ISBN: 978-81-992068-8-5

Matter & Motion

EXPLORATIONS IN PHYSICAL AND CHEMICAL SCIENCE

VOLUME I

Editors:

Dr. Shakuntala A. Shinde
Dr. Kushal R. Lanjewar
Dr. Rajanish Saikia
Mr. Swagatam Deva Nath

Bhumi Publishing, India

First Edition: August 2025

Matter & Motion: Explorations in Physical and Chemical Science Volume I

(ISBN: 978-81-992068-8-5)

DOI: https://doi.org/10.5281/zenodo.17038395

Editors

Dr. Shakuntala A. Shinde

Department of Physics,

SharadChandra Arts, Commerce and

Science College, Naigaon, Dist-Nanded, M.S.

Dr. Kushal R. Lanjewar

Department of Chemistry,

Mohsinbhai Zaweri Mahavidyalaya,

Desaiganj (Wadsa), Dist. Gadchiroli, M.S.

Dr. Rajanish Saikia

Department of Physics,

Nanda Nath Saikia College,

Titabar, Assam

Mr. Swagatam Deva Nath

Department of Physics,

Nanda Nath Saikia College,

Titabar, Assam

Bhumi Publishing

August 2025

Title: Matter & Motion: Explorations in Physical and Chemical Science Volume I

Editors: Dr. Shakuntala A. Shinde, Dr. Kushal R. Lanjewar,
Dr. Rajanish Saikia, Mr. Swagatam Deva Nath

First Edition: August 2025

ISBN: 978-81-992068-8-5

DOI: https://doi.org/10.5281/zenodo.17038395

Published by Bhumi Publishing,

a publishing unit of Bhumi Gramin Vikas Sanstha

Bhumi Publishing

Nigave Khalasa, Tal – Karveer, Dist – Kolhapur, Maharashtra, INDIA 416 207

E-mail: bhumipublishing@gmail.com

PREFACE

Science is the art of understanding nature through observation, reasoning, and experimentation. Among its vast domains, physical and chemical sciences form the very foundation of how we comprehend the universe—from the tiniest atoms to the grandest galaxies. This book, Matter & Motion: Explorations in Physical and Chemical Science, is a journey into the fundamental principles that govern the behavior of matter and the forces that drive motion and change.

The title reflects the dual essence of science explored within these pages. "Matter" encompasses the structures, properties, and transformations that define chemistry, while "Motion" captures the dynamism central to physics—movement, energy, force, and interaction. Together, these themes weave a rich narrative of the natural world and its intricate mechanics.

Designed for students, educators, and curious minds alike, this book presents complex ideas in an accessible, inquiry-based format. It encourages readers not only to learn but to explore, question, and connect scientific phenomena with real-world applications. Each chapter builds on core concepts, supported by illustrative examples, simple experiments, historical insights, and problem-solving opportunities that foster critical thinking.

In an age where science and technology shape every facet of human life, scientific literacy is not merely an academic goal but a societal need. Whether it is understanding climate change, navigating energy solutions, or exploring the possibilities of space, the principles of matter and motion remain central.

We hope this book ignites curiosity, nurtures understanding, and inspires future explorations. As you turn the pages, may you see not just equations and reactions, but the elegant patterns of nature—unfolding through the lens of physical and chemical science.

- Editors

TABLE OF CONTENT

REVOLUTIONIZING CHEMICAL PROCESSES: SUSTAINABLE SOLVENTS AND CATALYSTS FOR A CLEANER ENVIRONMENT

Chencharam Tulasi*[1], M. Vijaya Bhargavi[1] and M. Sumakanth[2]
[1]Department of Pharmaceutical Chemistry,
RBVRR Women's College of Pharmacy, Narayanguda, Hyderabad, 500027
[2]RBVRR Women's College of Pharmacy,
Osmania University, Hyderabad, 500027, India
*Corresponding author E-mail: chencharamtulasi2001@gmail.com

Abstract:

Solvents and catalysts play an important role in the context of green chemistry, which seeks to reduce the environmental impact and improve efficiency in chemical processes. The chapter discusses various minimization strategies imparted by sustainable solvents and novel catalysts in reducing waste, energy usage, and hazardous by-products. Various solvent systems that meet requirements for greener reaction environments, with a strong focus on bio-based and ionic solvents, are discussed. In addition, the advancement of catalytic methods — including heterogeneous, enzymatic and photocatalytic technologies for selective transformations with lower environmental footprints are critically examined. Using case studies and comparative analysis, we demonstrate the utility of these strategies across a range of applications, from pharmaceuticals to materials synthesis. This review brings home the point that solvent and catalyst developments must be viewed in the larger landscape of sustainable chemistry, providing valuable guidance to the researcher or industrialist working on designing an environment friendly chemical process.

Keywords: Green Chemistry, Sustainable Solvents, Bio-Based Solvents, Heterogeneous Catalysis, Enzymatic Catalysis, Photocatalysis

Introduction:

Designing chemical products and processes that reduce or eliminate the usage and manufacture of hazardous compounds is the goal of the cutting-edge field of "green chemistry". (U.S. Environmental Protection Agency. "Basics of Green Chemistry."). The main objective is to reduce the environmental impact and health hazards related to the production and use of chemicals.

The 12 Principles of Green Chemistry, first presented by Paul Anastas and John Warner in 1998, serve as the cornerstone of this field. By focusing on waste reduction, optimizing atom efficiency, employing safer synthesis pathways, creating non-toxic chemical products, and choosing ecologically friendly solvents and auxiliary materials, these guidelines provide a framework for sustainable chemical practices. (Anastas PT, Warner JC,2000) (American Chemical Society. "12 Principles of Green Chemistry.")

Industry use of green chemistry techniques directly supports a number of Sustainable Development Goals (SDGs) of the UN, such as:

- SDG 6: Clean Water and Sanitation – minimizing chemical pollutants released into water systems.
- SDG 7: Affordable and Clean Energy – promoting energy-efficient chemical processes.
- SDG 12: Responsible Consumption and Production – fostering sustainable industrial practices.
- SDG 13: Climate Action – curbing greenhouse gas emissions from chemical operations.

In industrial operations and chemical synthesis, solvents and catalysts are essential. However, many traditional solvents contain volatile organic compounds (VOCs), which are harmful to human health and contribute to pollution of the air and water. Furthermore, because of difficulties in separation and recovery, conventional catalysts frequently depend on hazardous or rare metals, raising environmental issues. (Sheldon,2012)

This chapter examines the ways in which sophisticated catalytic systems and sustainable solvents support environmentally friendly chemical reactions. We'll look at creative ways to cut down on waste, energy use, and dangerous byproducts, emphasizing bio-based solvents, ionic liquids, and deep eutectic solvents (DESs) as viable substitutes. Furthermore, we will investigate state-of-the-art catalytic technologies that improve reaction selectivity while reducing their negative effects on the environment, such as heterogeneous, enzymatic, and photocatalytic approaches. We will illustrate how these green alternatives are influencing sectors like industrial manufacturing, materials synthesis, and pharmaceuticals through case studies and comparative analysis.

1. Sustainable Solvents: A Path to Greener Chemistry

In order to achieve chemical processes that are environmentally responsible, the choice of solvent is essential. Because of their toxicity, volatility, and persistence in ecosystems, traditional organic solvents frequently present major health and environmental risks. Green solvents, which are either made from renewable resources or are engineered to cause the least amount of ecological harm, are becoming more and more popular as sustainable substitutes.

1.1 Bio-Based Solvents

Renewable biological sources, such plants or microbial fermentation, are the source of bio-based solvents. When compared to substitutes made from petroleum, these solvents typically show reduced toxicity and biodegradability. (Cvjetko *et al.,* 2015)

- *Ethanol*: A widely used solvent, ethanol is produced by fermenting sugars from crops like corn and sugarcane. It finds applications in pharmaceuticals, cosmetics, and fuel additives. (Jessop, Mercer, Hildebrant, 2012)

- *Ethyl Lactate*: Derived from lactic acid and ethanol, both sourced from biomass, ethyl lactate is commonly used in coatings, cleaning solutions, and pharmaceutical production. (Kerton, Marriott,2013)
- *2-Methyltetrahydrofuran (2-MeTHF):* A sustainable substitute for petroleum-based tetrahydrofuran (THF), 2-MeTHF is obtained from lignocellulosic biomass and is used in various synthetic reactions. (Tuck *et al.,* 2012)

1.2. Ionic Liquids (ILs)

Salts that stay liquid at or close to room temperature are known as ionic liquids, and they have several benefits, including low vapor pressure, excellent thermal stability, and adjustable solubility (Smith, Abbott, Ryder ,2014)

- *Applications*: ILs are widely employed in catalysis, electrochemistry, and as solvents for challenging-to-dissolve compounds. Their non-volatile nature significantly reduces air pollution. (Sheldon, 2007)
- *Environmental Considerations*: While ionic liquids offer numerous benefits, their ecological footprint varies depending on their chemical composition. Recent advancements focus on biodegradable and renewable-derived ILs to further enhance sustainability. (Horváth, Anastas, 2007)

1.3. Deep Eutectic Solvents (DESs)

DESs are formed by mixing two or more components that, when combined, create a low-melting-point liquid. These solvents are composed of cost-effective, readily available, and biodegradable substances. (Smith, Abbott, Ryder,2014)

Common Composition: A well-known DES is choline chloride mixed with urea, which remains liquid at room temperature. (Cvjetko *et al.,* 2015)

- ***Uses**:* DESs are increasingly used in metal processing, pharmaceutical formulations, and as solvents for chemical reactions and extractions. Their low toxicity and ease of preparation make them ideal for sustainable applications. (Pollet *et al.,* 2014)

1.4. Supercritical Fluids

Supercritical fluids exist at temperatures and pressures above their critical points, where they exhibit unique properties between liquids and gases. (Clarke *et al.,* 2018)

- *Supercritical Carbon Dioxide (scCO₂):* Widely applied in coffee decaffeination and essential oil extraction, $scCO_2$ is non-toxic, non-flammable, and easily separable by depressurization. (Jessop, Mercer, Hildebrant, 2012)
- *Advantages*: The tunable solvent properties of supercritical fluids enable selective extractions and reactions, reducing dependence on harmful organic solvents. (Sheldon, 2007)

1.5. Water as a Green Solvent

Water remains one of the most eco-friendly solvents due to its non-toxic, non-flammable, and abundant nature. Its high polarity and heat capacity make it ideal for many chemical transformations. (Horváth, Anastas, 2007)

- *Application***s**: Water-based systems are employed in Diels-Alder and Claisen rearrangement reactions, replacing hazardous organic solvents and enhancing safety in chemical manufacturing.

