DPC (mL)	Total Dilution (mL)	Absorbance (540 nm)	Concentration (ppm)
1.	RS1	5	1	50	0.015	0.0002
2.	RS2	5	1	50	0.030	0.0223
3.	US1	5	1	50	0.020	0.0076
4.	US2	5	1	50	0.036	0.0312
5.	IS1	5	1	50	0.022	0.0106
6.	RP1	5	1	50	0.103	0.129
7.	RP2	5	1	50	0.167	0.224
8.	UP1	5	1	50	0.057	0.062
9.	UP2	5	1	50	0.054	0.057
10.	IP1	5	1	50	0.072	0.084

*RS1 – Rural Neem Soil Sample, RS2 – Rural Tulsi Soil Sample, US1 – Urban Neem Soil Sample, US2 – Urban Tulsi Soil Sample, IS1 – Industrial Neem Soil Sample, RP1 – Rural Neem

Plant Sample, RP2 – Rural Tulsi Plant Sample, UP1 – Urban Neem Plant Sample, UP2 – Urban Tulsi Plant Sample, IS1 – Industrial Neem Plant Sample



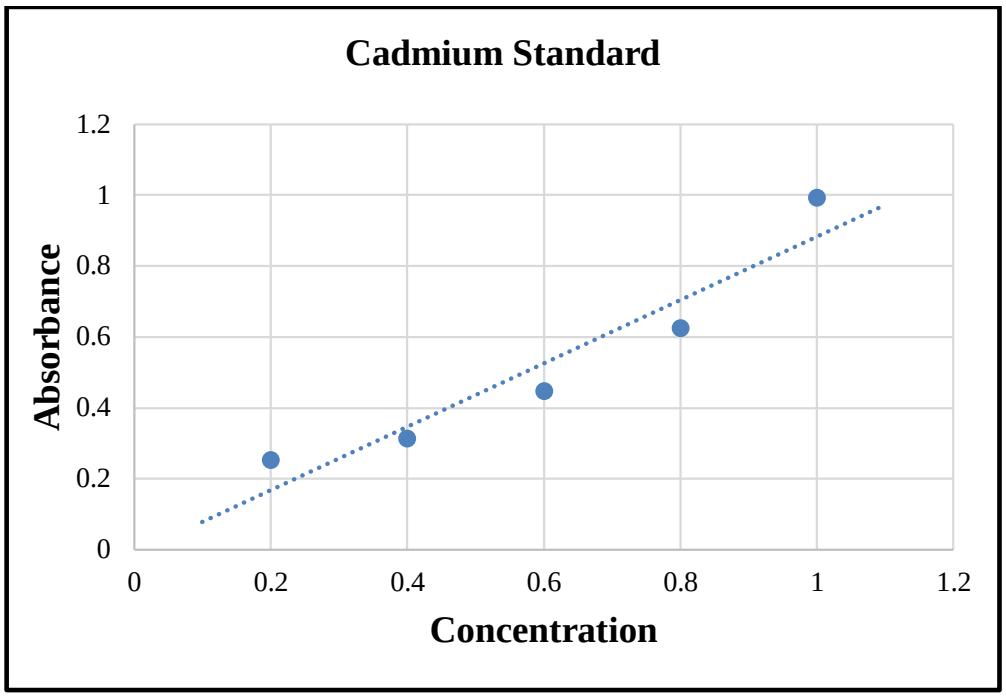
Graph 1 – Graph of Chromium Standard Solution (Absorbance vs Concentration)

The concentration for sample solution is calculated using $y = 0.679x + 0.0148$ formula.

4.2 Cadmium

Table 5 – Absorbance of Cadmium

Sr. No	*Sample	Vol. of pH 4 buffer (mL)	Vol. of 0.25% Dithizone (mL)	Total Dilution (mL)	Absorbance (485 nm)	Concentration (ppm)
1.	RS1	2.5	2.5	50	0.010	0.0005
2.	RS2	2.5	2.5	50	0.021	0.0117
3.	US1	2.5	2.5	50	0.013	0.0027
4.	US2	2.5	2.5	50	0.026	0.0173
5.	IS1	2.5	2.5	50	0.015	0.0050
6.	RP1	2.5	2.5	50	0.017	0.0676
7.	RP2	2.5	2.5	50	0.098	0.0978
8.	UP1	2.5	2.5	50	0.027	0.0184
9.	UP2	2.5	2.5	50	0.019	0.0095
10.	IP1	2.5	2.5	50	0.013	0.0229



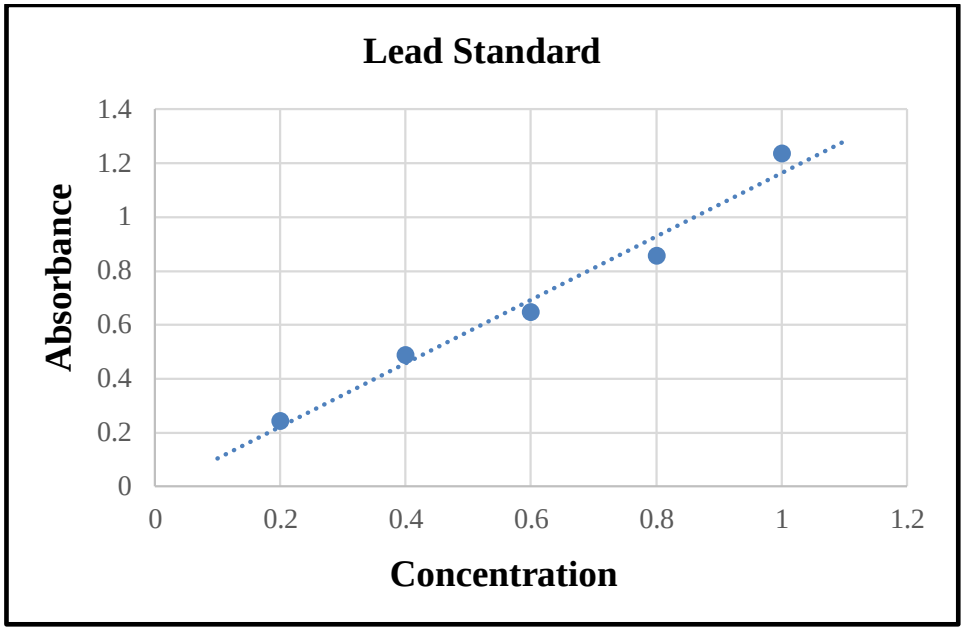
Graph 2 – Graph of Cadmium Standard Solution (Absorbance vs Concentration)

The concentration for sample solution is calculated using **y = 0.8945x - 0.0105** formula.

4.3 Lead

Table 6 – Absorbance of Lead

Sr. No	*Sample	Vol. of pH 9 buffer (mL)	Vol. of 0.25% Dithizone (mL)	Total Dilution (mL)	Absorbance (485 nm)	Concentration (ppm)
1.	RS1	2.5	2.5	50	0.009	0.0181
2.	RS2	2.5	2.5	50	0.010	0.0189
3.	US1	2.5	2.5	50	0.008	0.0172
4.	US2	2.5	2.5	50	0.009	0.0181
5.	IS1	2.5	2.5	50	0.013	0.021
6.	RP1	2.5	2.5	50	0.015	0.023
7.	RP2	2.5	2.5	50	0.012	0.020
8.	UP1	2.5	2.5	50	0.010	0.018
9.	UP2	2.5	2.5	50	0.009	0.018
10.	IP1	2.5	2.5	50	0.016	0.024



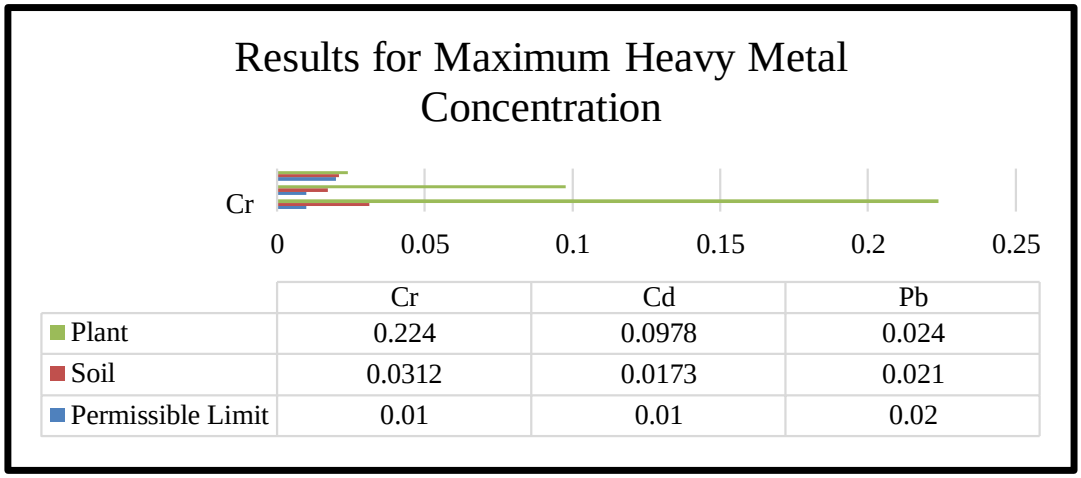
Graph 3 – Graph of Lead Standard Solution (Absorbance vs Concentration)

The concentration for sample solution is calculated **y = 1.1765x - 0.0123** formula.

Result

Table 7 – Maximum absorbance and concentration of Heavy Metal

Samples	Heavy Metal	Maximum Absorbance	Concentration (ppm)
Urban soil sample for Tulsi (Badlapur Residential area)	Chromium (Cr)	0.036	0.0312
Rural Tulsi Plant sample (Wada near Agriculture field)		0.167	0.224
Urban soil sample for Tulsi (Badlapur Residential area)	Cadmium (Cd)	0.026	0.0173
Rural Tulsi plant sample (Wada near Agricultural area)		0.098	0.0978
Industrial Neem soil sample (Ambarnath MIDC)	Lead (Pb)	0.013	0.021
Industrial Neem plant sample (Ambarnath MIDC)		0.016	0.018



	Cr	Cd	Pb
Plant	0.224	0.0978	0.024
Soil	0.0312	0.0173	0.021
Permissible Limit	0.01	0.01	0.02

Conclusion

Heavy metal pose a serious environmental and health risk. Heavy metals persist in soil and water, affecting ecosystems. They enter the food chain, leading to biomagnification where higher concentration is found in predators including humans.

According to WHO's limit published long ago which were out dated. According to research conducted by me, the concentration were very high as compare to previous limits it's a sign that WHO or FDA should published new limits as well as precautionary measures to avoid consumption of these heavy metals by humans or any other creatures.

From the conducted research it was found that Urban region had maximum amount of heavy metal. Moderate amount of heavy metal was found in Industrial region due to industrial emission and effluent disposal. Least amount of heavy metal concentration was determined in Rural region with notable level.

Chromium –

The concentration for chromium in soil sample was found maximum in Badlapur near Residential area i.e.,0.0312 ppm.

The concentration for chromium in plant sample was found maximum in Wada agriculture field i.e., 0.224 ppm.

Cadmium –

The concentration for cadmium in soil sample was found maximum in Badlapur near Residential area i.e.,0.0173 ppm.

The concentration for cadmium in plant sample was found maximum in Wada agriculture field i.e., 0.0978 ppm.

Lead –

The concentration for lead in soil sample was found maximum in Ambarnath MIDC i.e.,0.021 ppm.

The concentration for lead in plant sample was found maximum in Ambarnath MIDC i.e., 0.024 ppm.

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India in Girmitya Memory: A Literary Reflection on the Capildeo Family

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Abstract

Diaspora" (from the Greek word for "scattering") refers to the dispersion of people from their homeland. Diaspora literature are works that are written by authors who live outside their native land. The Indian Diaspora is one of the largest Diasporas in the world. Indians have a long history of emigration to other parts of the world. The Indian indenture system was a system of indentured servitude. About two million Indians were transported to labour in European colonies, as a substitute for slave labour. The system expanded after abolition of the Slavery in the early ninteenth century, British Empire in 1833, in the French colonies in 1848, and in the Dutch Empire in 1863. Indian indentureship lasted till the 1920s. This resulted in the development of a large Indian diaspora in the Caribbean, Natal, Mauritius, Sri Lanka, Malaysia, Myanmar, to Fiji, as well as the growth of Indo-Caribbean, Indo-African, Indo-Fijian, Indo-Malaysian, and Indo-Singaporean populations. The term "girmitya" is a malapropism of an English word "agreement, referring to the Agreement of the British Government with the Indian.

Indo-Caribbeans or Indian-Caribbeans, are people of Indian descent who live in the Caribbean. They are mostly descendants of the original Jahaji Indian indentured workers. Indo-Caribbeans have migrated to the United States, Canada, the Netherlands, France, the United Kingdom and Ireland. The Capildeo family is an Indo-Trinidadian family, 2001 Nobel laureate V. S. Naipaul and mathematician and politician Rudranath Capildeo are most notable members of this family. Pundit Capildeo, travelled to Trinidad as an indentured labourer in 1894 from his village in Uttar Pradesh. This paper concerns with the study of Capildeo family in terms of their representation of India in Literature.

Key words: Diaspora, Indian Indenture System, Alienation, Girmitya, Indo Caribbeans, Capildeo Family,

The Indian Diaspora is one of the largest Diasporas in the world. The term is particularly used for people like expatriates, immigrants, exiles, refugees and other ethnic minorities. Migration is a physical and psychological displacement leading to alienation, nostalgia, identity crisis and language barriers. People find alienated in a new land. Indian diasporic writers such as Bharti Mukharjee, Sujata Bhatt, Meena Alexander, Uma Parameswaran, Chitra Banarjee, Salman Rushdie, V.S. Naipaul, Kiran Desai, Jhumpa Lahiri and Hanif Kureishi have migrated across the world to Canada, America, Australia and to the

island countries such as Mauritius, Trinidad, Guyana, Malaysia, Fiji and many more. During the British rule in India, there emerged a new kind of slavery in the form of Indentureship around 1830s after the abolition of slavery. Many Indian natives were brought to the British colonies as cheap and hardworking labourers. The system was a new version of slavery, in which labourers signed an agreement with British rulers. Under this Indenture system, more than 60000 Indians were lured by the labor contractors of British rulers. They were transported in ships across the ocean. Some labourers could not survive the dangerous voyage, whereas some of them survive the hardship. But they were caught within a system of unfree labor which is bound by a signed or forced contract (indenture) to work without pay for the owner of the indenture for a period of time. Three and a half million Indians were transported to various colonies to provide labour for the plantations. After the end of slavery, attempts were made to bring in workers from Ireland, Germany, Malta, and Madeira,. All these efforts failed to satisfy the labour needs of the colonies due to high mortality of the new arrivals and their reluctance to continue working at the end of their indenture. On 16 November 1844, the British Indian Government legalized emigration to Jamaica, Trinidad and Demerara. The Indian indenture system was finally banned in 1917. After banishment these labours settled in those colonies were they were transported by European powers were they were transported by European powers. They become a major part of the population in migrated countries and there originated new form of culture which is visibly held an Indian taste.