By integrating sustainable solvent strategies, industries can improve process safety, reduce environmental impact, and advance greener chemical manufacturing. (Anastas, Zimmerman, 2019)

2.Catalytic Innovations for Sustainable Chemical Processes

Catalysis is a cornerstone of green chemistry, allowing for higher reaction efficiency, lower energy consumption, and reduced waste generation. (Anastas, Eghbali, 2010) Innovations in catalytic methods—including heterogeneous, enzymatic, and photocatalytic systems—are reshaping chemical processes by enabling selective transformations under milder, more sustainable conditions.

2.1. Heterogeneous Catalysis

- Heterogeneous catalysts exist in a different phase than the reactants (e.g., solid catalysts in liquid or gas-phase reactions). They offer stability, ease of separation, and recyclability. (Sheldon, 2007)

Green Catalysts for Industrial Use

- *Metal-Based Catalysts*: Transition metals like palladium, platinum, and nickel are widely used in hydrogenation and oxidation reactions. New research focuses on reducing metal usage while maintaining catalytic performance. (Biffis *et al.,* 2018)
- *Zeolites and MOFs (Metal-Organic Frameworks*)**:** These materials, known for their high surface area and tunable acidity, are increasingly utilized for petrochemical and biomass conversion.

2.2. Enzymatic Catalysis

Enzyme-based catalysis offers high specificity, efficiency at ambient conditions, and biodegradability. Enzymes facilitate reactions at room temperature and atmospheric pressure, cutting energy consumption. (Sheldon, Woodley, 2018)

Advancements in Biocatalysis

- *Directed Evolution & Protein Engineering*: Innovations in enzyme engineering have yielded highly stable biocatalysts tailored for industrial applications. (Arnold,2017)

2.3. Photocatalysis

Photocatalysis leverages light energy to drive chemical reactions, replacing conventional high-energy processes. (Fujishima, Zhang, 2006)

- *Titanium Dioxide (TiO_2):* A widely studied photocatalyst used in environmental remediation and water splitting. (Kudo, Miseki, 2009)
- *Visible-Light-Activated Photocatalysts*: Emerging materials like bismuth oxides and metal sulfides are improving efficiency under visible light. (Wang, Domen, Maeda, 2018)

Through the development of catalytic techniques, industries can drastically cut energy consumption, limit byproducts, and improve selectivity, resulting in more environmentally friendly and effective chemical production. (Anastas, Eghbali, 2010)

3.Waste and Energy Reduction Strategies

In order to achieve sustainable chemical processes, waste reduction and energy efficiency optimization are essential objectives. Conventional manufacturing techniques frequently need high energy inputs and produce considerable amounts of harmful byproducts, which raises worries about the environment and the economy. Innovative solvent systems, state-of-the-art catalytic technologies, and process intensification techniques can help industry drastically cut down on energy use and waste output.

The main strategies for attaining greener chemical processes are examined in this part, including energy-efficient reaction conditions, solvent and catalyst optimization, process intensification, and atom economy.

3.1. Atom Economy and Process Efficiency

Trost established the idea of "atom economy" in 1991. It focuses on avoiding the production of waste by-products and optimizing the incorporation of reactants into the end product. Catalytic hydrogenations and rearrangements are examples of high atom economy processes that increase overall efficiency and lessen the demand for dangerous chemicals. (Trost,1995)

3.1.1 Process Intensification

Through the optimization of reaction conditions or the integration of several reaction steps into a single process, process intensification (PI) seeks to increase the efficiency of chemical manufacturing. (Stankiewicz, Moulijn, 2000)

Key PI strategies include:

- *Microreactor Technology*: Continuous-flow microreactors increase mass and heat transfer, which lowers energy consumption and increases reaction efficiency. (Jensen, 2017)
- *Membrane Separation Techniques*: These methods replace energy-intensive distillation, significantly reducing energy costs in solvent recovery and purification. (Baker, 2023)

3.2. Green Solvent Selection and Minimization

Since conventional organic solvents contribute to volatile organic compound (VOC) emissions and hazardous waste, selecting the right solvents is crucial for reducing environmental impact. Several strategies can help in minimizing solvent waste.

3.2.1 Solvent-Free and Aqueous-Based Reactions

- *Solvent-Free Synthesis*: Eliminating solvents altogether can drastically reduce waste generation. Techniques such as mechanochemical reactions and solid-state synthesis offer promising alternatives. (Friščić,2010)
- *Aqueous-Phase Reactions*: Water is a preferred green solvent due to its non-toxic nature and availability. Various catalytic transformations, including Suzuki-Miyaura cross-coupling and enzymatic biotransformations, have successfully adapted to water-based conditions. (Li, Chen, 2006)

3.2.2 Ionic Liquids and Supercritical Fluids

- *Ionic Liquids (ILs):* These non-volatile solvents serve as sustainable alternatives to traditional organic solvents, reducing emissions and solvent losses. (Wasserscheid, Welton, 2008)
- *Supercritical Carbon Dioxide (scCO$_2$):* Widely employed in extraction and catalytic processes, scCO$_2$ provides a cleaner, more energy-efficient alternative to traditional solvents. (Anastas, Leitner, Jessop, 2014)

3.3. Waste Valorization and By-Product Utilization

Rather than treating waste as an inevitable by-product, industries are increasingly seeking ways to convert waste into valuable resources.

3.3.1 Biorefinery Approaches

- *Lignocellulosic Biomass Utilization*: Agricultural waste and plant-based biomass can be converted into biofuels, bioplastics, and specialty chemicals, reducing reliance on fossil resources. (Ragauskas *et al.,* 2006)
- *Glycerol Upcycling*: A by-product of biodiesel production, glycerol can be repurposed into high-value chemicals such as propanediol and epichlorohydrin. (Pagliaro, Rossi, 2010)

3.3.2 CO$_2$ Utilization and Circular Economy

- *Carbon Capture and Utilization (CCU):* Captured CO$_2$ can be transformed into fuels, polymers, and specialty chemicals, contributing to a more circular carbon economy. (Aresta, Dibenedetto, Angelini, 2013)
- *Industrial Symbiosis*: By repurposing waste from one industry as a raw material for another, industries can maximize resource efficiency and minimize waste generation. (Chertow,2000)

By implementing these waste and energy reduction strategies, chemical industries can significantly decrease their environmental impact while improving process sustainability.

4. Case Studies in Sustainable Solvents and Catalysts

The best way to illustrate the real-world impact of green chemistry is through case studies in various industries.

4.1. Greener Synthesis of Ibuprofen in the Pharmaceutical Industry

Background

Ibuprofen, a commonly used nonsteroidal anti-inflammatory drug (NSAID), was historically manufactured using a six-step process that required stoichiometric reagents, resulting in excessive waste generation. The traditional Hoechst synthesis had an Environmental Factor (E-Factor) of ~45, meaning that for every 1 kg of ibuprofen produced, 45 kg of waste was generated (Sheldon, 1992).

Green Chemistry Approach

BHC Company (now BASF) developed a three-step catalytic process that:

- Uses heterogeneous catalysts (such as palladium-based systems) to enhance reaction selectivity.
- Eliminates hazardous reagents like aluminium trichloride.
- Reduces the E-Factor from ~45 to 6, drastically cutting waste production (Jensen, 2006).

Impact

This optimized process has become a benchmark for sustainable pharmaceutical synthesis, lowering solvent consumption, reducing hazardous by-products, and significantly improving atom economy. (Rogers, Jensen, 2019)

4.2. Bio-Based Solvents in Agrochemical Formulations

Background

Traditional pesticide formulations rely heavily on petroleum-based solvents, which contribute to air pollution and pose health risks. (Anastas, Warner, 2000)

Green Chemistry Approach

- Bio-based solvents, such as γ-valerolactone (GVL) and limonene-derived solvents, have replaced conventional petroleum-derived solvents. (Clark, Farmer, Sherwood, 2012)
- These alternatives are non-toxic, biodegradable, and sourced from renewable feedstocks.
- Solvent-free formulations using nano-encapsulation and microemulsions have further *reduced reliance on VOC-based solvents.* (Li, Wasserscheid, Stark, 2010)

Impact

The adoption of bio-based solvents has enhanced worker safety, minimized solvent waste, and significantly improved environmental sustainability in the agrochemical sector.