Many Of the Girmitya population celebrate traditional Indian festivals and cherished Indian values. Indian Arrival Day is a holiday celebrated on May 30 in Trinidad and Tobago each year since the 1990s. in which day their ancestors were brought to new land as indentured labourers. Many writers from this region revolve around the theme of identity crisis, diaspora, loneliness as a result of their rootless life. Indo-Caribbeans or Indian-Caribbeans, are people of Indian descent who live in the Caribbean. They are mostly descendants of the original Jahaji Indian indentured workers brought by the British, the Dutch, and the French during colonial times. The majority of the Indians living in the English-speaking Caribbean and fiji island came from eastern Uttar Pradesh and Western Bihar. They are Hindi speakers. Satendra Prasad Nandan, one of the twice banished Indian Diasporic writer of Girmitiya Origin. His collection of poems *Lines Across Black Waters* Portrays History of Girmitiyas and their dangerous journey across black water. His *The wounded sea* and *In a far country* envisage assimilation to a alien culture. Gaiutra Bahadur is an award-winning Guyanese-American writer. She is best known for *Coolie Woman: The Odyssey of Indenture* was published in 2013. It is partly a narrative history of indentured women in the Caribbean and partly a family history, focusing on her great-grandmother, Sujaria, who left Calcutta for British Guiana in 1903, to work as an indentured plantation labourer. *Coolie Woman* is not only a family history, but a broader social and narrative history of indenture; the system that, for roughly eighty years after the abolition of slavery in the British empire, provided exploitable bonded labour to plantation owners across the globe. She collaborated with the poet and translator Rajiv Mohabir to recover the only known text by an indentured immigrant in the Anglophone Caribbean, a songbook by Lal Bihari Sharma first published as a pamphlet in India in 1915. Mohabir's English translation, *I Even Regret Night: Holi Songs of Demerara, w*as published in 2019. It is a voice that raises above the burden of indentured servitude and affection for culture, language and identity.

Raymond R. Ramcharitar is a Trinidadian poet, playwright, fiction writer.His *The Island Quintet,* four short stories and a novella that convey a complex vision of the Caribbean,

this breakthrough collection is written with a profound and disturbed sense of the history and destorted human relation as a result of colonialism. Samuel Selvon is a Trinidad-born writer. In the novel *The Lonely Londoners,* he used creolized English. His first Novel *A Brighter Sun*(1952) portrays the East Indian community of Southern Trinidad before the war. *An Island Is a World* deals with the theme of cultural mixing and nationality. *Cereus Blooms at Night*(1996) is the first novel published by a film-maker, artist, and writer Shani Mooto, which set in a fictional Caribbean town, it explores trauma, gender identity, and colonial legacies.

The Capildeo family is an Indo-Trinidadian family of politicians and writers. Nobel laureate V. S. Naipaul and mathematician and politician Rudranath Capildeo are notable members of this family. The ancestral home of the Capildeo family is known as Anand Bhavan ("The Lion House"), it is situated in Chaguanas, Caroni county, Trinidad and Tobago. The family has its root in Mahadeva Dubey Village, Baratgara Tehsil, Maharajganj, Gorakhpur, Uttar Pradesh, India. Pundit Capildeo, travelled to Trinidad as an indentured labourer in 1894 from his village in Uttar Pradesh. He was maternal father of VS Naipaul. His father Seepersad Naipaul married to Droapatie Capildeo, daughter of pandit Capildeo. Seepersad Naipaul was a writer, His only book, *The Adventures of Gurudeva*, is a collection of linked comic short stories that was first published in Trinidad and Tobago in 1943 under the title Gurudeva and Other Indian Tales. The Adventures of Gurudeva is a collection of one novelette and nine short stories. V. S. Naipaul, who provides the foreword for the book. V. S. Naipaul states that Gurudeva "is a unique record of the life of the Indian or Hindu community in Trinidad in the first fifty years of the century" (p. 19). The book was not published in London until after Seepersad's death. It was rewritten during the period between 1943 to 1953. It lament on the disintegration of the customs of the rural Indian community, trans-planted from India to Trinidad. Many customs and superstitious beliefs were represented in these stories.

In *"The Engagement"* Seepersad Naipaul states the belief that fourteen is the ideal age for a boy to enter into the usual arranged marriage. He portrays about ostracism in those days. He defines the status of women in those days through Leela of *The Wedding Came.* This story follows Leela, a girl who never attended school, and whose father is increasingly anxious because she remains unmarried after the age of ten. The father's guilt and fear of community shame is so intense it's described metaphorically, as if "the caverns of hell" are opening for his "defaulting soul."This story powerfully illustrates the patriarchal anxiety and superstition around women's sexuality, education, and social reputation.Another, and more important, illustration of the erosion of the society is the fact that the "*Bamboo wedding"* a traditional Hindu wedding ceremony is no longer considered sacred. The story implies that once-revered Hindu marriage rituals had become so informal and stripped down that they no longer held spiritual or social weight." *They Named him Mohun.*" he depicts the superstitious belief that the six-fingered boy being an evil omen. People begin to associate bad events with his presence. He portrayed man-women relationship throughout his stories like obedience and silence are expected from women, they eat only after the men, showing hierarchy even in daily routines. woman's laughter or independence is seen as inappropriate, especially if she's newly married. a male child is the best gift a woman can give to her husband,violence against wives is normalized and it described as a "privilege" of men, reflecting the harsh social norms of the time.

Vidiadhar Surajprasad Naipaul was a Trinidadian and Tobagonian British writer. His work, *An Area of Darkness* conveys the sense of disillusionment which the author experiences

on his first visit to his ancestral land. It was an Indian trilogy which includes A *Wounded Civilization a*nd *A Million Mutinies Now*. The book was immediately banned in India for its "negative portrayal of India and its people". Naipaul expresses serious misgivings about Indian attitudes and the Indian way of life.

"In India I had so far felt myself a visitor. Its size, its temperatures, its crowds : I had prepared myself for these, but its very extremes, the country was alien. Looking for the familiar , I had again, in spite of myself, become an islander : I was looking for the small and manageable (An Area of Darkness, p. 140).

He depicts India as,

"India lay about us in thing; in a string bed… in plaited straw mats; in innumerable brass Vessels… in brightly coloured pictures of deities on pink lotus or radiant against Himalaya snow; and in all the paraphernalia of the prayer room." (An Area of Darkness, p. 29)

"The emergency was over. And so was my year. The short winter was fading fast; it was no longer pleasant to sit out in the sun; the dust would not now be laid until the monsoon. ... India had not worked its magic on me. It remained the land of my childhood, an area of darkness; like the Himalayan passes, it was closing up again, as fast as I withdrew from it, into a land of myth; it seemed to exist in just the timelessness which I had imagined as a child, into which, for all that I walked on Indian earth, I knew I could not penetrate. In a year I had not learned acceptance. I had learned my separateness from India, and was content to be a colonial, without a past, without ancestors. (An Area of Darkness (1964).p 252)

Naipaul's second travelogue on India, India : A Wounded Civilization (1979) is nothing but the larger and more representational and sensible version of the first travelogue An Area of Darkness.it is divided into three parts, namely. 'A Wounded Civilization', 'A New Claim on the Land' and 'Not Ideas, but Obsessions'. he writes that;

"India is for me a difficult country. It isn't my home and cannot be my home; and yet I cannot reject it or be indifferent to it; I cannot travel only for the sights. I am at once too close and too far"

"A hundred years had been enough to wash me clean of many Indian religious attitudes; and without these attitudes the distress of India was – and is – almost insupportable". (IWC-9)

Naipaul has failed to recognize the sacredness and the virtues of the Indian religion. He Is an unhappy Trinidad-Indian, visits India with a Western eye and prejudice. Indian critics state that it is, because of his lost identity and double alienation, Naipaul writes negatively about India. It is his own confusion regarding his confused identity has contributed a lot to his negativity. *Mystic Masseur* (1957), Naipaul's first published novel, is considered to be his maiden effort in presenting the expatriate sensibility and the most serious picture of native Trinidad. The Suffrage of Elvira is a Satire that showing the effects of the election on various ethnic groups and consequence of political change. *A House for Mr Biswas* on of his worldwide acclaimed work, in which Mohun Biswas, a Hindu Indo-Trinidadian who marries into the influential Tulsi family and dominated by it. It has some biographical elements from the experience of the author's father. His birth was considered as omen as he has an extra finger. The pundit advises that the boy be kept "away from trees and water. His father drowned in an Attempt to save him which fulfil the prophecy. This leads to the dissolution of the family. He got married in early age, and his marriage was a failure. Mr Biswas becomes very unhappy with his wife Shama (based on Droapatie Naipaul) and her overbearing family. The Tulsis (based on the Capildeo family), and the big decaying Hanuman House (based on Anand Bhavan aka The Lion House) where they live, represent the communal way of life which is traditional throughout Asia. He attempts to build a house of his own, so he can lead

a independent life. The house symbolize his identity which overcome rootlessness and alienation. Naipaul portrays a man sandwiched between modernity and tradition.

In *Finding the Centre* Naipaul asserts that for him India was a far-off dream because he knew nothing about his ancestral roots. But later he came to know about his family history. His grandfather came to Trinidad as a child with his mother who was an indenture laborer in the sugar cane fields in Trinidad and he was trained to be a Pundit so as to follow the family tradition. Naipaul's father Seepersad Naipaul was also trained to be a Pundit, but he never wished to be a pundit and therefore he took a job of sign painting at the beginning of his career. I*n a Free State* Is a novel consist of framing narrative and three short stories - "One out of Many," "Tell Me Who to Kill," and the title story, "In a Free State." The first tale concerns an Indian servant, Santhosh from Bombay. Santosh emigrates from India to America and has to cope with the situation of being an illegal immigrant and finding a new identity.

Shiva Naipaul was the younger brother of novelist V. S. Naipaul . Shiva Naipaul wrote his first novel, *Fireflies* (1970), which won the Winifred Holtby Memorial Prize from the Royal Society of Literature for best regional novel. *The Chip-Chip Gatherers* is a novel Reveal comic story following a cast of colorful Hindu and Muslim characters of Indian descent in a large village in Trinidad. Both novels share dysfunctional families, marriages, horrible conditions for women, and the problem of class and race. Surya Vahni Priya Capildeo is a Trinidadian Scottish writer, and a member of the extended Capildeo family .Her notable works are N*o Traveller Returns (2003), One Scattered Skeleton, Person Animal Figure (2005), Undraining Sea (2009) and Dark & Unaccustomed Words (2012).* Neil Devindra Bissoondath was another writer from cauldron family. He was the nephew of authors V.S. Naipaul and Shiva Naipaul, grandson of Seepersad Naipaul, grandnephew of Rudranath Capildeo and Simbhoonath Capildeo, and cousin of Vahni Capildeo. *A Casual Brutality* is a powerful, dark novel about the failure of a decent man to come to terms with the moral disintegration of the Caribbean island of his birth. *The Soul of all Great Designs* about a young woman forced to balance her Indian immigrant parents' strict traditions.

Savitri (Savi) Naipaul Akal was born in Trinidad, the fifth child and fourth daughter of Seepersad and Droapatie Naipaul, sister of Vidia and Shiva is also creative writer. Her family memoir The Naipauls of Nepaul Street will be published in May 2018.This is a moving story of a family's beginnings, growth in the context both of time and Trinidadian societyand its inevitable dispersal. She depicts the influence of parents in their life, they are so different Individuals but equal in their contribution to their large family. It is an account of family loyalty, sacrifice, and sometimes tensions. She observed picture of cultural change in Trinidad from colony to independent nation, of being Indian in a Creole society, of the role of education, and her parents' encouragement of their children to make independent lives for themselves. The memoir gives an clear analysis of the pressures that led many of the family to emigrate. Once she explain an experience when her brother V S Naipaul awarded the 2001 Nobel Prize in Literature, She was proud of him, but disappointed when he failed to acknowledge and mention Trinidad, the land of his birth. He called his prize 'a great tribute to both England, my home, and India, the home of my ancestors'.

Feeling of alienation after dispersal from homeland constitutes the core of diasporic sensibility. a state of mind in which they search for locating and relocating their identity. Their quest for the past and their bitter realization of dislocation and marginalization lead to state of 'ambivalence'. Most of the members in capildeo family know little about India. The only link with their home land was Indian- style large house known as Anand Bhavan. Their belongingness to an uprooted traditional Hindu family indentured by the colonial power puts

him to an odd indefinable situation where all the immigrants live in a predicament of rootlessness and homelessness. The Indian immigrants Hardly connect with outer world. Therefore ancestral homeland also became a distant illusion for the new generation. This illusion can be seen throughout the works especially in travelogues by VS Naipaul. The history become dark before their eyes, that is why VS Naipaul called Indian as "An Area of Darkness." For many Girmityas, India remained a sacred, distant place—the source of culture, religion, and identity. It existed more in memory and imagination than in material reality. When descendants of Girmityas visited or reconnected with India, it was far from the imagination.

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The synthesis of CoMoO4 (CMO) and the activated carbon-CoMoO4 (AC-CMO) by co-precipitation method

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Abstract:
In the present study the synthesis of CoMoO4 (CMO) and the activated carbon- CoMoO4 (AC-CMO) by simple and low cost method is co-precipitation method. In this method, we produce two unique nonmaterial's, starting with the synthesis of CoMoO4 (CMO) as the initial component. Next, we enhance this process by incorporating activated carbon, resulting in the formation of the activated carbon-CoMoO4 hybrid (AC-CMO), a powerful combination ready to explore new possibilities in energy storage. We selected the co-precipitation method for our synthesis due to its remarkable adaptability, which allows for precise control over the composition and characteristics of the material. This technique's ability to uniformly integrate activated carbon within the CoMoO4 matrix ensures a cohesive interaction between the components. Additionally, the method's scalability and practicality, along with its operation at room temperature, perfectly align with our aim of developing an efficient and viable energy storage solution. This method serves as the optimal pathway to create the activated carbon-CoMoO4 hybrid, enabling us to fully harness its potential for improved supercapacitor performance.

Keywords: *CoMoO4 (CMO), activated carbon CMO, Co-precipitation, etc.*

Introduction:

Co-precipitation refers to the concurrent precipitation of several precursor ions from a solution, leading to the creation of solid particles. This technique allows for the precise formation of uniform mixtures and the generation of materials with clearly specified compositions. Co-precipitation is widely used for creating metal oxides, hydroxides and composite materials [1-6].As we bid adieu to this overview of synthesis methods, our focus now shifts toward the unfolding chapters, where we will unveil our own experimental journey. We explore the route of co-precipitation, a chemical synthesis method that enables us to develop the activated carbon-CoMoO4 hybrid material. This technique, functioning at room temperature, offers unique benefits as we examine its details and reveal its possibilities. Our experimental strategy aims to provide a fresh perspective on the synthesis procedure, generating knowledge about the interrelationship of variables, the complex interactions of precursors, and the emergence of a hybrid material with significant potential. The subsequent section focuses on investigating this process, clarifying the experimental conditions, and highlighting the critical elements that contribute to the successful creation of this exceptional hybrid material.

Experimental:

The development of hybrid materials has become a crucial pathway for improving the efficiency of energy storage devices and catalytic systems. This study explores the methods used to synthesize the activated carbon-CoMoO4 hybrid material, which shows promise for cutting-edge supercapacitor applications. This section describes the key approaches, techniques, and

considerations involved in the production of this hybrid material. It emphasizes the selection of activated carbon and CoMoO4 as essential components, focusing

on their unique properties that enhance the synergistic performance of the hybrid material. The following sections examine the sequential synthesis processes, including the preparation of precursors, mixing techniques, and reaction kinetics. In order to attain accurate control over the final structure and characteristics of the activated carbon-CoMoO4 hybrid material, a detailed examination of the synthesis methods is presented. Both physical and chemical approaches are explored at length, highlighting their distinct benefits and drawbacks. The section further investigates the experimental parameters influencing the synthesis, which include variables such as temperature, reaction duration, precursor ratios, and choices of solvents.

The synthesis of CoMoO4 (CMO) and the activated carbon- CoMoO4 (AC-CMO) by simple and low cost method is co-precipitation method, carefully carried out to guarantee the accurate formation of these materials. The synthesis of CMO commenced with a sequential procedure. Initially, 1 mmol of ammonium Molybdate (NH4)2 MoO4 was added to 50 ml of distilled water, followed by continuous stirring at room temperature for 30 minutes using a magnetic stirrer. Subsequently, 1 mmol of Cobalt Chloride CoCl2 was incorporated into the same solution, with consistent stirring maintained under the same conditions. The chemical reaction was completed with the addition of 30 mmol of NaBH4 into a 50 ml mixture of ammonium Molybdate (NH4)2MoO4 was added to 50 ml of distilled water. Followed by continuous stirring at room temperature for 30 minutes using a magnetic stirrer. This resulting aqueous solution then subjected to continuous stirring for an additional 30 minutes. The synthesis procedure foe AC-CMO was similar to that of CMO, with the addition of 200 mg of activated carbon into 50 ml of distilled water as the first step.



(A) (B)

Photographsof(A)HotairOven(B)Magneticstirrer

After completing the three- step synthesis process for each variant, the reaction solution were

allowed to remain undisturbed for 12 hours, promoting the development of precipitate. Subsequently, the Supernatant and precipitate were separated using a decanting process, which was carefully performed six times for each material variant.

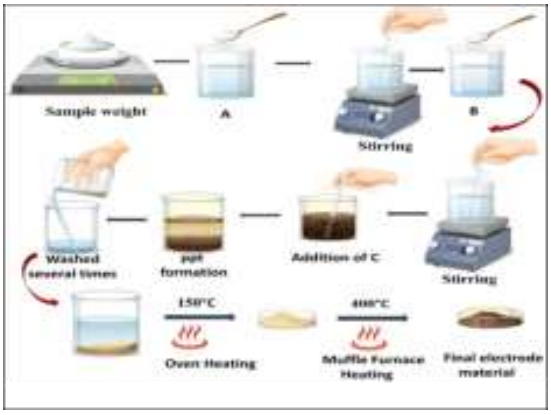


Figure1Schematic representation of Co-precipitation experimental method for CMO (A)-addition of (NH4)2MoO4,(B)-addition of CoCl2,(C)-addition of NaBH4

The resulting precipitate was isolated by draining excess supernatant after all extra water-soluble byproducts had been removed. Then, the material was heated in a hot air oven for 12 hours at 150°C to effectively remove any remaining moisture content. Following that, the material was cooled and further crushed using mortar and pestle, which refined the particle size into the nanoscale range. Next, the substance was placed into an alumina boat (specimen holder), which was then placed into a muffle furnace and held there for four hours at 400°C. After this heat treatment was finished, the material was allowed to cool before being ground further with a mortar and pestle. After this procedure, the resulting powder was ready for further steps in electrode production and thorough material characterization.

Reaction:

Thereactionmechanisminvolved informationofCoMoO4,is stated below.

$2(NH_4)_2MoO_4+2CoCl_2+NaBH_4+7H_2O \rightarrow 2CoMoO_4(ppt) + NaCl + 4NH_4OH+B(OH)_3+3HCL+4H_2\uparrow$

As we can see in this reaction mechanism, on the product side CoMoO4 is formed in the form ofpptandallotherwater-solublebyproductsareeliminatedwiththehelpofdecantingprocess. Cycles of decanting-washing was performed till neutral pH was achieved.

Conclusion:

The coprecipitation method is the simple and low-cost method for the synthesis of CoMoO4 (CMO) and the activated carbon- CoMoO4 hybrid (AC-CMO). With this method, it is possible to produce materials with precisely regulated compositions and create homogeneous mixtures in a controlled manner. The co-precipitation technique is commonly employed to produce composite materials, hydroxides, and metal oxides.

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"Symbiotic Architects of the Soil: Roles and Applications of Arbuscular Mycorrhizal Fungi in Ecosystem Function and Resilience"

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Abstract

Arbuscular mycorrhizal fungi (AMF), which are over 400 million years old and members of the phylum Glomeromycota, are fundamental mutualists in terrestrial ecosystems. These ancient symbionts significantly influence plant-soil interactions by forming complex and advantageous relationships with the roots of almost 80% of vascular plant species. AMF greatly improves the uptake of essential nutrients, especially phosphorus and micronutrients, which are frequently scarce in soils, through their hyphal networks. Better response to biotic and abiotic challenges, including drought, heavy metal toxicity, and pathogen infections, is made possible by this nutrient exchange, which promotes plant growth and resilience. By encouraging soil particle aggregation through the release of glomalin, a glycoprotein that improves soil porosity and water retention, AMF ecologically play a critical role in stabilizing soil structure. Additionally, they serve as a biological interface that connects plant roots to the larger soil biome by influencing the makeup and activity of nearby microbial populations. Their capacity to regulate ecosystem functions such as carbon sequestration, nitrogen cycling, and successional dynamics in both wild and managed settings accounts for their keystone status. In the applied sciences, AMF's contributions are becoming more widely acknowledged, especially in the areas of phytoremediation, reforestation, and sustainable agriculture. By acting as biofertilizers, they lessen the need for chemical inputs, improving the health of the environment. Their promise in ecological engineering and restoration ecology is highlighted by their use in improving plant performance under environmental stress and restoring degraded lands. To fully utilize AMF's potential in fostering ecosystem stability and resilience in the face of global change, it is imperative to comprehend their diversity, functional characteristics, and ecological responsibilities.

I. Introduction

The stability and productivity of terrestrial ecosystems are supported by the symbiotic connections that exist between plants and soil microbes. Because of their ecological significance and evolutionary age, arbuscular mycorrhizal fungi (AMF) belonging to the phylum Glomeromycota stand out among these. According to Redecker, et al., (2000), these fungi are thought to have co-evolved with land plants for around 450 million years, indicating

their presence during the colonization of terrestrial environments. AMF facilitates a finely tuned mutualism by forming highly specialized intracellular structures called arbuscules within the root cortex of host plants. In return, the fungi receive carbon from photosynthetic plants, and AMF improves nutrient acquisition, particularly phosphorus and nitrogen, which are frequently growth-limiting in terrestrial soils.

By enhancing both nutrient intake and resistance to abiotic stressors like drought, salt, and low soil fertility, the AMF-plant alliance dramatically increases plant fitness. Additionally, by inducing systemic resistance mechanisms, AMF significantly strengthens plant defense against root diseases and herbivores (Cameron et al., 2013). In order to improve soil structure and promote long-term soil health, these fungi also release glomalin, a glycoprotein that aids in soil aggregation and carbon storage (Rillig, 2004). AMF are so essential in both natural and agricultural systems because they mediate vital processes including nutrient cycling, water management, and biological resilience, acting as ecosystem engineers. The significance of protecting and incorporating AMF into plans for ecological restoration and sustainable land management is underscored by their ecological impact and widespread occurrence.

2. Taxonomy and Morphological Characteristics of AMF

Within the fungal kingdom, arbuscular mycorrhizal fungi (AMF) of the phylum Glomeromycota are distinguished by a set of distinctive physical and biochemical characteristics. These fungi, which are obligate biotrophs and depend totally on host plants for carbon to complete their life cycle, are distinguished by their coenocytic (non-septate) hyphae. AMF produce a variety of reproductive structures, such as vesicles (storage organs) and enormous multinucleate spores, both of which are essential to their survival and spread. AMF taxonomy has historically depended on spore size, color, wall construction, and morphology. However, these physical criteria did not adequately reflect evolutionary relationships and frequently obscured cryptic variety.

The classification of AMF has been improved since the development of molecular phylogenetics, specifically ribosomal DNA sequencing and multilocus gene studies. One of the most thorough molecular phylogenies was presented by Krüger et al. (2012), which increased the known diversity within Glomeromycota. By showing that physical characteristics by themselves were unable to capture evolutionary relationships, their work assisted in the delineation of new clades and taxa.

Nowadays, the orders Glomerales, Diversisporales, and Paraglomerales contain the majority of the well-characterized AMF species. Because of its genetic tractability and reliable symbiotic performance across plant hosts, Rhizophagus irregularis (previously Glomus intraradices) has become one of these often-researched model species (Tisserant et al., 2013). Deep insights into the symbiotic gene networks, signaling pathways, and functional modifications that characterize AMF-host relationships have been made possible by the genome's sequencing. For the advancement of ecological, agronomic, and genomic research on mycorrhizal systems, these taxonomic and morphological insights are essential.

3. Functional Role in Ecosystem Processes

3.1 Nutrient Cycling and Plant Nutrition

In the dynamics of terrestrial nutrients, particularly the uptake of phosphorus (P), arbuscular mycorrhizal fungi (AMF) play a crucial role. Plant roots frequently have trouble reaching immobile inorganic P in phosphorus-deficient soils. By extending their vast extraradical hyphal networks outside the nutrient depletion zone close to the root surface, AMF are able to get over this restriction. In order to facilitate uptake and return to the host plant, these hyphae scavenge and solubilize inorganic phosphate (Smith & Smith, 2011). The overall fitness and production of plants are enhanced by this effective nutrient foraging mechanism, which also helps with the uptake of nitrogen and micronutrients like copper and zinc (Smith & Read, 2008).

3.2 Soil Structure and Water Relations

AMF has a significant impact on the physical characteristics of soil. Glomalin, a hydrophobic glycoprotein released by AMF hyphae, encourages the aggregation of soil particles, improving the soil's porosity, structure, and ability to store water (Rillig, 2004). In arid and semi-arid regions, where soil stability and water conservation are essential for ecosystem resilience, these impacts are particularly significant. Plant-soil-microbe interactions are further strengthened by AMF's indirect support of microbial habitats and root penetration through improved soil aggregation (Wilson et al., 2009).

3.3 Microbial Community Dynamics

AMF are essential rhizosphere microbiome modulators. By changing soil chemistry and root exudation profiles, their symbiotic presence affects microbial assemblages and their functional roles. While competition with saprotrophs may impact decomposition rates and organic matter turnover, interactions between AMF and rhizobacteria can improve nutrient cycling and plant defense (Zhang et al., 2022). AMF is positioned as a key role in the co-regulation of soil biodiversity and ecosystem multifunctionality due to these dynamic connections.

4. Role as Keystone Mutualists

Due to their crucial role in influencing plant communities and more general ecosystem processes, arbuscular mycorrhizal fungi (AMF) are becoming more widely acknowledged as keystone mutualists. AMF have a disproportionate impact on plant resilience, production, and diversity despite their minuscule size. AMF promotes the coexistence of many plant species by improving nutrient intake and stress tolerance, which eventually boosts ecosystem stability and functional redundancy (Van der Heijden et al., 1998). Moreover, the presence of AMF interactions modifies the composition of microbial communities in the rhizosphere microbial network, which extends beyond plant roots. By suppressing soilborne pathogens and enhancing helpful microorganisms like plant growth-promoting rhizobacteria (PGPRs), AMF injection has been demonstrated to produce a protective microenvironment surrounding roots (Cheng et al., 2023). Because of these qualities, AMF plays a vital role in sustainable agriculture, ecosystem restoration, and the reduction of environmental stressors including salinity and drought.

5. Applications in Agriculture and Phytoremediation

Arbuscular mycorrhizal fungi (AMF) are revolutionary for environmental rehabilitation and sustainable agriculture. By improving the uptake of nutrients, especially nitrogen and phosphorus, AMF lessens the need for synthetic fertilizers, which lowers costs and lessens pollution in the environment (Smith & Smith, 2011). According to Baslam et al. (2014), their symbiotic relationship increases plant resistance to abiotic stressors such drought, salinity, and soil compaction, which is essential for climate-resilient agriculture. By binding heavy metals like cadmium, lead, and arsenic inside their hyphae or by changing the bioavailability of metals in the rhizosphere, AMF aid in the detoxification of contaminated soils through phytoremediation (Begum et al., 2023). By encouraging biomass buildup and soil aggregation, these fungi also aid in carbon sequestration. As a result, regenerative agriculture strategies that enhance soil health, biodiversity, and long-term ecosystem productivity are supported by incorporating AMF into agroecosystem design.