5. Challenges in Sustainable Solvents and Catalysts

5.1. Economic and Industrial Barriers

- *High Production Costs*: The synthesis of bio-based solvents and advanced catalysts often involves complex processes and expensive raw materials, making them less competitive than conventional options. (Jessop,2011)
- *Scalability Issues*: While promising at the laboratory scale, many green solvents and catalysts face hurdles in large-scale industrial applications. (Sheldon,2007)

5.2. Performance and Stability Issues

- *Solvent Compatibility*: Some bio-based solvents may not be fully compatible with existing industrial processes, requiring modifications. (Clarke *et al.,* 2018)
- *Catalyst Longevity*: Many sustainable catalysts, including enzymatic and photocatalytic systems, degrade under harsh conditions, limiting reusability. (Wasserscheid, Welton, 2008)

5.3. Regulatory and Environmental Concerns

- *Toxicity of Ionic Liquids (ILs)*: Some ILs exhibit cytotoxicity and poor biodegradability, necessitating further research into safer alternatives. (Pham, Cho, Yun, 2010)
- *End-of-Life Management*: Metal-based catalysts require appropriate disposal or recycling to prevent environmental contamination.

6. Future Directions in Sustainable Chemistry

6.1. Novel Solvent Development

- *Bio-Based Solvents from Waste Biomass*: Converting agricultural and forestry residues into solvents can enhance sustainability and lower costs. (Smith, Abbott, Ryder, 2014)
- *Deep Eutectic Solvents (DESs)*: DESs, derived from biodegradable components, are emerging as cost-effective, environmentally friendly alternatives to ILs.

6.2. Advancements in Catalysis

- *Nanocatalysts & MOFs*: Advanced nanostructured catalysts offer greater efficiency and selectivity.
- *Artificial Enzymes & Biomimetic Catalysts*: Inspired by nature, these engineered catalysts can enhance reaction efficiency and sustainability.

Industries can establish sustainable chemistry as the standard by advancing innovation, which will save waste, save energy, and promote a cleaner, greener future.

Conclusion:

An important development in green chemistry is the move toward sustainable solvents and catalysts, which opens the door to better environmental sustainability, waste reduction, and energy efficiency in chemical processes. As this chapter discusses, innovative catalytic techniques—such as heterogeneous, enzymatic, and photocatalytic systems—as well as bio-based and ionic solvents are demonstrating themselves to be game-changing options for lowering harmful byproducts and streamlining industrial processes. Agrochemical and pharmaceutical case studies show how these innovations are actively changing industrial processes to become more efficient and sustainable.

Nevertheless, several difficulties still exist despite these developments. Widespread acceptance of several alternative solvents and catalysts is still hampered by economic considerations, scaling issues, and environmental concerns.

Ongoing research to create affordable, biodegradable solvents, design long-lasting catalytic systems, and incorporate green chemistry concepts into industrial operations will be essential to the future of sustainable chemistry.

Chemical manufacturing companies can significantly reduce their environmental effect and help create a cleaner, safer, and more responsible future by prioritizing sustainability. The developments discussed in this chapter highlight how crucial green chemistry is becoming to creating a more sustainable industrial environment. Going forward, multidisciplinary cooperation between chemistry, engineering, and environmental science will be necessary for success in this subject in order to overcome current challenges and guarantee that sustainable chemical practices become the norm worldwide.

References:

1. American Chemical Society. (n.d.). *12 principles of green chemistry*. https://www.acs.org/green-chemistry-sustainability/principles/12-principles-of-green-chemistry.html
2. Anastas, P., & Eghbali, N. (2010). Green chemistry: Principles and practice. *Chemical Society Reviews, 39*(1), 301–312.
3. Anastas, P. T., Leitner, W., & Jessop, P. G. (2014). *Green solvents, Volume 4: Supercritical solvents*. John Wiley & Sons.
4. Anastas, P. T., & Warner, J. C. (2000). *Green chemistry: Theory and practice*. Oxford University Press.
5. Anastas, P. T., & Zimmerman, J. B. (2019). The periodic table of the elements of green and sustainable chemistry. *Green Chemistry, 21*(24), 6545–6566.
6. Aresta, M., Dibenedetto, A., & Angelini, A. (2013). The changing paradigm in CO_2 utilization. *Journal of CO_2 Utilization, 3*, 65–73.
7. Arnold, F. H. (2017). Directed evolution: Bringing new chemistry to life. *Angewandte Chemie International Edition, 57*(16), 4143.
8. Baker, R. W. (2023). *Membrane technology and applications*. John Wiley & Sons.
9. Biffis, A., Centomo, P., Del Zotto, A., & Zecca, M. (2018). Pd metal catalysts for cross-couplings and related reactions in the 21st century: A critical review. *Chemical Reviews, 118*(4), 2249–2295.
10. Chertow, M. R. (2000). Industrial symbiosis: Literature and taxonomy. *Annual Review of Energy and the Environment, 25*(1), 313–337.

11. Clark, J. H., Farmer, T. J., & Sherwood, J. (2012). Circular economy in the chemical industry. *Green Chemistry, 14*(3), 243–256.
12. Clarke, C. J., Tu, W. C., Levers, O., Brohl, A., & Hallett, J. P. (2018). Green and sustainable solvents in chemical processes. *Chemical Reviews, 118*(2), 747–800.
13. Corma, A., García, H., & Primo, A. (2007). Zeolites and MOFs as catalysts. *Chemical Reviews, 107*(6), 2411–2502.
14. Cvjetko Bubalo, M., Vidović, S., Radojčić Redovniković, I., & Jokić, S. (2015). Green solvents for green technologies. *Journal of Chemical Technology & Biotechnology, 90*(9), 1631–1639.
15. Dreyer, D. R., Park, S., Bielawski, C. W., & Ruoff, R. S. (2010). The chemistry of graphene oxide. *Chemical Society Reviews, 39*(1), 228–240.
16. Friščić, T. (2010). Supramolecular and solid-state synthesis with mechanochemistry. *Chemical Society Reviews, 39*(1), 138–150.
17. Fujishima, A., & Zhang, X. (2006). Titanium dioxide photocatalysis: Present situation and future approaches. *Comptes Rendus Chimie, 9*(5–6), 750–760.
18. Horváth, I. T., & Anastas, P. T. (2007). Innovations and green chemistry. *Chemical Reviews, 107*(6), 2169–2173.
19. Jensen, K. F. (2017). Flow chemistry—Microreaction technology comes of age. *AIChE Journal, 63*(3), 858–869.
20. Jessop, P. G., Mercer, S. M., & Heldebrant, D. J. (2012). CO_2-triggered switchable solvents, surfactants, and other materials. *Energy & Environmental Science, 5*(6), 7240–7253.
21. Jessop, P. G. (2011). Searching for green solvents. *Green Chemistry, 13*(6), 1391–1398.
22. Kerton, F. M., & Marriott, R. (2013). *Alternative solvents for green chemistry*. Royal Society of Chemistry.
23. Kudo, A., & Miseki, Y. (2009). Heterogeneous photocatalyst materials for water splitting. *Chemical Society Reviews, 38*(1), 253–278.
24. Li, C. J., & Chen, L. (2006). Organic chemistry in water. *Chemical Society Reviews, 35*(1), 68–82.
25. Li, C. J., Wasserscheid, P., & Stark, A. (2010). Green solvents. In W. Leitner & P. G. Jessop (Eds.), *Green solvents* (Vol. 4). Wiley-VCH.
26. Nicewicz, D. A., & MacMillan, D. W. (2008). Merging photoredox catalysis with organocatalysis: The direct asymmetric alkylation of aldehydes. *Science, 322*(5898), 77–80.
27. Pagliaro, M., & Rossi, M. (2010). *The future of glycerol*. Royal Society of Chemistry.
28. Pham, T. P., Cho, C. W., & Yun, Y. S. (2010). Environmental fate and toxicity of ionic liquids: A review. *Water Research, 44*(2), 352–372.
29. Pollet, P., Davey, E. A., Ureña-Benavides, E. E., Eckert, C. A., & Liotta, C. L. (2014). Solvents for sustainable chemical processes. *Green Chemistry, 16*(3), 1034–1055.

30. Polshettiwar, V., & Varma, R. S. (2010). Green chemistry by nano-catalysis. *Green Chemistry, 12*(5), 743–754.
31. Prier, C. K., Rankic, D. A., & MacMillan, D. W. (2013). Visible light photoredox catalysis with transition metal complexes: Applications in organic synthesis. *Chemical Reviews, 113*(7), 5322–5363.
32. Ragauskas, A. J., Williams, C. K., Davison, B. H., Britovsek, G., Cairney, J., Eckert, C. A., Frederick Jr, W. J., Hallett, J. P., Leak, D. J., Liotta, C. L., & Mielenz, J. R. (2006). The path forward for biofuels and biomaterials. *Science, 311*(5760), 484–489.
33. Rogers, L., & Jensen, K. F. (2019). Continuous manufacturing—the Green Chemistry promise? *Green Chemistry, 21*(13), 3481–3498.
34. Sheldon, R. A., & Woodley, J. M. (2018). Role of biocatalysis in sustainable chemistry. *Chemical Reviews, 118*(2), 801–838.
35. Sheldon, R. A. (2012). Fundamentals of green chemistry: Efficiency in reaction design. *Chemical Society Reviews, 41*(4), 1437–1451.
36. Sheldon, R. A. (1992). Organic synthesis—Past, present and future. *Chemistry and Industry, (23)*, 903–906.
37. Sheldon, R. A. (2007). The E factor: Fifteen years on. *Green Chemistry, 9*(12), 1273–1283.
38. Smith, E. L., Abbott, A. P., & Ryder, K. S. (2014). Deep eutectic solvents (DESs) and their applications. *Chemical Reviews, 114*(21), 11060–11082.
39. Stankiewicz, A. I., & Moulijn, J. A. (2000). Process intensification: Transforming chemical engineering. *Chemical Engineering Progress, 96*(1), 22–34.
40. Sustainable Manufacturing Expo. (n.d.). *Sustainable manufacturing expo*. https://sustainablemanufacturingexpo.com
41. Trost, B. M. (1995). Atom economy—A challenge for organic synthesis: Homogeneous catalysis leads the way. *Angewandte Chemie International Edition in English, 34*(3), 259–281.
42. Tuck, C. O., Pérez, E., Horváth, I. T., Sheldon, R. A., & Poliakoff, M. (2012). Valorization of biomass: Deriving more value from waste. *Science, 337*(6095), 695–699.
43. U.S. Environmental Protection Agency. (n.d.). *Basics of green chemistry*. https://www.epa.gov/greenchemistry/basics-green-chemistry
44. U.S. Environmental Protection Agency. (n.d.). *Green chemistry*. https://www.epa.gov/greenchemistry
45. Wang, Q., Domen, K., & Maeda, K. (2018). Visible-light-driven photocatalysts for hydrogen production from water splitting. *Nature Reviews Materials, 3*, 368–384.
46. Wasserscheid, P., & Welton, T. (Eds.). (2008). *Ionic liquids in synthesis*. Wiley-VCH.