6. Future Perspectives

Despite the well-established ecological significance of arbuscular mycorrhizal fungi (AMF), there are still important knowledge gaps. Due to their obligate symbiotic nature and host dependency, one of the main obstacles is the mass manufacturing and commercialization of AMF inoculants (Ijdo et al., 2011). Moreover, little is known about the specificity of AMF-plant interactions in different environmental settings, especially when exposed to stresses brought on by climate change such as increased CO_2, warmth, and extreme weather.

Metagenomics, transcriptomics, and metabolomics are examples of emerging -omics technologies that provide new ways to understand the molecular basis of AMF interactions with coexisting soil bacteria and host plants (Schlaeppi & Bulgarelli, 2015). The creation of customized AMF consortia for certain ecosystem services may be made possible by these strategies. The development of affordable, scalable AMF formulations that maintain their viability and efficacy in a variety of field situations is also essential to achieving widespread use.

7. Conclusion

The ecological foundation of plant-soil systems is made up of arbuscular mycorrhizal fungi (AMF), particularly those belonging to the Glomeromycota. They are keystone mutualists that improve productivity, resilience, and biodiversity because of their functions in microbial modulation, soil structure, and nutrient cycling. AMF-based solutions provide sustainable means of restoring soil fertility, cutting back on chemical inputs, and promoting regenerative agriculture as the earth experiences increasing ecological stress due to land degradation and climate change. To fully utilize AMF in both natural and controlled environments, more multidisciplinary research combining ecology, genetics, and agronomy is essential.

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The Rann of Kutch and Other Wetlands: Ecological Significance and Conservation Strategies

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Abstract

Wetlands in Gujarat, including the Rann of Kutch, Nalsarovar Lake, Thol Lake, and Khijadiya Bird Sanctuary, are ecologically significant ecosystems that support biodiversity, regulate water cycles, and contribute to local livelihoods. This research paper explores the geographical distribution, ecological significance, pollution challenges, and conservation strategies for wetlands in Gujarat. It highlights the impact of pollution from industrial discharge, agricultural runoff, and waste mismanagement, which threatens the health of these wetlands. The paper also emphasizes the vital role of community involvement in wetland conservation through eco-tourism, sustainable livelihoods, and citizen science initiatives. Effective pollution control measures, waste management strategies, and government-community partnerships are essential for the long-term protection of Gujarat's wetlands. The study concludes by advocating for sustainable practices, increased awareness, and policy interventions to preserve these fragile ecosystems.

I. Introduction

Wetlands are among the most productive and ecologically significant ecosystems on Earth, providing a range of environmental, social, and economic benefits. In India, Gujarat is home to several vital wetlands, with the Rann of Kutch being one of the most prominent. The Rann of Kutch, divided into the Great Rann and the Little Rann, is a unique seasonal salt marsh located in the Thar Desert. It is not only a remarkable geographical feature but also a critical habitat for diverse flora and fauna, including the endangered Indian Wild Ass (Equus hemionus khur) and migratory birds like flamingos, pelicans, and cranes.

Apart from the Rann of Kutch, Gujarat hosts other significant wetlands, including Nalsarovar Lake, Thol Lake, and Khijadiya Bird Sanctuary, which are recognized for their rich biodiversity and ecological importance. These wetlands play a vital role in groundwater recharge, flood control, and carbon sequestration, while also supporting local livelihoods through activities like fishing, agriculture, and eco-tourism.

However, Gujarat's wetlands face growing threats due to climate change, industrial expansion, unsustainable agricultural practices, and urbanization. The degradation of these ecosystems not only impacts biodiversity but also disrupts the ecological balance, affecting both the environment and local communities.

2. Geographical and Ecological Overview of Wetlands in Gujarat

2.1 Geographical Distribution of Wetlands in Gujarat

Gujarat, located in western India, has a diverse landscape that includes coastal regions, river basins, salt marshes, and freshwater wetlands. The state is home to both inland

and coastal wetlands, making it ecologically significant. According to the Wetlands Atlas of India, Gujarat has around 34,350 km² of wetlands, accounting for approximately 17.5% of the state's geographical area.

The major types of wetlands in Gujarat include:

Inland Wetlands: Rivers, lakes, reservoirs, and marshes (e.g., Nalsarovar Lake, Thol Lake).

Coastal Wetlands:

Mangroves, mudflats, estuaries, and salt pans (e.g., Gulf of Kutch, Khijadiya Bird Sanctuary).

Salt Marshes:

The Rann of Kutch, a unique seasonal salt marsh, is one of the largest wetlands in India.

2.2 The Rann of Kutch: A Unique Wetland Ecosystem

The Rann of Kutch, spanning over 30,000 km², is a distinctive salt marsh located in the Thar Desert.

Great Rann of Kutch: Situated in the north, it features expansive salt flats that flood during the monsoon and transform into a shallow wetland, attracting migratory birds.

Little Rann of Kutch: Located to the southeast, it is famous for the Indian Wild Ass Sanctuary, which supports the endangered Indian Wild Ass (Equus hemionus khur).

Ecological Importance of the Rann of Kutch:

Biodiversity hotspot:

It hosts several migratory bird species, including flamingos, pelicans, cranes, and raptors.

Breeding ground:

It serves as an important breeding site for the Greater Flamingo (Phoenicopterus roseus).

Salt production:

The region is also a major center for salt farming, contributing significantly to the economy but also posing ecological challenges.

2.3 Other Major Wetlands in Gujarat

Apart from the Rann of Kutch, Gujarat is home to several significant wetlands:

1.Nalsarovar Lake Location: Ahmedabad District

Type: Freshwater lake and marsh

Ecological Significance:

Declared a Ramsar site in 2012.

Home to over 200 species of migratory birds, including flamingos, pelicans, and ducks.

2.Thol Lake

Location: Mehsana District Type: Freshwater wetland Ecological Significance:

Known for its large population of Sarus Cranes and other waterfowl. Important for birdwatching and eco-tourism.

A breeding site for several bird species.

3.Khijadiya Bird Sanctuary Location: Jamnagar District

Type: Coastal wetland (mix of freshwater and marine ecosystems)

Ecological Significance:

Recognized as a Ramsar site in 2022.

Hosts coastal and freshwater bird species, including herons, egrets, and ibises. Critical for biodiversity conservation.

4.Gulf of Kutch Marine National Park Location: Jamnagar District

Type: Coastal wetland and marine ecosystem

Ecological Significance:

Known for mangroves, coral reefs, and marine biodiversity.

Supports species like green sea turtles, dugongs, and various fish species. Important for marine conservation.

5.Porbandar Bird Sanctuary Location: Porbandar District Type: Freshwater wetland Ecological Significance:

Hosts both resident and migratory birds. Supports local fisheries and tourism activities.

2.4 Ecological Functions of Wetlands in Gujarat

Gujarat's wetlands provide a range of ecological services, including:

Biodiversity Conservation: Wetlands are vital for the survival of migratory and resident bird species, supporting their breeding and feeding grounds.

Water Regulation: Wetlands help in groundwater recharge, maintain water tables, and control floods.

Climate Regulation: Coastal wetlands and mangroves act as carbon sinks, reducing the impact of climate change.

Livelihood Support: Wetlands support fishing, salt production, and eco-tourism, providing income to local communities.

Nutrient Cycling: Wetlands improve water quality by filtering pollutants and promoting nutrient cycling.

3.Ecological Significance of Wetlands

Wetlands are among the most ecologically significant ecosystems, providing a wide range of environmental, social, and economic benefits. In Gujarat, wetlands such as the Rann of Kutch, Nalsarovar Lake, Thol Lake, and Khijadiya Bird Sanctuary play a crucial role in maintaining ecological balance, supporting biodiversity, and offering ecosystem services.

3.1 Biodiversity Hotspots

Wetlands in Gujarat serve as critical habitats for a variety of plant and animal species, including many that are endangered or migratory

Flora Diversity:

Wetlands support aquatic vegetation, including reeds, sedges, and floating plants, which provide food and shelter for various species.

Fauna Diversity:

Avian species: Wetlands in Gujarat are major stopover points for migratory birds. For example:

Rann of Kutch: Breeding ground for the Greater Flamingo.

Nalsarovar Lake: Hosts over 200 species of migratory birds, including pelicans, cranes, storks, and ducks.

Khijadiya Bird Sanctuary: Supports both freshwater and marine birds, making it a unique ecological site.

Mammals:

The Little Rann of Kutch is home to the endangered Indian Wild Ass (Equus hemionus khur).

Marine and aquatic life:

Coastal wetlands, such as the Gulf of Kutch Marine National Park, support coral reefs, fish, turtles, and dugongs.

3.2 Water Regulation and Hydrological Functions

Wetlands in Gujarat play a vital role in water regulation and hydrological balance:

Groundwater Recharge:

Wetlands act as natural reservoirs, replenishing groundwater levels during monsoons.

Flood Control:

Wetlands absorb excess rainwater during the monsoon, reducing the risk of floods.

Water Quality Improvement:

Wetlands act as natural filters, trapping sediments and pollutants, thus improving water quality.

3.3 Climate Regulation and Carbon Sequestration

Wetlands play a key role in climate regulation by capturing and storing carbon dioxide (CO_2):

Carbon Sinks:

Wetlands store large amounts of organic carbon in their soils, helping mitigate the effects of climate change.

Temperature Regulation:

Wetlands maintain local microclimates by retaining moisture and regulating temperature.

Resilience Against Droughts:

Wetlands act as natural water reservoirs, providing water during dry periods.

3.4 Support for Livelihoods and Local Communities

Wetlands in Gujarat provide economic benefits by supporting local livelihoods: Fisheries and Aquaculture:

Wetlands like Nalsarovar Lake and Khijadiya Bird Sanctuary support local fishing communities.

Salt Production:

The Little Rann of Kutch is a major center for salt farming, contributing significantly to Gujarat's economy.

Tourism and Recreation:

Wetlands attract tourists, birdwatchers, and nature enthusiasts, boosting eco-tourism.

Traditional Practices:

Many local communities depend on wetlands for farming, grazing, and collecting medicinal plants.

3.5 Wetlands as Ecological Buffers

Wetlands act as natural buffers, protecting against environmental hazards: Coastal Protection:

Mangrove forests along Gujarat's coast protect against storm surges, erosion, and sea-level rise.

Disaster Mitigation:

Wetlands reduce the impact of floods, droughts, and cyclones, providing natural disaster resilience.

4. Pollution Control and Waste Management in Wetlands

Wetlands in Gujarat, including the Rann of Kutch, Nalsarovar Lake, Thol Lake, and Khijadiya Bird Sanctuary, are increasingly threatened by pollution and waste mismanagement. Rapid urbanization, industrialization, agricultural runoff, and unregulated tourism have led to the contamination of these fragile ecosystems. Effective pollution control and waste management strategies are essential for preserving the ecological integrity and sustainability of Gujarat's wetlands.

4.1 Sources of Pollution in Gujarat's Wetlands

Wetlands in Gujarat face pollution from various sources, including:

1. Industrial Discharge:

Gujarat's industrial hubs release untreated or partially treated effluents into nearby water bodies, contaminating wetland ecosystems.

Chemical pollutants from textile, dye, and chemical industries near the Gulf of Kutch and Khijadiya Bird Sanctuary degrade water quality.

2. Agricultural Runoff:

Excessive use of fertilizers and pesticides in nearby farmlands leads to nutrient pollution in wetlands.

3. Solid Waste and Plastic Pollution:

Tourism activities generate large quantities of plastic waste, food wrappers, and bottles, especially during events like the Rann Utsav.

4. Sewage and Domestic Waste:

Unregulated sewage discharge from nearby towns and villages contaminates wetland water.

5. Oil Spills and Marine Pollution:

Coastal wetlands such as the Gulf of Kutch face oil spill risks due to shipping and port activities, impacting marine biodiversity.

4.2 Impacts of Pollution on Wetlands

Pollution significantly affects the health and functioning of Gujarat's wetlands: Biodiversity Loss:

Water contamination reduces the population of fish, amphibians, and invertebrates, affecting the entire food chain

Eutrophication:

Excess nutrients from agricultural runoff and sewage lead to algal blooms, which reduce oxygen levels in the water.

Degradation of Water Quality:

Industrial and sewage pollutants increase water toxicity, making wetlands unfit for aquatic life and human use.

Soil Contamination:

Wetland soil absorbs heavy metals and toxins from polluted water, affecting its fertility and plant health.

Threat to Livelihoods:

Pollution reduces fish stocks, impacting the livelihoods of local fishermen.

4.3 Pollution Control and Waste Management Strategies

To protect Gujarat's wetlands from pollution, the following strategies are essential:

1. Strengthening Pollution Control Regulations:

Strict enforcement of the Water (Prevention and Control of Pollution) Act, 1974 and the Environment Protection Act, 1986.

Regular monitoring of industrial effluents and strict penalties for violations.

2. Wastewater Treatment and Management:

Installation of sewage treatment plants (STPs) near wetland regions to prevent raw sewage discharge.

3. Agricultural Runoff Management:

Promoting organic farming practices to reduce chemical runoff.

Establishing buffer zones with vegetation around wetlands to absorb excess nutrients. Implementing sustainable irrigation techniques to reduce water contamination.

4. Solid Waste and Plastic Management:

Ban on single-use plastics in wetland areas.

Installing waste collection and segregation bins at tourism hotspots like the Rann of Kutch and Nalsarovar Lake.

5. Oil Spill Prevention in Coastal Wetlands:

Strengthening monitoring systems for oil spills in the Gulf of Kutch.

Installing oil containment booms and quick-response units to contain and clean oil spills.

4.4 Community Involvement and Awareness Programs Local Participation:

Engaging local communities in wetland monitoring and clean-up activities.

Providing training on waste management practices to local stakeholders.

Awareness Campaigns:

Conducting educational programs on the impact of pollution on wetlands.

Promoting eco-friendly tourism practices.

Citizen Science Initiatives:

Encouraging citizens to report pollution incidents through mobile apps and local networks.