NANOPARTICLES IN FOOD PRESERVATION AND PROCESSING: APPLICATIONS, SAFETY, AND FUTURE TRENDS

Madhuri K. Patil[1], Shital G. Chaudhari[2], Amod S. Patil*[2] and Vikram Jadhav[3]
[1]Department of Physics,
R. C. Patel English Medium Junior College, Shirpur, Dist. Dhule 425405
[2]Department of Pharmaceutical Chemistry,
R. C. Patel Institute of Pharmacy, Shirpur, Dist. Dhule 425405
[3]Bench Chemist MDTL, Office of the ADC (I), CDSCO,
International Air Cargo Complex, Sahar Village, Andheri, Mumbai–400099.
*Corresponding author E-mail: patilamod.s@gmail.com

Abstract:

The advent of nanotechnology has significantly influenced the food industry, offering novel approaches to enhance food quality, safety, and shelf life. This chapter provides a comprehensive overview of the applications of nanoparticles in food preservation and processing, emphasizing their multifunctional roles in modern food systems. The antimicrobial, antioxidant, and barrier-enhancing properties of nanoparticles—particularly those of silver, zinc oxide, titanium dioxide, and biopolymer-based nanocomposites—are explored in the context of active and intelligent packaging solutions. Furthermore, the chapter examines the use of nano-encapsulation techniques to improve the stability, controlled release, and bioavailability of bioactive compounds and nutrients during processing and storage. Attention is also given to the potential toxicological implications, regulatory frameworks, and consumer acceptance issues associated with the use of nanomaterials in food applications. By integrating recent advancements and current challenges, this chapter aims to contribute to the global discourse on the responsible and effective use of nanotechnology in ensuring food security and sustainability.

Keywords: Nanoparticles; Food Preservation; Nano-Encapsulation; Active Packaging.

1. Introduction:

Nanotechnology, defined as the design, production, and application of materials and devices at the nanometer scale (1–100 nm), has emerged as a transformative technology across diverse sectors, including medicine, agriculture, energy, and food science. In the food industry, nanotechnology offers innovative solutions for improving food quality, safety, packaging, and shelf life. Nanoparticles exhibit unique physicochemical properties—such as increased surface area, reactivity, and controlled release capabilities—that make them highly suitable for applications in food preservation and processing (Chaudhry *et al.,* 2008; Sozer & Kokini, 2009).

Nanomaterials are being incorporated into a variety of food systems, either directly as additives and carriers or indirectly through packaging. For instance, silver and zinc oxide nanoparticles have shown potent antimicrobial activity, while nano-encapsulation techniques are being employed to enhance the stability and bioavailability of sensitive nutrients and bioactives (Silva *et al.,* 2012). Additionally, intelligent and active packaging systems utilizing nanosensors and controlled-release agents are revolutionizing how food quality is maintained and monitored during distribution and storage.

Food preservation and processing are fundamental to ensuring the safety, nutritional quality, sensory acceptability, and year-round availability of food products. As global populations grow and food supply chains become increasingly complex and extended, maintaining food quality from farm to fork presents significant challenges. The World Health Organization (WHO) estimates that each year, unsafe food causes 600 million cases of foodborne illnesses globally, highlighting the urgent need for more robust preservation technologies (WHO, 2020). Moreover, food spoilage due to microbial contamination, oxidation, and enzymatic activity results in substantial post-harvest losses—especially in perishable categories like fruits, vegetables, dairy, and meat (Kumar *et al.,* 2021).

Traditional preservation methods such as refrigeration, drying, salting, and chemical additives have been instrumental in reducing spoilage and extending shelf life. However, these techniques often come with limitations. For instance, thermal processing can lead to the degradation of heat-sensitive nutrients and bioactive compounds, while chemical preservatives may raise consumer health concerns and regulatory scrutiny (Gyawali & Ibrahim, 2014). Furthermore, in the context of modern consumer demands for minimally processed, clean-label, and nutrient-rich foods, there is growing pressure on the food industry to adopt preservation strategies that are not only effective but also safe, sustainable, and aligned with health-conscious preferences.

Advanced technologies, particularly those at the nanoscale, are now being explored as complementary or alternative preservation tools. Nanoparticles offer enhanced antimicrobial activity, superior barrier properties in packaging materials, and improved retention of food quality during storage. Their unique physicochemical properties enable the development of smart delivery systems and active packaging that respond dynamically to environmental conditions—ushering in a new era of intelligent and responsive food preservation solutions (Ravichandran, 2010).

Nanotechnology introduces precision-based interventions that enhance microbial safety, reduce the need for chemical preservatives, and extend shelf life with minimal nutrient loss. Moreover, in food processing, nanoparticles contribute to improved emulsification, texture modification, flavor protection, and nutrient delivery—offering a new paradigm in food innovation (McClements & Xiao, 2017).

This chapter aims to explore the current and emerging applications of nanoparticles in food preservation and processing. It presents an in-depth discussion of the types of nanoparticles used in the food industry, their mechanisms of action in antimicrobial protection and nutrient stabilization, and their incorporation into packaging systems and processing technologies. Additionally, the chapter addresses safety concerns, regulatory frameworks, and consumer perspectives associated with the use of nanotechnology in food systems. By bridging scientific innovation with practical applications, this chapter offers valuable insights into how nanotechnology can contribute to a more sustainable and secure global food supply.

2. Types of Nanoparticles Used in Food Applications

Nanoparticles used in food preservation and processing can be broadly categorized based on their composition and functional properties. Each type offers distinct advantages in enhancing food safety, shelf life, and nutrient delivery. This section outlines the major classes of nanoparticles, their characteristics, and their relevance to food applications.

2.1 Metallic Nanoparticles

Metallic nanoparticles, particularly silver (Ag) and gold (Au) nanoparticles, are widely studied for their potent antimicrobial properties. Silver nanoparticles (AgNPs) disrupt microbial cell membranes, interfere with DNA replication, and generate reactive oxygen species, making them effective against a broad spectrum of bacteria, fungi, and viruses (Rai *et al.,* 2012). These properties have made AgNPs ideal candidates for active packaging, surface coatings, and edible films.

Gold nanoparticles, while less antimicrobial than AgNPs, are valued for their biocompatibility, optical properties, and potential use in biosensing and targeted delivery systems for food fortification and diagnostics (Daniel & Astruc, 2004).

2.2 Metal Oxide Nanoparticles

Metal oxide nanoparticles such as zinc oxide (ZnO), titanium dioxide (TiO_2), and magnesium oxide (MgO) have demonstrated both antibacterial and UV-blocking capabilities, making them effective for food packaging and preservation.

ZnO NPs show strong inhibitory effects against Gram-positive and Gram-negative bacteria and are generally regarded as safe (GRAS) by the FDA (Emamifar *et al.,* 2011).

TiO_2 NPs, due to their photocatalytic activity, are used in UV-protective coatings and can degrade ethylene gas, slowing down fruit ripening.

MgO NPs exhibit antifungal and antibacterial properties and have also been proposed for extending the shelf life of produce and dairy products (Huang *et al.,* 2015).

2.3 Polymeric Nanoparticles

Polymeric nanoparticles are synthesized from natural or synthetic polymers and are mainly used for encapsulation and controlled release of bioactive compounds such as vitamins, antioxidants, flavors, and probiotics.

Natural polymers like chitosan, alginate, and gelatin are biodegradable, non-toxic, and often possess inherent antimicrobial activity (Sinha *et al.,* 2004).

These nanoparticles can protect sensitive ingredients during processing and digestion, enhancing their stability and bioavailability.

2.4 Lipid-Based Nanoparticles

Lipid-based nanoparticles, including solid lipid nanoparticles (SLNs) and nanostructured lipid carriers (NLCs), are widely applied in food systems for encapsulation of hydrophobic compounds. These structures provide sustained release, improved solubility, and targeted delivery of lipophilic nutrients, flavors, and functional ingredients (McClements, 2012). Lipid nanoparticles are also compatible with food-grade emulsifiers and are generally safe for ingestion.

2.5 Silica Nanoparticles

Amorphous silica nanoparticles are used as anti-caking agents, delivery vehicles, and flavor carriers in various dry and liquid food products. They are thermally stable, chemically inert, and have a large surface area that supports adsorption and controlled release (Dekkers *et al.,* 2011). Their porous structure also makes them suitable for incorporating antioxidants and enzymes in dry food formulations.