5. Community Involvement in Wetland Conservation

Community involvement plays a vital role in the conservation, management, and sustainable use of wetlands. In Gujarat, wetlands such as the Rann of Kutch, Nalsarovar Lake, Thol Lake, and Khijadiya Bird Sanctuary are not only rich in biodiversity but also support local livelihoods through fishing, salt production, and eco-tourism. Engaging local communities, NGOs, and stakeholders in conservation efforts is essential for ensuring the long-term protection and sustainable management of these fragile ecosystems.

5.1 Importance of Community Involvement in Wetland Conservation Involving local communities in wetland conservation offers several benefits: Traditional Knowledge and Sustainable Practices:

Local communities possess valuable traditional knowledge about wetland ecosystems, which can aid in sustainable management.

Enhanced Conservation Outcomes:

Participatory management improves the effectiveness of conservation programs by ensuring local support.

Involving locals fosters a sense of ownership and responsibility, encouraging sustainable practices.

Improved Livelihoods:

Community-led eco-tourism initiatives generate income while promoting wetland conservation.

Environmental Awareness and Education:

Community involvement spreads awareness about the ecological importance of wetlands.

5.2 Community-Based Conservation Initiatives in Gujarat

Several community-driven wetland conservation initiatives have been implemented in Gujarat:

1. Eco-Tourism and Community Participation in the Rann of Kutch:

The Rann of Kutch is famous for the Rann Utsav, a major tourist event that attracts thousands of visitors.

Local communities, including Kutch artisans, camel herders, and salt farmers, actively participate in eco-tourism activities.

Community-led eco-tourism programs promote sustainable tourism by:

Generating income for locals through handicraft sales, guided tours, and cultural performances.

2. Wetland Restoration Programs Involving Local Farmers:

In Nalsarovar Lake, farmers and fisherfolk participate in restoration and conservation activities.

Community-driven wetland restoration programs focus on: Reducing agricultural runoff through sustainable farming practices. Planting buffer vegetation around the wetland to prevent soil erosion.

3. Salt Farmers and Wetland Protection in the Little Rann of Kutch:

The Little Rann of Kutch is known for its salt production, which is a major source of livelihood for local communities.

Initiatives have been introduced to:

Promote sustainable salt farming practices that minimize environmental impact. Encourage water conservation and reduce the over-extraction of groundwater.

4. Community Involvement in Bird Monitoring and Conservation:

In wetlands such as Khijadiya Bird Sanctuary, local birdwatchers and conservationists participate in bird monitoring programs.

Community groups collaborate with forest departments and NGOs to:

Conduct bird census surveys during the migratory season.

5.3 Challenges in Community Involvement

Despite its benefits, involving local communities in wetland conservation faces several challenges:

Lack of Awareness and Education:

Many local communities are unaware of the ecological value of wetlands.

Lack of environmental education reduces their willingness to participate in conservation activities.

Limited Financial Support:

Community-led initiatives often lack financial resources and government support.

Conflicts Between Livelihood and Conservation:

Local communities dependent on wetlands for fishing, farming, or salt production may prioritize economic activities over conservation.

Unregulated Tourism:

Mass tourism events like the Rann Utsav generate income but also lead to waste accumulation and pollution.

5.4 Strategies to Enhance Community Involvement

To strengthen community participation in wetland conservation, the following strategies are recommended:

1. Capacity Building and Training:

Providing training programs on wetland conservation, sustainable farming, and eco-tourism.

Equipping locals with skills in waste management, biodiversity monitoring, and eco-friendly practices.

Offering financial incentives for adopting wetland-friendly practices.

2. Promoting Sustainable Livelihoods:

Encouraging eco-tourism enterprises managed by local communities.

Supporting sustainable fishing and farming practices to reduce wetland degradation.

3. Community-Based Monitoring and Reporting:

Engaging local communities in wetland monitoring through citizen science programs. Establishing community-based reporting systems to identify pollution or illegal activities.

4. Awareness and Education Campaigns:

Organizing environmental education programs in local schools and villages. Using folk art, street plays, and traditional storytelling to raise awareness.

5. Strengthening Government and NGO Partnerships:

Collaborating with government agencies, NGOs, and local groups for capacity building. Ensuring financial support and resources for community-led initiatives.

6. Conclusion

Gujarat's wetlands, including the Rann of Kutch and other inland and coastal ecosystems, play a crucial role in biodiversity conservation, water regulation, and climate resilience. They serve as habitats for migratory birds, endangered species, and diverse flora and fauna. Wetlands also contribute to local economies through fishing, salt production, and eco-tourism.

However, these ecosystems are under increasing threat from pollution, unregulated tourism, agricultural runoff, and industrial activities. Pollution degrades water quality, reduces biodiversity, and disrupts the ecological balance. Additionally, climate change and habitat loss further exacerbate the vulnerability of wetlands.

To ensure the long-term conservation and sustainability of Gujarat's wetlands, the following measures are essential:

Strengthening pollution control regulations and enforcement mechanisms.

Promoting community-led conservation programs and eco-friendly tourism practices. Enhancing awareness campaigns and educational initiatives.

Establishing collaborative partnerships between government agencies, NGOs, and local communities.

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Synthesis of trimellitic acid by base hydrolysis

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Abstract

Trimellitic acid (TMA), a benzene tricarboxylic acid, is a crucial intermediate in the production of polymers, coatings, and plasticizers. This study explores efficient synthetic methodologies for TMA, focusing on the base-catalysed hydrolysis of trimellitic anhydride using NaOH, KOH, and sodium bicarbonate. The impact of reaction conditions, including base type, temperature, and reaction time, on the yield and purity of TMA was investigated. This research aims to address existing gaps in the synthesis of trimellitic acid by exploring cheaper reagent and reaction conditions that could enhance yield rates while reducing energy consumption. The synthesized TMA will contribute towards sustainable development goals within chemical industries globally today and highlights its untapped potential in diverse industries.

Keywords – Trimellitic acid, base-catalysed hydrolysis, trimellitic anhydride, sustainable development

Introduction

Trimellitic acid (TMA) or benzene-1,2,4-tricarboxylic acid is a three-functional aromatic compound that has the chemical formula $C_9H_6O_6$.Trimellitic acid has the CAS number 528-44-9 [1]. Being one of three isomers of benzene tricarboxylic acid, TMA has three carboxylic acid groups located asymmetrically on a benzene ring, which accounts for its high chemical reactivity and industrial value.

Physically, TMA appears as white crystalline solid with a melting point between 218–234 °C, poor water solubility (about 21 g/Lat 25 °C), but good solubility in a variety of organic solvents.

It has a high boiling point (~505.5 °C) and a moderate flash point (~273.6 °C), indicative of its thermal stability[2].

Chemically, the compound's triprotic character makes it capable of undergoing a great variety of esterification and amination reactions, and is thus a good intermediate in organic synthesis. As an anhydride form, trimellitic anhydride, it is very widely used for the production of polyimides, high-strength polymers prized for their thermal and mechanical stability in electrical and aerospace equipment[3].

TMA is also a promising ligand for metal-organic frameworks (MOFs), wherein its three -COOH groups facilitate versatile coordination geometries. Such versatility is useful in the design of MOFs with controllable pore architecture and high thermal and chemical stability. Chemical-modified MOFs with TMA incorporated have shown higher adsorption performance, especially for contaminants like dyes in water[4].

Industrial synthesis of TMA usually comprises oxidation of pseudocumene with nitric acid under temperature and pressure control[5]. Modern studies focus on refining this process

through greener and more energy-conserving approaches and alternative oxidizing agents to minimize environmental degradation.

Major applications of TMA and its derivatives are:

1. Plasticizers: Sulfonated esters employed to render flexibility to PVC materials.
2. Polymer Resins: Polyimides based on TMA for application in electronics.
3. Coatings: Improved water resistance and durability in paint and surface coatings.
4. MOFs: Flexible frameworks for gas storage, catalysis, and separation technologies.

trimellitic acid is a chemically valuable compound with far-reaching potential in many fields. Its
functionality in polymer and MOF chemistry, along with prospects for environmentally friendly production, highlights its value in pushing materials science as well as green chemistry endeavours forward.

METHODOLOGY

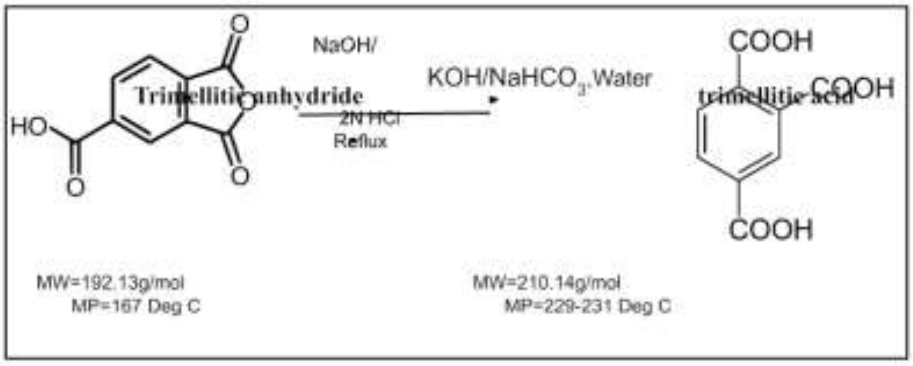
Base hydrolysis using NaOH/ KOH/NaHCO3

1. Requirements :

Chemicals- trimellitic anhydride, Sodium hydroxide/ potassium hydroxide/ sodium bicarbonate distilled water, Hydrochloric acid

Instruments and apparatus- magnetic stirrer, conical flask, beaker, whatman filter paper, Buchner funnel, oven.

2. Reaction scheme :



3. Stoichiometric Table

Sr N	Chemicals	Qty(g)	Mol,wt	Purity	Mole	Mol Eq
1	Trimellitic anhydride	5	192.13	99	0.026	1
2	$NaHCO_3$	7.651	84	98	0.091	3.5
3.	KOH	6.7903	74.55	98	0.091	3.5
4.	$NaHCO_3$	7.651	84	98	0.091	3.5
3	Water	18.737	18	99	1.040	40
4	2N HCl/7.3% HCl	46.843	36.5	7.3	0.093	3.6

4. **Procedure :**

1. Assemble the reaction assembly with Single neck 250ml RBF with vertical condenser with chilled water circular.
2. Weigh accurately 5g, 0.0260 mole of Trimellitic anhydride and poured into a dry round bottom flask flask.
3. Weigh accurately 3.74g, 0.09 mole of sodium hydroxide or 6.79g, 0.09 mole of potassium hydroxide or 7.65 g, 0.09 mole of sodium bicarbonate and 18.73 ml distilled water into the reaction mass.
4. Heat the reaction mass at 80-90°C in a water bath and keep stirring with a magnetic stirrer for about 35-45 min.
5. Cool the reaction mass at ambient temperature (20-25 °C) and add 2N HCl into the reaction mass.
6. Adjust the pH of reaction mass below 7(acidic condition.)
7. Cool the reaction mass at 0-5 °C and observe the Crystallization of the product , continue the stirring for 3-4hr for complete Crystallization.
8. Filter the product through whatman-41 (Pore size ~20) filter paper using Buchner funnel.
9. Isolated Wet cake is transferred to the dryer in a glass petri dish with the help of spatula.
10. Dry the product in the air oven at 110 °C till constant weight of the product is obtained.
11. The final Product is white Crystalline Powder.

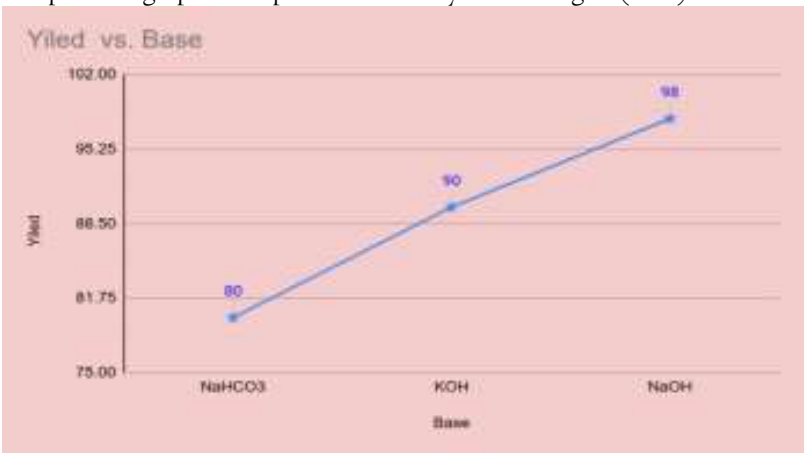
5. **Results and Conclusion :**

parameter	Value
Theoretical Yield (g)	5.469
Isolated Dry Qty(g) by NaOH	5.350
Isolated Dry Qty(g) by(KOH)	4.923
Isolated Dry Qty(g) by($NaHCO_3$)	4.377
Purity % (by HPLC) (for NaOH)	98.58%
Practical Yield (%)	97.830(by NaOH) 90.021(by KOH) 80.037(by $NaHCO_3$)

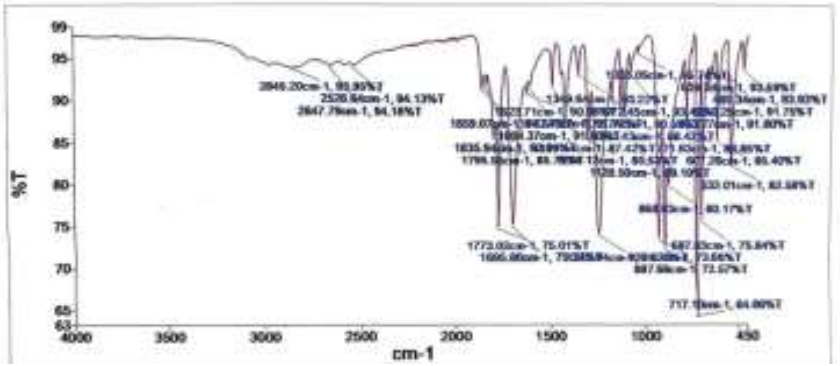
6. Conclusion:

Hydrolysis of Trimellitic anhydride in presence of strong base (NaOH) produces ~98% yield of TMA with purity NLT 98% (by HPLC) and confirmed by IR spectrum and mass analysis.