2.6 Sources and Synthesis Methods

Nanoparticles used in food applications can be synthesized via top-down or bottom-up approaches: Top-down methods include mechanical milling, high-pressure homogenization, and laser ablation, which break down bulk materials into nanoscale particles.

Bottom-up approaches involve the chemical or biological assembly of nanoparticles from atoms or molecules. These include precipitation, sol-gel synthesis, emulsion-based methods, and green synthesis using plant extracts, microbes, or enzymes (Iravani, 2011).

Biogenic or green synthesis methods are gaining popularity due to their eco-friendliness, lower toxicity, and compatibility with food systems. The choice of synthesis method significantly influences the particle size, shape, surface charge, and overall stability—parameters critical to nanoparticle function in food matrices. The types of NPs are summarized in Table 1.

Table 1: Types of NPs and their properties and Applications in food preparation and preservation.

Type of Nanoparticle	Material Examples	Properties / Functions	Applications in Food
Metallic NPs	Silver (Ag), Gold (Au)	Antimicrobial, optical properties	Active packaging, surface coatings, biosensing
Metal Oxide NPs	Zinc oxide (ZnO), Titanium dioxide (TiO_2), Magnesium oxide (MgO)	Antimicrobial, UV-blocking, photocatalytic	Shelf-life extension, UV-protective films
Polymeric NPs	Chitosan, Alginate, Gelatin	Biodegradable, controlled release, antimicrobial	Nano-encapsulation of nutrients, edible coatings
Lipid-based NPs	Solid lipid NPs (SLNs), Nanostructured lipid carriers (NLCs)	Hydrophobic nutrient delivery, biocompatibility	Encapsulation of flavors, antioxidants, vitamins
Silica NPs	Amorphous silica	Large surface area, inert, porous structure	Anti-caking agents, enzyme carriers, dry foods

3. Applications in Food Preservation

Nanoparticles play a significant role in enhancing the safety, stability, and shelf life of food products. Their unique surface properties, reactivity, and functional versatility enable applications that go beyond traditional preservation methods. This section discusses key nanoparticle-based strategies used in food preservation, with a focus on antimicrobial and antioxidant mechanisms, as well as smart packaging innovations.

3.1 Antimicrobial Activity

Nanoparticles, especially metallic (e.g., Ag, ZnO, CuO) and metal oxide nanoparticles, have been widely studied for their broad-spectrum antimicrobial effects. These nanoparticles can effectively inhibit the growth of spoilage organisms and foodborne pathogens such as Escherichia coli, Listeria monocytogenes, Salmonella spp., and Staphylococcus aureus.

3.1.1 Mechanisms of Microbial Inhibition

The antimicrobial action of nanoparticles involves multiple mechanisms:

- Disruption of microbial cell membranes, causing leakage of intracellular contents
- Generation of reactive oxygen species (ROS), which induce oxidative stress and damage DNA, proteins, and lipids
- Interaction with microbial enzymes and proteins, leading to metabolic dysfunction

- Release of metal ions (e.g., Ag^+ or Zn^{2+}) that interfere with cellular respiration and replication (Rai *et al.,* 2012)

These mechanisms make nanoparticles less susceptible to resistance development compared to conventional antimicrobials.

3.1.2 Use in Inhibiting Spoilage and Pathogenic Organisms

Nanoparticles have demonstrated substantial efficacy in controlling spoilage and pathogenic microorganisms when applied through various delivery systems in food preservation. One of the most common applications is their incorporation into edible coatings for fresh produce, meats, and dairy products. These coatings act as barriers to moisture and gas exchange while simultaneously releasing antimicrobial agents directly onto the food surface. For instance, silver and zinc oxide nanoparticles have been incorporated into chitosan-based edible films to preserve strawberries and chicken, significantly reducing microbial contamination and prolonging shelf life (Emamifar *et al.,* 2011).

In addition to coatings, nanoparticles are also integrated into packaging materials such as polymeric films and containers to form antimicrobial packaging systems. These nanocomposite materials prevent external contamination and reduce microbial proliferation on food surfaces during storage. Silver nanoparticles embedded in polyethylene films, for example, have shown effectiveness against common foodborne pathogens such as Escherichia coli and Staphylococcus aureus (Rai *et al.,* 2012). Another innovative application is the use of sprayable nanoparticle-based preservatives, which can be applied directly to food surfaces or processing equipment. These sprays often contain nanoemulsions of essential oils or metal nanoparticles, offering broad-spectrum antimicrobial action while maintaining the sensory and nutritional properties of foods (McClements, 2012). For example, nanoemulsified thyme or oregano oils have been used to treat fresh-cut vegetables, effectively inhibiting microbial growth without altering taste or appearance. Collectively, these nanoparticle-enabled approaches reduce microbial load, delay spoilage, and improve food safety, making them promising alternatives or adjuncts to traditional preservation technologies.

3.2 Antioxidant Properties

In addition to microbial protection, some nanoparticles exhibit antioxidant activity, which is crucial for preventing oxidative deterioration in food.

3.2.1 Prevention of Oxidation and Rancidity

Oxidation of fats, oils, pigments, and vitamins leads to rancidity, discoloration, and nutritional loss. Nanoparticles—such as cerium oxide, selenium nanoparticles, and nanoencapsulated polyphenols—can scavenge free radicals or delay oxidation reactions (Silva *et al.,* 2012). These are often embedded in packaging materials or delivery systems that release antioxidants in a controlled manner.

3.3 Shelf-Life Extension

By inhibiting microbial growth and oxidative spoilage, nanoparticles help extend the shelf life of perishable foods. Their integration into various delivery forms—such as coatings, encapsulated preservatives, or active packaging—enhances the protection of foods during transport and storage.

3.3.1 Integration into Packaging and Direct Food Application

Nanoparticles are increasingly being integrated into food packaging systems or applied directly to food surfaces to enhance preservation and safety. Nanocomposite films incorporating antimicrobial or antioxidant nanoparticles—such as silver, zinc oxide, or titanium dioxide—have been shown to significantly extend the shelf life of dairy, meat, fresh produce, and baked goods by reducing microbial growth and oxidative degradation (Emamifar *et al.,* 2011; Huang *et al.,* 2015). Nanoemulsions formulated with bioactive compounds, such as essential oils or natural antioxidants, are used as surface treatments or spray preservatives, forming a uniform, protective layer that combats spoilage organisms while maintaining food quality (McClements, 2012). Additionally, biodegradable nanocoatings, often composed of polysaccharides, proteins, or lipids embedded with nanoparticles, function as edible barriers that limit moisture and gas exchange, thereby delaying spoilage without generating non-degradable waste (Iravani, 2011).

3.4 Smart and Active Packaging Systems

Nanotechnology has enabled the development of active packaging, which interacts dynamically with the food or its surrounding environment to maintain quality, and smart packaging, which provides real-time monitoring of food freshness and safety. For example, silver nanoparticle-embedded films can continuously inhibit microbial growth, while pH-sensitive nanomaterials in smart labels can signal spoilage through visible color changes (Rai *et al.,* 2012).

3.4.1 Indicators and Sensors

Nanoparticles play a crucial role in colorimetric indicators that change color in response to pH shifts, gas emissions (such as carbon dioxide or ethylene), or microbial growth, providing a simple visual cue of food quality (Dekkers *et al.,* 2011). Nanosensors, incorporating materials like gold nanoparticles or quantum dots, can detect trace levels of spoilage compounds such as ammonia or ethylene, enabling early intervention before food safety is compromised. These sensors can be integrated directly into packaging films, labels, or container linings for continuous monitoring throughout the supply chain.

3.4.2 Controlled Release of Preservatives

Nanocarriers—such as lipid-based nanoparticles, polymeric nanospheres, and silica nanocapsules—are being designed for the controlled release of preservatives in response to specific environmental triggers, including changes in temperature, moisture, or microbial load. This targeted release ensures that active compounds are delivered precisely when needed, reducing the risk of overexposure, maintaining sensory quality, and improving overall safety. For example, nano-encapsulated nisin in biodegradable films has been shown to release antimicrobial activity only under high-humidity storage conditions, preventing unnecessary loss of activity during dry storage (Ravichandran, 2010).

4. Applications in Food Processing

4.1 Nano-encapsulation of Bioactives

Nano-encapsulation has gained significant attention in the food industry as an efficient strategy for incorporating bioactive compounds such as vitamins, probiotics, flavors, and essential oils into functional food products. This technique involves enclosing active ingredients within nanocarriers—such as liposomes, nanoemulsions, or biopolymer nanoparticles—which improves solubility, stability, and bioavailability while protecting them from degradation during processing, storage, and digestion (McClements, 2012; Augustin & Sanguansri, 2009). For example, vitamin D encapsulated in protein-based nanoparticles has shown enhanced stability against heat and light, making it suitable for fortification in dairy beverages (Qian *et al.,* 2012). Similarly, nanoemulsions containing essential oils like thyme or oregano have demonstrated improved antimicrobial efficacy in fresh produce preservation without adversely affecting sensory attributes (Donsì *et al.,* 2011).

4.2 Targeted Delivery Systems

Nanotechnology-based targeted delivery systems have emerged as a promising approach to enhance the functional performance of bioactive compounds in food. These systems are designed to protect sensitive ingredients during processing and storage while enabling their controlled release during digestion at specific sites in the gastrointestinal tract (Weiss *et al.,* 2006; McClements *et al.,* 2009). Nanocarriers such as liposomes, solid lipid nanoparticles, and biopolymer-based nanogels can encapsulate nutrients, flavors, or nutraceuticals, shielding them from degradation in acidic gastric conditions and releasing them in the small intestine where absorption is optimal (Chen *et al.,* 2006). For example, liposomal encapsulation of probiotics has been shown to significantly improve their viability through gastric transit and enhance colonization efficiency (Krasaekoopt *et al.,* 2003). Similarly, nano-structured lipid carriers have been developed for the controlled release of omega-3 fatty acids, thereby reducing oxidative degradation and off-flavors while improving bioavailability (Patel *et al.,* 2012). These targeted delivery strategies not only optimize nutrient utilization but also contribute to enhanced sensory quality and consumer acceptance of functional foods.

4.3 Improving Texture and Sensory Properties

Nanotechnology plays a significant role in enhancing the texture, appearance, and overall sensory qualities of food products. Nanostructured emulsions, nanofoams, and nanogels are increasingly used to manipulate rheological properties, mouthfeel, and stability of food systems (Weiss *et al.,* 2006; McClements, 2012). For example, nanoemulsions with droplet sizes below

200 nm provide improved optical clarity, creaminess, and flavor delivery in beverages, sauces, and dairy products (Qian and McClements, 2011). Nanogels derived from proteins or polysaccharides can form fine, uniform gel networks that improve water retention, elasticity, and smoothness in products such as yogurt, desserts, and meat analogues (Patel and Velikov, 2011). Additionally, nanoparticle-based thickeners and stabilizers can enhance the stability of foams and emulsions, prevent phase separation and extend shelf life (McClements and Rao, 2011). By precisely controlling particle size and surface characteristics at the nanoscale, food manufacturers can create products with superior texture and consumer appeal without relying heavily on artificial additives.

4.4 Enhancing Nutrient Retention during Processing

Food processing often involves exposure to heat, light, oxygen, and mechanical stress, which can degrade sensitive nutrients such as vitamins, carotenoids, polyphenols, and unsaturated fatty acids. Nanotechnology offers innovative approaches to protect these labile compounds, thereby preserving their nutritional value throughout processing, storage, and distribution (Huang *et al.,* 2010; Augustin and Sanguansri, 2009). Nano-encapsulation and nanoliposome-based delivery systems can shield bioactive compounds from oxidative degradation, light exposure, and thermal breakdown (Ravichandran, 2010). For instance, vitamin C encapsulated in lipid-based nanoparticles exhibits improved stability during pasteurization and prolonged shelf life in fortified beverages (Oehlke *et al.,* 2014). Similarly, polyphenols and omega-3 fatty acids incorporated into nanostructured carriers show enhanced retention during baking, frying, and high-pressure processing (Sanguansri and Augustin, 2006). By providing a physical barrier at the nanoscale and controlling the release of bioactives, these technologies not only improve nutrient stability but also help maintain the intended functional and sensory properties of food products.

5. Safety, Toxicity, and Regulatory Considerations

The incorporation of nanoparticles into food products and packaging offers promising benefits but also raises concerns regarding potential health risks and toxicity. Nanoparticles, owing to their small size and large surface area, can exhibit unique physicochemical properties that may lead to biological interactions different from their bulk counterparts (Bouwmeester *et al.,* 2009). Potential toxicity mechanisms include oxidative stress, DNA damage, membrane disruption, and inflammatory responses, which depend on factors such as particle size, shape, surface charge, concentration, and exposure duration (Oberdörster *et al.,* 2005; Singh & Nalwa, 2011).

Globally, regulatory bodies have established varying guidelines for the safe use of nanomaterials in food. The European Food Safety Authority (EFSA) mandates comprehensive risk assessments for any engineered nanomaterial intended for food contact or direct incorporation (EFSA Scientific Committee, 2018). The U.S. Food and Drug Administration (FDA) evaluates nanoparticles under existing food additive regulations, with specific guidance for nanotechnology-enabled food ingredients and packaging materials (FDA, 2014). In India, the Food Safety and

Standards Authority of India (FSSAI) has developed draft guidelines for assessing the safety of nanomaterials in food systems, focusing on toxicological evaluation, migration studies, and labelling requirements (FSSAI, 2021).

Risk assessment protocols typically involve characterization of nanoparticle physicochemical properties, in vitro and in vivo toxicity studies, migration testing for packaging materials, and assessment of bioaccumulation potential. These evaluations help ensure that the benefits of nanoparticle applications do not compromise consumer health.

In addition to scientific and regulatory challenges, consumer perception plays a critical role in the adoption of nanotechnology in the food sector. Public concerns often center around the perceived unnaturalness of nanoparticles in food, possible long-term health impacts, and ethical considerations regarding transparency and informed choice (Siegrist *et al.,* 2007). Addressing these concerns through clear labelling, public education, and transparent safety assessments is essential for enhancing consumer trust and acceptance.

6. Challenges and Future Perspectives

The application of nanotechnology in the food sector presents remarkable opportunities, yet its large-scale adoption faces several challenges. One of the primary hurdles is the scale-up and commercialization of laboratory-developed nanomaterials into economically viable products. While numerous nanoparticle-based systems have demonstrated efficacy in research settings, transitioning these innovations to industrial production often encounters technical, cost, and infrastructure constraints (Kumar *et al.,* 2019). Issues such as maintaining nanoparticle stability, ensuring batch-to-batch consistency, and integrating nano-enabled solutions into existing food processing lines remain significant obstacles (Weiss *et al.,* 2006).

Another major concern is the need for standardized testing and regulatory protocols. Currently, variations in analytical methods, toxicity testing models, and labeling regulations across countries impede global harmonization (EFSA, 2018; FDA, 2014). Establishing universally accepted frameworks for risk assessment, quality control, and product approval will be critical for consumer safety and international trade.

In parallel, recent research has emphasized advances in green synthesis and biodegradable nanomaterials as a sustainable pathway for the food industry. The development of nanoparticles using plant extracts, microbial systems, or food-grade biopolymers offers an eco-friendly alternative to conventional chemical synthesis methods, reducing environmental impact and enhancing biocompatibility (Singh *et al.,* 2017; Rai *et al.,* 2012). These innovations also align with the growing consumer demand for environmentally responsible technologies.

Looking ahead, future trends in nano-enabled food systems are likely to involve the integration of multiple functionalities within a single nanomaterial platform—such as combining antimicrobial activity, oxygen scavenging, and freshness sensing in one packaging material

(Huang *et al.,* 2015). Advances in nanobiosensors, smart packaging, and precision nutrient delivery will further enhance food quality, safety, and nutritional value. However, sustained progress will require interdisciplinary collaboration among material scientists, food technologists, toxicologists, and regulatory bodies to address safety, scalability, and public perception challenges.

Conclusion:

Nanotechnology has emerged as a transformative tool in food science, offering innovative solutions for preservation, processing, safety, and quality enhancement. This chapter has highlighted the diverse applications of nanoparticles, including their roles in antimicrobial packaging, antioxidant systems, targeted nutrient delivery, and smart sensing technologies. These advancements demonstrate the vast potential of nanomaterials to revolutionize the food sector by extending shelf life, improving nutritional value, enhancing sensory properties, and ensuring consumer safety.

However, the success of nanotechnology in food systems depends on more than just scientific innovation. Responsible development requires thorough safety evaluations, compliance with regulatory standards, and the adoption of eco-friendly synthesis methods. Equally important is fostering consumer trust through transparent communication about the benefits and risks of nanotechnology.

Looking ahead, the integration of green synthesis approaches, biodegradable nanomaterials, and multifunctional nano-enabled systems offers a promising pathway toward sustainable food production. By balancing technological progress with ethical and environmental considerations, nanoparticles can play a pivotal role in shaping a future where food is not only safer and longer-lasting but also produced in harmony with global sustainability goals.

Acknowledgment:

The authors gratefully acknowledge the support of the R. C. Patel Institute of Pharmacy, Shirpur, for providing access to library facilities.

List of Abbreviations:

- **Ag** – Silver
- **AgNPs** – Silver Nanoparticles
- **Au** – Gold
- **AuNPs** – Gold Nanoparticles
- **CuO** – Copper Oxide
- **DNA** – Deoxyribonucleic Acid
- **EFSA** – European Food Safety Authority
- **FDA** – U.S. Food and Drug Administration
- **FSSAI** – Food Safety and Standards Authority of India

- **GRAS** – Generally Recognized as Safe
- **MgO** – Magnesium Oxide
- **NLCs** – Nanostructured Lipid Carriers
- **NPs** – Nanoparticles
- **pH** – Potential of Hydrogen (measure of acidity/alkalinity)
- **ROS** – Reactive Oxygen Species
- **SLNs** – Solid Lipid Nanoparticles
- **TiO_2** – Titanium Dioxide
- **UV** – Ultraviolet
- **WHO** – World Health Organization
- **ZnO** – Zinc Oxide

References:

1. Augustin, M. A., & Sanguansri, L. (2009). Nanoemulsions in functional food delivery. *Nano Today, 4*(3), 209–218.
2. Augustin, M. A., & Sanguansri, L. (2009). Nanostructured materials in the food industry. *Advances in Food and Nutrition Research, 58*, 183–213.
3. Bouwmeester, H., Dekkers, S., Noordam, M. Y., Hagens, W. I., Bulder, A. S., de Heer, C., ten Voorde, S. E. C., Wijnhoven, S. W. P., Marvin, H. J. P., & Sips, A. J. A. M. (2009). Review of health safety aspects of nanotechnologies in food production. *Regulatory Toxicology and Pharmacology, 53*(1), 52–62.
4. Chaudhry, Q., Castle, L., & Watkins, R. (2008). Nanotechnologies in food. *Food Additives & Contaminants: Part A, 25*(3), 241–258.
5. Chen, L., Remondetto, G. E., & Subirade, M. (2006). Food protein-based materials as nutraceutical delivery systems. *Trends in Food Science & Technology, 17*(5), 272–283.
6. Daniel, M. C., & Astruc, D. (2004). Gold nanoparticles: Assembly, supramolecular chemistry, quantum-size-related properties, and applications toward biology, catalysis, and nanotechnology. *Chemical Reviews, 104*(1), 293–346.
7. Dekkers, S., Krystek, P., Peters, R. J. B., Lankveld, D. P. K., Bokkers, B. G. H., van Hoeven-Arentzen, P. H., Bouwmeester, H., & Oomen, A. G. (2011). Presence and risks of nanosilica in food products. *Nanotoxicology, 5*(3), 393–405.
8. Donsì, F., Annunziata, M., Vincensi, M., & Ferrari, G. (2012). Design of nanoemulsion-based delivery systems of natural antimicrobials: Effect of the emulsifier. *Journal of Biotechnology, 159*(4), 342–350.