Table : Comparative graphical representation of yield vs reagent(base)



Results :



The trimellitic acid that was created went through a systematic characterization utilizing a multi-technique analytical method. Fourier-transform infrared spectroscopy (FT-IR) confirms the presence of characteristic carboxylic acid functional groups, as evidenced by absorption bands located at ~2500-3300 cm^{-1} (O-H stretch) and 1680-1740 cm^{-1} (C=O stretch)[fig.1]. High-performance liquid chromatography (HPLC) with ultraviolet (UV) detection (205-232 nm) demonstrated the effective separation and high purity (>98%) of the target compound relative to the retention times of trimellitic acid.

The HPLC method separation had no interferences of the anhydride derivatives to demonstrate specificity analytically[fig.2]. Liquid chromatography-mass spectrometry (LC-MS) was successful in confirming the compound's molecular identification via exact mass (m/z 210 for [M-H]-)[fig.3] and also by fragmentation pattern, which confirmed the tricarboxylic acid structure. The identification was important because the LC-MS effectively differentiated between trimellitic acid and potential anhydride impurities by indicating variation in the mass spectral signal. Further characterization with X-ray diffraction (XRD) demonstrated that the compound formed a crystalline structure consistent with orthorhombic symmetry and demonstrated characteristic peaks of $2\theta = 15.8°$, 25.3°, and 28.7° consistent with known crystal lattice parameters for anhydrate trimellitic acid. The sharp peaks of the diffraction patterns also indicated high crystallinity and high phase purity. The unit cell simple cubic dimension computations also were consistent with literature values (a = 7.42 Å, b = 10.55 Å, c = 9.87 Å)[fig.4].

Fig.1 FT-IR Spectrum

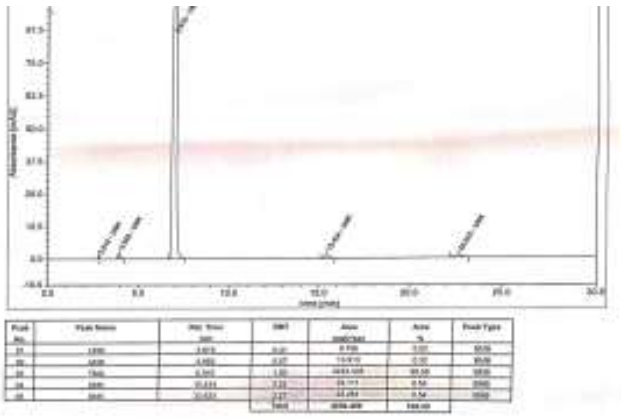


Fig.2 HPLC Chromatogram

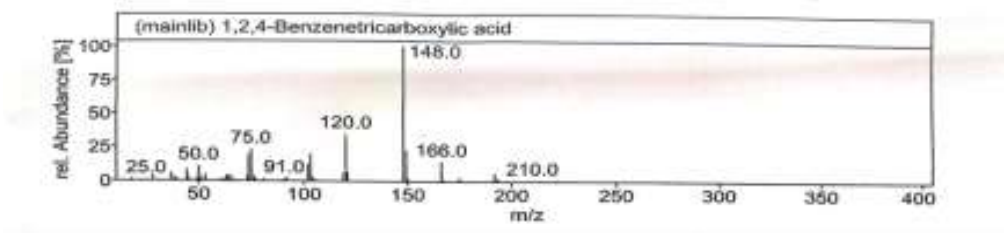


Fig.3 LC-MS

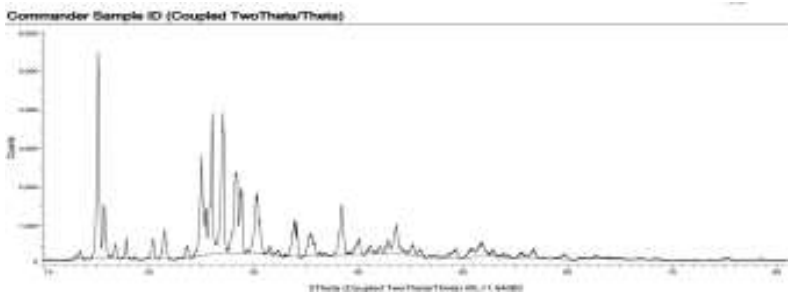


Fig.4 XRD

Conclusion

This study successfully synthesized trimellitic acid through the base-catalyzed hydrolysis of trimellitic anhydride. The experimental procedures, including varying base catalysts, temperatures, and reaction times, have provided valuable insights in optimizing the TMA production process. Further research should focus on refining these methodologies, exploring novel catalysts, and implementing green chemistry principles to enhance efficiency and sustainability. Future work could explore hybrid materials combining TMA-based MOFs with other functional components to enhance performance further. Ultimately, this work helps bridge current research gaps by offering innovative solutions for synthesizing trimellitic acid efficiently while highlighting its untapped

potential in diverse industries. This comprehensive approach will not only enhance economic viability but also contribute towards greener chemical production methodologies essential for future sustainability goals.

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“A comparative study of rice cultivation, cereal cultivation, pulse cultivation, as well as fruit cultivation and flower cultivation in Vikramgad taluka.”

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Abstract:

Rice farming is done on a large scale in Vikramgad taluka. Agriculture is the main occupation of the people here. The people of Vikramgad taluka have a large economic base from agriculture. Various crops are grown in Kharif, Rabi and Zaid seasons in Vikramgad taluka. Rice is the main crop in Kharif season. During the Rabi season, gram, tur and other pulses are grown, while during the Zaid season, vegetables, flowers and fruits are grown. The rice variety 'Wada Kolam' from Vikramgad taluka is famous not only in Maharashtra but also all over India. There is a huge demand for Wada Kolam rice. This rice is exported to other states in large quantities from Vikramgad taluka. After the rice harvest, crops like gram and tur are grown in the Rabi season because the moisture and cool weather they require are available in this season, while various fruits and flowers are grown in the Zaid season. Mango and Chiku fruits from here are in great demand across India. Mogra flowers are also produced in large quantities here. These flowers are in great demand in cities like Mumbai, Pune and Nashik. Although the rainfall in Vikramgad taluka is high, due to water shortage in summer, double sowing is done in very small quantities. Flower cultivation is done on a large scale in Vikramgad taluka. The farmers here are getting huge financial benefits due to flower cultivation and flower production. In particular, the flower Mogra is produced in large quantities. Along with Mogra, flowers like Sonchafa and Rose are also produced in large quantities. There is a large market for these flowers too. Sunflower and Mogra are also cultivated in some places in Vikramgad taluka.

The climate of Vikramgad taluka is very favorable for flower farming. Therefore, there is a large scope for flower farming in this taluka. However, there has not been enough progress in flower farming. The agriculture department should pay special attention to the betterment of agriculture here.

Special efforts should be made to increase flower and fruit cultivation. Agricultural fairs should be organized to guide farmers about agriculture. The vagaries of nature, the uncertain amount of rainfall, the increasing temperature, and the crisis of crop diseases have put agriculture in trouble here.

Keywords: *Rice farming, Flower farming, Fruit farming, Kharif season, Rabi season*

Introduction:

Vikramgad taluka is one of the eight talukas of Palghar district. This taluka is located in the middle of Palghar district. Vikramgad taluka is a tribal-dominated taluka. Tribal tribes like Warli, Katkari, Konkana, Thakur, Mahadev Koli and Malhar Koli etc. live in this taluka. Most of

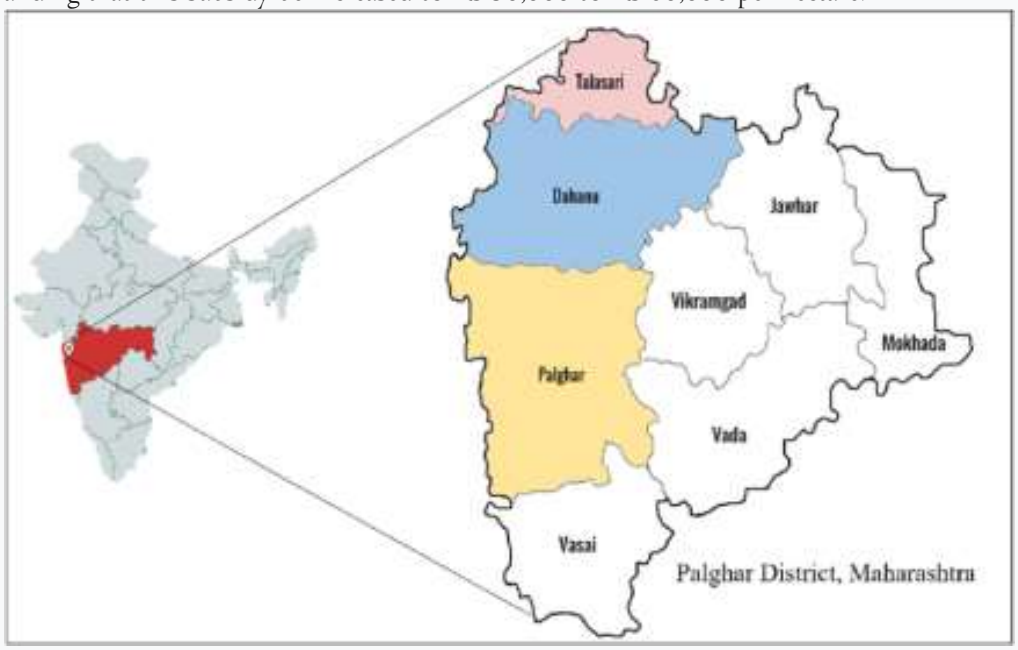
this taluka is surrounded by dense forests. A large part of Vikramgad taluka is covered with forest. The average rainfall here is 250 cm to 300 cm. Of course, this rainfall is very high. The rainfall is very high in the four months of the monsoon season, while the rainfall is very low in the other months. Agriculture is the main occupation of the people of Vikramgad taluka. Most of the people of Vikramgad taluka are engaged in agriculture. The main crop of the people is rice. A huge production of rice is done in this taluka. Along with rice, gram, tur, moong, urad, khurasani, groundnut, sesame, rabi sesame, vegetables, orchards and flower cultivation are done on a large scale in Vikramgad taluka.



Vikramgad Taluka, Source:Google Maps

Flower farming is done on a large scale in Vikramgad taluka, especially the production of Mogra flower is done on a large scale in Vikramgad taluka. Along with grain crops, the farmers are getting financial benefits. Also, by abandoning traditional agriculture and turning to flower farming, the farmers are also getting financial benefits to a large extent. Mogra flowers from Vikramgad taluka are sent for sale in the cities of Mumbai, Pune and Nashik. These flowers are also in great demand in the above cities. The specialty of Mogra flower is that its production can be taken for about eight months. Today, Vikramgad taluka is famous not only in Palghar district but also in Maharashtra and India for Mogra cultivation. Mogra crop has been cultivated on a large scale in the villages of Ughanipada, Sakhra, Mann, Pochada, Krunjeh and Khand. Along with Mogra flower, many farmers have also cultivated Rose flower. Farmers in Vasuri, Wakdupada, Umbarpada and Hatane areas have cultivated Rose flower on a large scale. Also, farmers in Deharja and Onde villages have cultivated large quantities of Sonchafa and Mogra flowers. Mogra, rose, and Sonchafa flowers from Vikramgad taluka are sent for sale in the Mumbai market. There is also a huge demand for these flowers from Pune and Nashik districts. Farmers in Vikramagad taluka are earning good money from this flower cultivation. They are making a lot of money. In

recent times, due to good communication facilities, it has been possible for farmers to send their farm produce to nearby markets. Marigold flowers are also cultivated in a small quantity in Vikramagad taluka. Farmers are being given information about planting flowers through the Agriculture Department and Panchayat Samiti of Vikramagad taluka. Farmers are also being encouraged to plant flowers. Mogra flowers are generally getting a price of Rs. 800 to Rs. 1000 per kg. Also, for plucking Mogra flowers, the laborer is generally getting a price of Rs. 40 to Rs. 60 per kg. Therefore, along with the farmers, the laborer is also happy. When some farmers were asked about flower cultivation, they said that they are getting very little subsidy from the government for flower cultivation. The government should increase this subsidy and schemes like drip irrigation scheme and frost irrigation scheme for floriculture should also be implemented. Farmers here say that the government should provide subsidies for this. Currently, the farmers here are in distress due to the huge increase in the prices of seedlings from nurseries, fertilizers, expensive medicines, and spraying machines for flower farming. The government is providing a subsidy of about Rs 23,500 for drip irrigation for flower farming. The farmers here are demanding that this subsidy be increased to Rs 50,000 to Rs 60,000 per hectare.



Location Map of Vikramgad

Marigold flowers have been planted in about 30 acres in the village of Onde. Three to four tons of marigold flowers are being produced from this farm every day. Marigold flowers have a good price in the market in Mumbai. These flowers are sold at a minimum price of Rs 30 to 35 per kg and a maximum price of Rs 50 to 60 per kg. Marigold cultivation does not cost much. Marigold flowers are in great demand for ceremonies like Dussehra, Deepawali, and weddings. In the local market of Vikramagad, marigold flowers are also getting a price of Rs 30 to 40 per kg for sale of flower garlands and retail flowers. Along with rice farming and floriculture, orchards have also started being produced on a large scale in Vikramagad taluka. Especially, crops like chiku, mango, guava, lemon, banana (cardamom), coconut etc. have started being produced in Vikramagad. The government has implemented many schemes for orchard cultivation. The cultivation of watermelon has started in large quantities in Vikramgad taluka. The demand for watermelon is high in summer. Also, the farmers here are getting good profit from the sale of watermelon. In summer, shops are available in the market of Vikramgad for selling watermelon. Many shops selling watermelon have been started on both sides of the roads of Vikramgad Wada,

Vikramgad Palghar, Vikramgad Jawhar, Vikramgad Dahanu. Due to this, the farmers are getting a lot of money.

Prof. Dinesh Nahire, Head, of the Department of Geography, College of Arts, Commerce and Science, Onde, Vikramgarh, prepared a survey report on agriculture in some villages of Vikramgarh taluka. A questionnaire on agriculture was prepared and about 150 farmers of Vikramgarh taluka were involved. In this questionnaire,

- What is your name?
- How many members are there in your family?
- How many female members are there?
- How many male members are there?
- How many elders are there in the house?
- How many children are there?
- Do they go to school?
- If so, in which grade?
- Do you currently have a farm?
- How many acres of land are there?
- What crops do you grow in the field?
- Do you use fertilizers?
- If so, which ones?
- Do you farm organically?
- Do you use mechanization for farming?
- What implements do you use in the field for farming?
- What machinery do you use for farming? For example, plow, seed machine, irrigation system, tractor, etc.
- What problems do you face as a farmer?
- How do you solve them?
- Do you do animal husbandry along with farming?
- If you do animal husbandry, what livestock have you raised? For example, chickens, goats, sheep, cows, buffaloes, bulls, etc.
- Do you send your farm produce to the market?
- Do you sell it to other people?
- How do you market your farm produce? Are you a member of a farmers' organization?
- Or are you a member of a cooperative?
- Do you have any Fair Trade, Non-GMO, Organic or other certifications for your farm?
- Do you have any plans to increase your farm production in the future?
- Do you want to buy more farms?
- What methods do you follow in your farm?
- Do you farm sustainably?
- Do you use technology or digital tools to manage your farm?
- Do you use water conservation, crop rotation, compost fertilizer, etc. in your farm?
- Do you also use some environmental conservation methods?
- Have you taken any measures to modernize your farm?
- Do you want to improve agriculture so that you can flourish in the agricultural industry?
- What do you find challenging or what are the main difficulties you face while farming?
- Have you ever participated in an agricultural workshop?
- Have you visited an agricultural exhibition?
- Has an agricultural exhibition been organized by the Agriculture Department in your taluka?

- If not, do you think that the Agriculture Department should organize such an agricultural exhibition? How has farming affected your family?
- What is the main impact of farming on your life?
- How much annual income do you get from farming?
- Is this income sufficient for your family?
- Do you still need financial help to run your family?
- Which bank are you a member of?
- Have you taken a loan from a bank for farming?

Through such a questionnaire, we tried to go to the farmers of Vikramagad taluka and get information about their farming. With the help of students, we tried to collect this information and study farming life. From it, we got very useful information about farming and the life of farmers. Based on that information, a survey report was prepared. The students got invaluable cooperation in this work. They were able to get first-hand information about the problems of farmers and the difficulties they face. The students themselves went to the farmers' homes and surveyed them and obtained information. To collect this information, the primary information (questionnaire) method was adopted. Also, to get secondary information, we contacted the Agriculture Department, Agricultural Officer Vikramagad taluka and asked the Agricultural Officer about what crop production targets were set in Vikramagad taluka for the years 2023-24, 2024-25 and 2025-26. In this, information was obtained about the total area under cultivation of cereal crops in Vikramagad taluka in the year 2023-2024, the total production of cereal crops, and agricultural productivity. Information was obtained about rice, jowar, bajra, gram, maize and other cereals among the cereal crops. From this information, it was understood that the highest production and the largest area under cultivation among the cereal crops is rice. It was also understood that rice is the main crop in Vikramagad taluka. The total area under cultivation under rice crop in 2023-2024 was 7164 hectares, while the area under jowar was 0 hectares. The area under cultivation under bajra was also 0 hectares. Also, the area under cultivation of maize was zero hectares. From this, it was understood that jowar, bajra and maize crops are not grown in Vikramagad taluka. After rice, the cereal crop of gram is grown. The total area under gram was 976 hectares while the area under other cereal crops was 135.53 hectares. In 2023-2024, the production of rice was 14686.2 tons while the productivity of rice was 2050 kg per hectare.

In the year 2024 25, the area under rice cultivation was 7163 hectares, while the production of rice was 15106.47 tons, while the productivity of rice was 2109 kg per hectare. The area under gram was 974 hectares, while the production was 15106.47 tons, while the productivity was 652 kg per hectare. The area under other cereal crops was 135 hectares, while the production was 99.90 tons, while the productivity was 740 kg per hectare. The Agriculture Department has set a target of 7163 hectares under rice cultivation for the year 2025-2026, while the production was 16618.16. Productivity was set at 2320 kg per hectare. Also, 974 hectares of area was determined for the gram crop, the production was determined as 698.36 tons, while the productivity was determined as 717 kg per hectare. The target area under cultivation of other cereal crops was determined as 135 hectares. While the production was determined as 109.89 tons, while the productivity was determined as 2106.67 kg per hectare.

In the year 2023-2024, the total area under cereal crops was 8275.53 hectares, while the total production of cereal crops was 15315.72 tons, while the productivity was 1850.72 kg per hectare. In the year 2024-2025, the total area under cereal crops was 8272 hectares, while the total production of cereal crops was 15841.72 tons. While the productivity was 1915.10 kg per hectare. In the year 2025-2026, the total area under cereal crops was set at 8272 hectares. Production was set at 17426.41 tons, while the productivity was set at 2106.67 kg per hectare.

The information on the area under the crop of Tur, Moong, Urid and other pulses and their production and productivity in the year 2023-2024 is as follows: This year, the area under Tur was 199.92 hectares, while the production of Tur was 126.95 tons, while the productivity of Tur was 635 kg per hectare. The area under the cultivation of Urid was 260.48 hectares, while the production was 91.69 tons, while the productivity was 352 kg per hectare. The area under the cultivation of Moong was zero hectares. While the production was also zero. That is, there was no area under the cultivation of this crop. The area under the cultivation of other pulses was two hectares, while the production was 0.70 tons. While the productivity was 350 kg per hectare. In this year, the total area under the cultivation of pulses was 426.40. Production was 219.34 tonnes and productivity was 474.35 kg per hectare.

In the year 2024-2025, the area under Tur crop was 230 hectares. The production was 149.50 tons and the productivity was 650 kg per hectare. This year too, the area under Moong crop was 0 hectares, which means that Moong crop was not produced in Vikramgad taluka this year too. The area under Urid crop was 263 hectares. The production was 94.68 tons and the productivity was 360 kg per hectare. The area under other pulses was 3.40 hectares and the production was 1.19 tons and the productivity was 350 kg per hectare. In the year 2025-2026, the area under Tur crop was 230 hectares and the production was 164.45 tons and the productivity was 715 kg per hectare. This year, the area under urad crop was determined to be 263 hectares. The production was determined to be 104.15 tons and the productivity was determined to be 396 kg per hectare. The area under other cereals was determined to be 3.40 hectares, while the production was determined to be 1.31 and the productivity was determined to be 385 kg per hectare. Thus, the total area under cereals was determined to be 496.40. The production was determined to be 269.91 tons and the productivity was determined to be 543.73 per hectare. In the same year, the total area under food grains was determined to be 8768.40 hectares, while the production was determined to be 17696.32 tons and the productivity was determined to be 2018.19 kg per hectare.

The information on groundnut, sesame, khurasani, sunflower, soybean and other milled grains in the year 2023-2024 is as follows: This year, the area under groundnut crop was 7 hectares, while the production of groundnut was 8.72 tons, while the productivity of groundnut crop was 1245 kg per hectare. In the same year, the area under sesame cultivation was 6 hectares, while the production was 2.64 tons. The productivity was 440 kg per hectare. The area under khurasani cultivation was 16 hectares, while the production was 7.68 tons, while the productivity was 480 kg per hectare. This year, sunflower and soybean crops were not cultivated in Vikramgad taluka. This year, the total area under crushed grains cultivation was 29 hectares, the production was 19.04 tons, and the productivity was 656.38 kg per hectare. In the year 2024-2025, the area under cultivation was not available. The area under cultivation of sesame was 6.20 hectares, and its production was 2.73 tons, and the productivity of sesame was 440 kg per hectare. The total area under crushed grains cultivation was 21.40 hectares, and the production was 10.02 tons. The productivity was 468.41 per hectare. In the year 2025-2026, the area under cultivation of this crop was 5 hectares, and if the production is fixed at 6.25 tons, the productivity will be 1250 kg per hectare. If the area under sesame is determined to be 6.20 hectares, then the production of sesame is determined to be 3 tons, then the productivity is determined to be 484 kg per hectare. If the area under the cultivation of khurasani is determined to be 15.20 hectares, then the production is determined to be 8.03 tons. The productivity is determined to be 528 kg per hectare. If the area under the cultivation of total milled grain is determined to be 26.40 hectares, then the production is determined to be 17.28 tons, then the productivity is determined to be 654.41 kg per hectare.

In the year 2023-2024, the area under cultivation of Rabi sesame was 92.35 hectares, the production was 40.63 tons, and the productivity was 440 kg per hectare. The area under

cultivation of Rabi sunflower was 7 hectares, the production was 10.50 lakh tons, and the productivity was 1500 kg per hectare.

Conclusion and Suggestions:

 The climate in Vikramagad taluka is very conducive to rice cultivation. But the efforts that should be made to increase the yield of rice are not being done as much as they should be.
 Agricultural exhibitions are held very rarely, their number should be increased.
 Farmers should be guided from time to time.
 Irrigation facilities should be provided for agriculture in Vikramagad taluka.
 Farmers should be guided from time to time for flower and fruit production.
 Guaranteed prices should be provided for the agricultural produce of the farmers.
 Fraud of farmers by brokers and agents should be stopped.

S. N.	Crop Name	2023-24 Final			2024-25 Forecast			2025-26 Target		
		Area	Production	Productivity	Area	Production	Productivity	Area	Production	Productivity
1	Rice	7164.00	14686.2	2050	7163.00	15106.77	2109	7163.0	16618.16	2320
2	Jowar	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	Bajara	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	नाचणी	976.00	629.52	645	974	635.05	652	974.00	698.36	717
5	Maize	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6	इतरतृणधान्य	135.53	0.00	0.00	135.00	99.90	740	135.00	109.89	814
एकूण		8275.5	15315.	1850.7	8272.0	15841.	1915.1	8272.0	17426.	2106.6

तृणधान्य		3	72	2	0	72	0	0	41	7
7	तूर	199.92	126.95	635	230.0	149.5	650	230.0	164.45	715
8	मुग	0.00	0.00	642	0.00	0.00	0.00	0.00	0.00	0.00
9	उडीद	260.48	91.69	352	263.00	94.68	360	263.00	104.15	396
10	इतर कडधान्य	2.00	0.70	350	3.40	1.19	350	3.40	1.31	385
एकूण कडधान्य		462.40	219.34	474.35	496.40	245.37	494.30	496.40	269.91	543.73
11	भुईमुग	7.00	8.72	1245	0.00	0.00	0	5.00	6.25	1250
12	तीळ	6.00	2.64	440	6.20	2.73	440	6.20	3.00	484
13	खुरासणी	16	7.68	480	15.20	7.30	480	15.20	8.03	528
14	सुर्यफुल	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	सोयाबीन	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1	इतर	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

6	गळीत धान्य	0	0	0	0	0	0	0	0	0
एकूण गळीतधान्य		29.00	19.04	656.38	21.40	10.02	468.41	26.40	17.28	654.41
17	उस	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
18	कापूस	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
एकूण खरीप		8759.93			8789.80			8856.00		

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Financial Literacy in India: Building the Foundation for Sustainable Growth

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Abstract

Financial literacy programs in India have shown positive results, with initiatives such as the Financial Education Program for Adults and the "RBI Kehta Hai" campaign helping people understand financial concepts and make informed decisions, but there is still a long way to go to achieve nationwide financial literacy.

Introduction

India's financial literacy rate stands at just 27%. This means four out of five Indians find it hard to make sound financial decisions. These numbers paint a worrying picture of our nation's economic future. The situation becomes more challenging in rural India. Bank accounts exist for only 35% of the rural population, while mobile banking usage remains at a low 7%. The knowledge gap doesn't just stop at personal finances. Research shows that financial literacy plays a vital role in achieving seven of the 17 Sustainable Development Goals, including poverty elimination and gender equality. The Reserve Bank of India's warning adds another layer of concern - climate-related challenges could put 4.5% of our country's GDP at risk by 2030. This makes informed financial decisions more important than ever.

This piece dives into India's current financial literacy landscape and its role in sustainable development. We'll also analyze the groundbreaking initiatives that are reshaping our nation's financial education. The focus will be on how digital transformation and government programs help bridge this significant knowledge gap.

Current State of Financial Literacy Rate in India

Financial literacy in India shows a mixed picture that varies by region, demographics, and economic factors. Studies and surveys have given us a clear view of Indians' financial awareness. This knowledge points to key areas we need to address for environmentally responsible economic growth.

Statistical Overview of 2023-2025 Progress

The Reserve Bank of India's survey from June 2023 showed financial literacy at 62.6%, measured through knowledge, behavior, and attitude parameters [1]. In spite of that, other complete national assessments tell a different story. The National Center for Financial Education found that all but one of these Indians lack proper financial knowledge [2]. Only 16.7% of students show a simple understanding of money management [3].

The RBI managed to keep its promise of promoting financial awareness through yearly programs like the Financial Literacy Week (FLW). The FLW 2025 ran from February 24-28 with "Financial

Literacy - Women's Prosperity" as its theme [4]. This campaign zeroed in on three vital areas: financial planning, saving and risk management, and credit access to stimulate growth [4]. Through collaboration with major financial institutions like NABARD and commercial banks, the campaign used multimedia and took a social-first approach to reach more people [5].

The challenges remain substantial. Reports show different financial literacy rates—some put it at 35%, which sits slightly above the world average of 33% [6]. These varying numbers show how hard it is to measure financial literacy with standard metrics and why we need consistent ways to assess it.

Urban vs. Rural Financial Literacy Gap

In stark comparison to what many believe, the RBI's pan-India 'Financial Literacy and Inclusion survey' found that urban and rural populations know about digital banking equally well. Both groups scored 11.7 on a scale of 21 [7]. Zone-wise numbers show little difference: North zone (11.5 for both rural and urban), East zone (12.1 for both), Central zone (12.5 urban, 12.1 rural), West zone (12.6 urban, 12.5 rural) [7]. The South zone stands out with urban areas at 11.2 and rural areas at 10.3 [7].

Yet other studies reveal an ongoing rural-urban divide. Data shows 33% of rural and 29% of urban populations don't have simple financial tools like bank accounts, credit/debit cards, or e-wallets [8]. Some regions face bigger challenges—states like Assam, Bihar, Manipur, Nagaland, and Uttar Pradesh consistently score below national averages in financial literacy [8].

Some regions shine brighter than others. Chandigarh, Goa, and Himachal Pradesh lead in financial literacy across both rural and urban areas [8]. Chandigarh stands out with over 90% of its urban population showing high financial literacy [8]. These regional differences show why we need targeted solutions based on each area's unique challenges.