9. EFSA Scientific Committee. (2018). Guidance on risk assessment of the application of nanoscience and nanotechnologies in the food and feed chain: Part 1, human and animal health. *EFSA Journal, 16*(7), e05327.
10. Emamifar, A., Kadivar, M., Shahedi, M., & Soleimanian-Zad, S. (2010). Evaluation of nanocomposite packaging containing Ag and ZnO on shelf life of fresh orange juice. *Innovative Food Science & Emerging Technologies, 11*(4), 742–748.
11. Food and Drug Administration (FDA). (2014). *Guidance for industry: Considering whether an FDA-regulated product involves the application of nanotechnology*. U.S. Food and Drug Administration. https://www.fda.gov
12. Food Safety and Standards Authority of India (FSSAI). (2021). *Draft guidelines for safety assessment of nanomaterials in food and food contact materials*. https://www.fssai.gov.in
13. Gyawali, R., & Ibrahim, S. A. (2014). Natural products as antimicrobial agents. *Food Control, 46*, 412–429.
14. Huang, Q., Yu, H., & Ru, Q. (2010). Bioavailability and delivery of nutraceuticals using nanotechnology. *Journal of Food Science, 75*(1), R50–R57.
15. Huang, S., Vignarooban, K., Xu, X., & Elankumaran, S. (2015). Nanotechnology in food science: Functionality and applications. *Food Science & Human Wellness, 4*(4), 155–161.
16. Huang, Y., Chen, S., Yang, Y., & Chen, Y. (2015). Effect of magnesium oxide nanoparticles on extending the shelf life of fresh-cut fruits. *Food Chemistry, 188*, 171–178.
17. Iravani, S. (2011). Green synthesis of metal nanoparticles using plants. *Green Chemistry, 13*(10), 2638–2650.
18. Krasaekoopt, W., Bhandari, B., & Deeth, H. (2003). Evaluation of encapsulation techniques of probiotics for yoghurt. *International Dairy Journal, 13*(1), 3–13.
19. Kumar, P., Mahato, D. K., Kamle, M., Mohanta, T. K., & Kang, S. G. (2019). Nanotechnology interventions in agri-food systems to improve nutrition and health. *Food Frontiers, 1*(1), 3–22.
20. Kumar, R., Bhardwaj, A., & Bhardwaj, R. (2021). Recent advances in food preservation using nanotechnology. *Food Reviews International, 37*(3), 244–270.
21. McClements, D. J. (2012a). Nanoemulsions versus microemulsions: Terminology, differences, and similarities. *Soft Matter, 8*(6), 1719–1729.
22. McClements, D. J. (2012b). Nanoemulsions for improving the bioavailability of hydrophobic foods. *Annual Review of Food Science and Technology, 3*, 219–243.
23. McClements, D. J. (2012). Nanoemulsions for improving the delivery of food ingredients. *Current Opinion in Colloid & Interface Science, 17*(4), 235–245.
24. McClements, D. J., Decker, E. A., & Weiss, J. (2009). Emulsion-based delivery systems for lipophilic bioactive components. *Journal of Food Science, 74*(7), R100–R111.

25. McClements, D. J., & Rao, J. (2011). Food-grade nanoemulsions: Formulation, fabrication, properties, performance, biological fate, and potential toxicity. *Critical Reviews in Food Science and Nutrition, 51*(4), 285–330.
26. McClements, D. J., & Xiao, H. (2017). Potential biological fate of ingested nanoemulsions: Influence of particle characteristics. *Food & Function, 8*(1), 15–27.
27. Oberdörster, G., Oberdörster, E., & Oberdörster, J. (2005). Nanotoxicology: An emerging discipline evolving from studies of ultrafine particles. *Environmental Health Perspectives, 113*(7), 823–839.
28. Oehlke, K., Adamiuk, M., Behsnilian, D., Gräf, V., Mayer-Miebach, E., Walz, E., & Greiner, R. (2014). Potential bioavailability enhancement of bioactive compounds using food-grade engineered nanomaterials: A review of the existing evidence. *Food & Function, 5*(7), 1341–1359.
29. Patel, A. R., & Velikov, K. P. (2012). Colloidal delivery systems in foods: A general comparison with oral drug delivery. *LWT - Food Science and Technology, 46*(2), 413–420.
30. Patel, A. R., & Velikov, K. P. (2011). Colloidal delivery systems in foods: A general comparison with oral drug delivery. *LWT - Food Science and Technology, 44*(9), 1958–1964.
31. Qian, C., Decker, E. A., Xiao, H., & McClements, D. J. (2012). Physical and chemical stability of β-carotene-enriched nanoemulsions: Influence of pH, ionic strength, and temperature. *Food Chemistry, 132*(3), 1221–1229.
32. Qian, C., & McClements, D. J. (2011). Formation of nanoemulsions stabilized by model food-grade emulsifiers using high-pressure homogenization: Factors affecting particle size. *Food Hydrocolloids, 25*(5), 1000–1008.
33. Rai, M., Yadav, A., & Gade, A. (2009). Silver nanoparticles as a new generation of antimicrobials. *Biotechnology Advances, 27*(1), 76–83.
34. Rai, M., Yadav, A., & Gade, A. (2012). Current trends in phytosynthesis of metal nanoparticles for applications in medicine and technology. *Journal of Nanomedicine & Nanotechnology, 3*(2), 1–7.
35. Ravichandran, R. (2010). Nanotechnology applications in food and food processing: Innovative green approaches, opportunities and uncertainties for global market. *International Journal of Green Nanotechnology: Physics and Chemistry, 1*(2), P72–P96.
36. Sanguansri, L., & Augustin, M. A. (2006). Nanoscale materials development – A food industry perspective. *Trends in Food Science & Technology, 17*(10), 547–556.
37. Siegrist, M., Stampfli, N., Kastenholz, H., & Keller, C. (2007). Perceived risks and perceived benefits of different nanotechnology foods and nanotechnology food packaging. *Appetite, 49*(2), 459–466.

38. Silva, H. D., Cerqueira, M. A., & Vicente, A. A. (2012). Nanoemulsions for food applications: Development and characterization. *Food and Bioprocess Technology, 5*(3), 854–867.
39. Singh, P., Kim, Y. J., Zhang, D., & Yang, D. C. (2016). Biological synthesis of nanoparticles from plants and microorganisms. *Trends in Biotechnology, 34*(7), 588–599.
40. Singh, P., & Nalwa, H. S. (2011). Medical applications of nanoparticles in biological imaging, cell labeling, antimicrobial agents, and anticancer nanodrugs. *Journal of Biomedical Nanotechnology, 7*(4), 489–503.
41. Sinha, V. R., Bansal, K., Kaushik, R., Kumria, R., & Trehan, A. (2004). Poly-ε-caprolactone microspheres and nanospheres: An overview. *International Journal of Pharmaceutics, 278*(1), 1–23.
42. Sozer, N., & Kokini, J. L. (2009). Nanotechnology and its applications in the food sector. *Trends in Biotechnology, 27*(2), 82–89.
43. Weiss, J., Takhistov, P., & McClements, D. J. (2006). Functional materials in food nanotechnology. *Journal of Food Science, 71*(9), R107–R116.
44. World Health Organization. (2020). *Food safety*. https://www.who.int/news-room/fact-sheets/detail/food-safety

APPLYING THE 12 PRINCIPLES OF GREEN CHEMISTRY TO NANOPARTICLE PRODUCTION

Rishabh Bhardwaj*[1], Meenal Maan[2], Vivek[2] and Mohd Nayeem Ali[3]
[1]Department of Chemistry,
[2]Faculty of Basic Science,
[3]Faculty of Agriculture,
Shri Ram College, Muzaffarnagar, U. P. 251 001
*Corresponding author E-mail: bhardwajrs14@gmail.com

Abstract:

Nanotechnology has emerged as a transformative field across industries, from medicine and energy to agriculture and environmental remediation. However, conventional nanoparticle synthesis methods often involve toxic chemicals, high energy consumption, and environmentally hazardous by-products. This chapter explores how the 12 Principles of Green Chemistry, proposed by Paul Anastas and John Warner, can be strategically applied to nanoparticle production. The integration of green chemistry in nanoparticle synthesis fosters environmentally benign, cost-effective, and sustainable practices, essential for the future of materials science and industrial innovation.

1. Introduction:

Nanoparticles possess unique physical and chemical properties due to their nanoscale size (1–100 nm), which enables diverse applications. Despite their potential, traditional synthesis techniques often neglect environmental and health safety. Green chemistry offers a robust framework for rethinking nanoparticle production to align with principles of sustainability. This chapter dissects each of the 12 principles and illustrates their relevance and application to nanoparticle synthesis and functionalization.