Demographic Analysis: Age, Gender, and Income Factors

The gender gap remains a big worry in India's financial literacy landscape. The 2020-21 National Center for Financial Education survey found only 21% of women financially literate compared to 27% of men [9]. This gap affects financial inclusion deeply—only 33% of women have active bank accounts while 45% of men do [9]. Women's lower wages make things worse, as they earn about 34% less than men for the same work [9].

Age plays a big role in financial awareness. Middle-aged adults show the highest levels of financial literacy, while young adults and elderly people lag behind [10]. To cite an instance, people aged 41-50 handle financial documents better than other age groups [10].

Income and education relate closely to financial literacy. People become more financially literate as their education level rises [8]. The same pattern shows up across income levels [8]. The type of job matters too—people with regular jobs and steady income usually know more about finance than self-employed or casual workers [8].

These complex demographic factors mean we need different approaches to financial education. Programs must meet each group's specific needs rather than using one solution for everyone to bridge these gaps effectively.

Financial Literacy as a Catalyst for Sustainable Development

Financial literacy does more than teach people how to manage money. It's a key driver of sustainable development in India, affecting economic, social, and environmental progress. When

people understand finance better, both individual prosperity and national development move forward together.

Connecting Financial Knowledge to SDG Achievement

Financial literacy directly helps achieve multiple Sustainable Development Goals (SDGs) and creates paths to inclusive growth. Research shows that better financial knowledge plays a vital role in sustainable development by speeding up financial inclusion [11]. People who understand finance can participate better in formal economic systems, which helps reduce poverty and inequality.

Financial literacy supports these key SDGs:

- No Poverty (SDG 1): Microfinance institutions give low-interest loans to financially educated people, which helps them manage risks and escape extreme poverty [12]
- Zero Hunger (SDG 2): Farmers who understand finance can get agricultural loans more easily, which boosts food production and security [12]
- Gender Equality (SDG 5): Women with financial knowledge make better economic decisions, which improves family welfare and promotes equal decision-making [13]

Research shows that when women control financial resources through better literacy, they create positive changes in their homes and communities [13]. Financial literacy acts as a powerful tool to achieve sustainable development goals. Studies confirm "encouraging, progressive, and highly positive effects of financial inclusion on sustainable development through financial literacy" [11].

Economic Stability Through Informed Financial Decisions

People who understand finance help create a stable economy by making smarter money choices. They build resilience at both personal and system-wide levels. Those with financial knowledge handle money challenges better and feel less stressed about their finances [14]. They can plan for retirement and make better long-term decisions [14].

Poor financial literacy leads to lower savings and investment rates, which limits economic growth [2]. But when people understand finance better, they use formal banking systems more often and invest more wisely. This creates a ripple effect that reduces financial hardships and defaults, making society more prosperous [14].

Environmental Impact of Financially Conscious Investments

Financial literacy now plays a crucial role in environmental sustainability. Green finance products help connect money with environmental goals [3]. Indians who understand finance can better participate in sustainable investments.

India needs ₹15,000-20,000 crores of annual Foreign Direct Investment just in renewable energy [6]. The government now allows 100% FDI in renewable power generation, with projects worth ₹16621.26 billion in progress [6]. People who understand finance can invest in these green projects and support climate resilience.

ESG investing (Environmental, Social, and Governance) gives another way to make finance work for the environment. This method puts money into companies that balance ethics with profits [15]. You can invest in sustainable projects no matter your income level, from small green deposits to large ESG portfolios.

Understanding climate risk as financial risk has become crucial in sustainable investing [16]. India's green finance hit record levels in 2021/22, but we still need to triple these investments to

meet climate targets [17]. Better financial education about environmental aspects helps people understand climate-related financial risks and support a low-carbon economy through smart investments.

Digital Transformation of Financial Education in India

The digital revolution has changed how Indians learn about finance. Technology has created new ways to access financial knowledge. Research shows 55% of Indians want to learn about managing money [18]. Digital tools have become powerful ways to meet this need as more people across the country get smartphones.

Mobile Apps Revolutionizing Financial Learning

Indians who want to improve their money management skills now turn to financial literacy apps. These apps provide interactive learning that traditional education cannot match. Fortune City stands out as a popular choice. Users can build a virtual city while they track expenses and set budget goals [19]. This makes learning about money fun instead of scary.

Rooster Money helps younger users learn simple money concepts through allowance tracking, chore management, and savings goals [7]. Savings Spree uses a game show format to teach children about saving, spending, donating, and investing [7]. These tools help kids develop good money habits early.

Investmate helps adults with straightforward financial courses about stocks, commodities, and trading strategies [19]. A 15-year-old from Gurgaon created DhanDanaDan in 2022. This free Hindi-language app serves tier 2 and 3 cities with animated videos that explain simple financial planning [20]. Local content like this matters because only 27% of India's population understands finance, with even lower rates in smaller cities [20].

AI-Powered Financial Advisory Platforms

AI has changed financial advisory services in India. The robo-advisory market should grow 33.4% each year from 2023-2030. Revenue could reach INR 181,839.87 million by 2030 [10]. Platforms like Zerodha's Nudge and Groww give automated investment guidance that costs much less than traditional advisors [10].

These AI systems quickly process big amounts of data and offer tailored recommendations based on each person's investment goals and risk tolerance [10]. Machine learning and predictive analytics help investors make evidence-based decisions [10]. Wealth management services used to target only rich individuals. Now AI has made these resources available to regular investors [10].

Jarvis, Finbingo, and Mool are gaining popularity in India's robo-advisory space [21]. WealthAI connects real-life events to relevant investment advice through cloud-deployed "advise-the-advisor" platforms [22]. Notwithstanding that, some problems remain—potential algorithmic biases, cybersecurity risks, and incomplete banking infrastructure integration need attention [10].

Digital Payment Systems as Educational Tools

Digital payment systems teach users about simple financial transactions through hands-on experience. UPI has become India's main fast payment system, improving the digital payment experience [23]. On top of that, IMPS, mobile banking, and Aadhaar-enabled payment systems create an environment where people learn finance through daily transactions [24].

The government wants to promote digital transactions. They set a target of 2,500 crore digital transactions in the 2017-18 Union Budget [25]. Common Service Centers (CSCs) support this by

providing digital services to rural citizens [25]. People need better digital financial literacy as they use these payment systems more [24].

Digital financial literacy helps users make safe transactions and protect themselves from phishing, pharming, and spyware [24]. Users also learn about their rights as consumers and what to do if they face fraud [24]. Digital payments make life easier and build a foundation to learn more about finance.

India's financial literacy future looks increasingly digital. Ongoing education, strong security measures, and better infrastructure will drive sustainable growth [9]. A mix of human advisors and AI-powered systems will likely expand investment opportunities and create meaningful connections across India's diverse population [10].

Government Initiatives Shaping Financial Literacy

India's government has worked to strengthen financial literacy through coordinated policies since 2013. Financial institutions and regulatory bodies cooperate to create a population that understands finance and makes smart money decisions.

National Strategy for Financial Education 2020-2025

The Reserve Bank of India launched the National Strategy for Financial Education (NSFE) 2020-2025 in August 2020. This strategy builds on the previous 2013-2018 initiative [8]. The National Center for Financial Education (NCFE) developed it with key stakeholders like RBI, SEBI, IRDAI, and PFRDA under the Technical Group on Financial Inclusion and Financial Literacy [26].

NSFE uses an innovative '5 C' approach:

- Content: Creating financial literacy materials for different groups
- Capacity: Improving expertise of financial education providers
- Community: Building sustainable community-driven financial literacy models
- Communication: Using technology and media to spread awareness
- Collaboration: Coordinating efforts between stakeholders [27]

The strategy focuses on school children, young adults, women, entrepreneurs, MSMEs, senior citizens, and persons with disabilities [27]. NSFE wants to reach 500 million Indians by 2025 to create a financially aware population [28].

RBI's Financial Literacy Programs

RBI runs several meaningful financial education programs. Financial Literacy Week happens each year with specific themes. February 2025's theme "Financial Literacy, Women's Prosperity" highlighted financial planning, saving, risk management, and credit access for growth [29].

RBI has built more than 1,500 Financial Literacy Centers (FLCs) across India, mostly in rural and semi-urban areas [28]. These centers give free advice about managing debt, savings, and investments [28]. The Centers for Financial Literacy (CFL) work at block level through NGOs and sponsor banks to help people aged 18-60 [30].

"RBI Kehta Hai" campaign stands out as another key initiative. This multilingual awareness program teaches safe banking through various media [4]. The Financial Education Program for Adults (FEPA) helps excluded groups like employees, self-help members, farmers, women groups, and MGNREGA cardholders [5].

State-Level Implementation Successes and Challenges

Financial literacy implementation varies across Indian states. Ministry of Finance monitoring shows NCFE conducted 54 financial literacy programs in northeastern states over three years [1]. Participants reported better understanding of financial concepts and fraud protection [1].

Chandigarh, Goa, and Himachal Pradesh lead in financial literacy metrics [31]. Chandigarh shows exceptional results with 90% of its urban population having high financial literacy [31].

Some challenges remain in nationwide implementation. Many people don't know about available resources despite plenty of public materials [32]. The 2017 Pan-India Financial Literacy and Inclusion survey across 29 states and 5 union territories showed uneven progress in knowledge, attitude, and behavior [4].

Experts suggest starting financial education early in schools and colleges [32]. The ongoing mid-term evaluation of NSFE 2020-2025 will show progress, identify gaps, and help improve strategies [33].

Measuring Impact: Beyond Financial Knowledge

Financial literacy programs show their real worth through noticeable changes in how people handle money and make economic choices. These programs go beyond just teaching theory - they change how people deal with money in their daily lives.

Behavioral Changes in Savings and Investment Patterns

Financial education reshapes how Indians handle their money. Studies show that people with financial education invest more often and put in larger amounts. They also spread their investments across different options [11]. People who learn about finance feel more confident when making money decisions and worry less about managing their finances [11].

Research shows a strong link between financial knowledge and saving habits across India [12]. Different groups show varying levels of financial understanding - self-employed and casual workers have moderate levels at 45.6% and 45.2% [12]. Better financial knowledge helps people make smarter investment choices among various options [12].

Reduction in Predatory Lending Victimization

Financial knowledge protects people from unfair lending practices. People who don't understand finance well tend to overspend, rely too much on credit, and pay too many fees. This hurts their ability to build wealth over time [34]. Better financial knowledge leads to smarter borrowing and better debt management [12].

People who understand finance are more likely to negotiate better mortgage terms and find cheaper ways to borrow [12]. Good financial knowledge helps people spot and avoid scams that promise unrealistic returns - protecting their life savings [35]. People who know more about finance usually have the right paperwork and can prove their income when applying for loans [12].

Financial Resilience During Economic Downturns

Financial education builds stronger economies at personal and system levels. The global economy has faced four major recessions since 1950 - in 1975, 1982, 1991, and 2009. These downturns affected many countries at once [36]. India felt these effects strongly because it imports lots of oil, making it sensitive to global oil prices [36].

Recent studies show India's financial system has grown stronger and more diverse. It handled the pandemic well [2]. Tests prove that banks and NBFCs have enough total capital to keep lending

even in tough economic times [2]. People who understand finance help make the system stronger by:

- Keeping their savings during tough times
- Continuing to invest when markets go up and down
- Not selling in panic during market drops

The IMF likes India's financial rules, especially the new bank-style Liquidity Coverage Ratio for big NBFCs [2]. India's insurance sector keeps growing steadily, helped by better rules and digital improvements [2].

Future Roadmap for Financial Literacy in India

India's financial literacy framework needs to advance through education integration, strategic collaborations, and advanced technology by 2030. The path to giving people financial ability must tackle structural challenges while building on current momentum.

Integration with Formal Education Curriculum

The National Education Policy (NEP) is a chance to make financial literacy mandatory in school education. Students should start learning about finance in secondary school and continue through higher education [37]. Australia and Canada's success stories show how compulsory financial literacy in national curricula can work, providing models for India [38]. Financial literacy shouldn't stand alone but should blend with mathematics, social studies, and economics [38].

NCFE's Money Smart School Program encourages schools to introduce financial literacy for students from classes VI to X [3]. This program uses special workbooks that naturally fit with current subjects and builds foundations for financially aware youth [3].

Public-Private Partnership Models

Public-private partnerships help scale financial literacy programs effectively. NITI Aayog promotes PPPs as preferred models for infrastructure projects and social development [6]. These cooperative models share risks between public and private sectors and make projects more sustainable [15]. A groundbreaking initiative emerged when the Investor Education and Protection Fund Authority joined forces with India Post Payments Bank to create "Niveshak Didi." This program runs over 4,000 financial literacy camps led by 40,000 women postal workers [17]. Their grassroots approach brings financial knowledge straight to underserved communities [17].

Technological Innovations on the Horizon

Advanced technology will remain vital to financial education's future. A tech-driven financial system using AI and advanced automation can provide individual-specific, available, and secure financial services [18]. Young digital natives connect well with interactive learning platforms that use engaging short videos and ground simulations [39].

Digital platforms create safe spaces where young learners gain practical financial knowledge without potential risks [39]. The trip toward financial independence now relies more on these digital tools, with guidance from parents, educators, and mentors [39].

Conclusion

Financial literacy is the life-blood of India's green practices for economic growth as we look toward 2025 and beyond. Digital transformation, government initiatives, and mutually beneficial alliances have shown results, yet only 27% of Indians are financially literate.

Chandigarh's success story demonstrates the power of targeted educational programs, with 90% of its urban residents showing high financial literacy. RBI's detailed approach through Financial

Literacy Centers works alongside technological innovations. Mobile apps and AI-powered advisory platforms create new ways for Indians to boost their financial knowledge.

The National Strategy for Financial Education 2020-2025 offers a reliable framework to reach 500 million Indians. Digital payment systems and formal education integration support this ambitious goal that strengthens our nation's financial resilience. Studies show that financially educated citizens choose better investments, stay away from predatory lending, and remain stable during economic downturns.

Building complete financial literacy needs sustained effort from all stakeholders. Government bodies, educational institutions, financial organizations, and citizens must work together. Our focus on digital innovation, curriculum integration, and grassroots education programs will help create a financially capable India ready to tackle future economic challenges.

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