2. Overview of the 12 Principles of Green Chemistry

The 12 Principles are:

1. Prevention
2. Atom Economy
3. Less Hazardous Chemical Syntheses
4. Designing Safer Chemicals
5. Safer Solvents and Auxiliaries
6. Design for Energy Efficiency
7. Use of Renewable Feedstocks
8. Reduce Derivatives

9. Catalysis
10. Design for Degradation
11. Real-time Analysis for Pollution Prevention
12. Inherently Safer Chemistry for Accident Prevention

Each principle is explored below in the context of nanoparticle production.

3. Applying the Principles to Nanoparticle Synthesis

3.1 Prevention

Traditional issue: Many nanoparticle synthesis methods generate toxic waste, especially in wet-chemical reduction and sol-gel methods.

Green solution: Use of plant extracts, microorganisms, and biodegradable templates avoids harmful waste. Biosynthesis methods inherently reduce by-products.

Example: Using Azadirachta indica (neem) extract for silver nanoparticle synthesis eliminates the need for toxic reducing agents.

3.2 Atom Economy

Traditional issue: Inefficient use of reagents results in significant waste.

Green solution: Optimizing reactions such that most of the starting materials are incorporated into the final nanoparticles.

Example: One-pot green syntheses using natural polymers as both reducing and stabilizing agents enhance atom economy.

3.3 Less Hazardous Chemical Synthesis

Traditional issue: Use of sodium borohydride, hydrazine, and organic solvents poses toxicity risks.

Green solution: Replace with benign alternatives like ascorbic acid, citric acid, or amino acids for reduction.

Example: Gold nanoparticles synthesized using glucose as a reducing agent in aqueous medium.

3.4 Designing Safer Chemicals

Traditional issue: Functionalized nanoparticles may introduce toxic surface coatings.

Green solution: Design biocompatible and biodegradable coatings—such as chitosan or dextran—to reduce toxicity.

Example: Iron oxide nanoparticles coated with dextran used in MRI imaging with reduced cytotoxicity.

3.5 Safer Solvents and Auxiliaries

Traditional issue: Organic solvents like toluene or DMF are often used.

Green solution: Employ water, ethanol, or supercritical CO_2 as safer alternatives.

Example: Green synthesis of ZnO nanoparticles in water-ethanol mixtures.

3.6 Design for Energy Efficiency

Traditional issue: High-temperature or prolonged reaction times increase energy use.

Green solution: Use microwave, sonochemical, or photochemical methods that reduce energy consumption.

Example: Rapid microwave-assisted synthesis of TiO_2 nanoparticles in <10 minutes under ambient conditions.

3.7 Use of Renewable Feedstocks

Traditional issue: Petroleum-derived stabilizers and surfactants.

Green solution: Use renewable materials like starch, cellulose, gelatin, or plant oils.

Example: Starch-mediated synthesis of gold nanoparticles serves both as a stabilizer and mild reductant.

3.8 Reduce Derivatives

Traditional issue: Functionalization steps often involve protecting groups or multi-step synthesis.

Green solution: Direct synthesis routes avoiding unnecessary intermediates.

Example: In-situ functionalization of silica nanoparticles with green silanes during formation, bypassing post-processing.

3.9 Catalysis

Traditional issue: Stoichiometric reagents used for reduction.

Green solution: Utilize nanocatalysts or enzyme-mediated synthesis that require only small quantities.

Example: Enzyme-assisted biosynthesis of palladium nanoparticles using Shewanella oneidensis.

3.10 Design for Degradation

Traditional issue: Persistent nanoparticles accumulate in the environment.

Green solution: Design nanoparticles to break down into non-toxic components.

Example: Poly (lactic acid)-coated nanoparticles degrade into water and CO_2 over time.

3.11 Real-time Analysis for Pollution Prevention

Traditional issue: Lack of in-process monitoring leads to overdosing or contamination.

Green solution: Integrate spectroscopic or electrochemical real-time monitoring during synthesis.

Example: In-situ UV-Vis monitoring of silver nanoparticle growth enables process control and minimizes waste.

3.12 Inherently Safer Chemistry for Accident Prevention

Traditional issue: High-pressure or explosive reagents (e.g., hydrazine) pose risks.

Green solution: Substitute with low-risk reagents and ambient-condition processes.

Example: Room-temperature synthesis of ZnO nanoparticles using lemon juice as reducing agent.

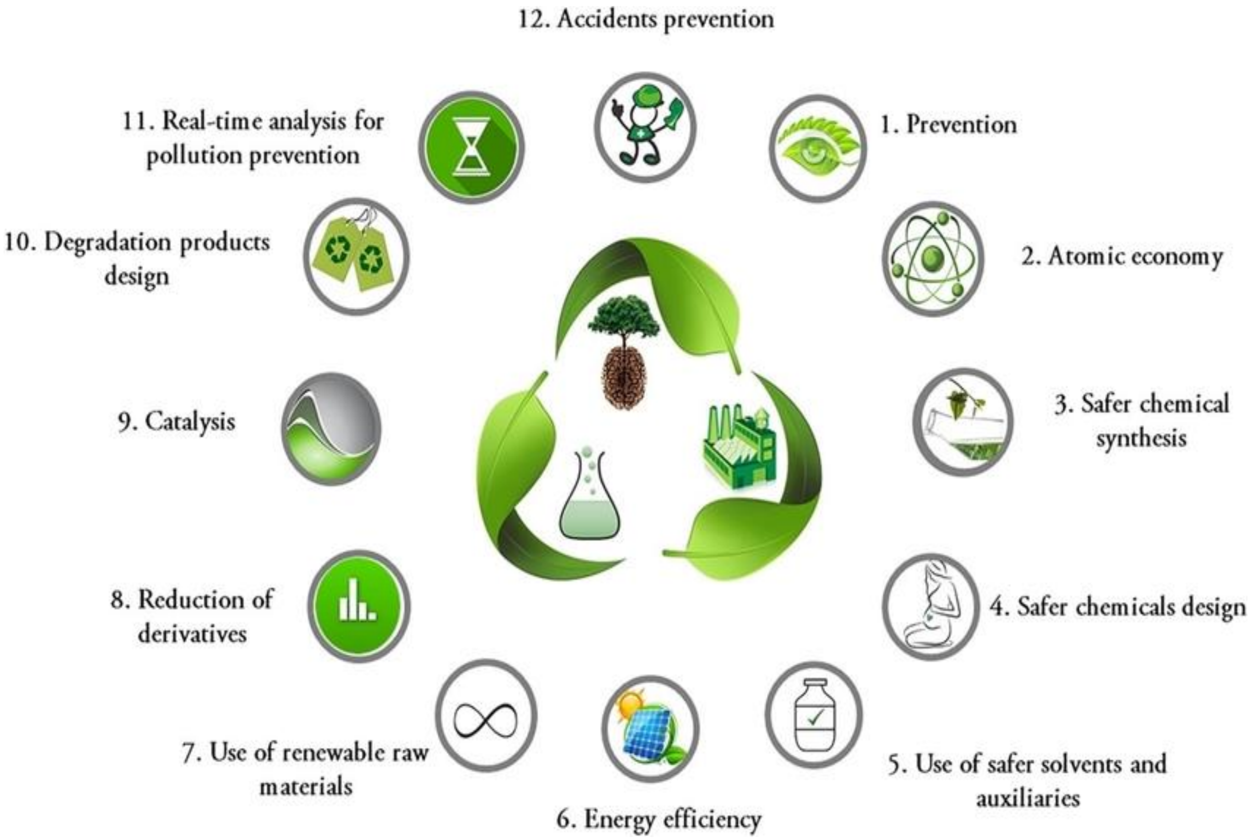


Figure 1: 12 Principles of Green Chemistry

4. Case Study: Green Synthesis of Silver Nanoparticles Using Citrus Peel Extract

Parameter	Conventional Method	Green Method
Reducing Agent	Sodium borohydride	Citrus peel extract (rich in ascorbic acid)
Solvent	Ethanol/Organic solvent	Water
Stabilizer	CTAB or PVP	Natural polyphenols
By-products	Borates	None
Toxicity	High	Low
Energy Requirement	High (heating required)	Ambient

5. Challenges and Future Prospects

- Standardization: Biosynthetic methods are difficult to reproduce across labs.
- Scalability: Green methods often have lower yields in industrial-scale processes.
- Toxicity Evaluation: Even green-synthesized nanoparticles require full environmental and biological impact assessments.

Emerging tools like machine learning, AI-driven process control, and life cycle assessments (LCA) can help address these challenges.

Conclusion:

Integrating the 12 Principles of Green Chemistry into nanoparticle production is not only environmentally imperative but also economically viable in the long run. By redesigning processes to align with these principles, researchers and industries can contribute to sustainable nanotechnology. The path forward lies in multidisciplinary collaboration, policy support, and continued innovation.

References:

1. Anastas, P. T., & Warner, J. C. (1998). *Green chemistry: Theory and practice*. Oxford University Press.
2. Iravani, S. (2011). Green synthesis of metal nanoparticles using plants. *Green Chemistry, 13*(10), 2638–2650.
3. Ahmed, S., Ahmad, M., Swami, B. L., & Ikram, S. (2016). A review on plants extract mediated synthesis of silver nanoparticles. *Arabian Journal of Chemistry, 9*(2), 113–130.
4. Sharma, V. K., Yngard, R. A., & Lin, Y. (2009). Silver nanoparticles: Green synthesis and their antimicrobial activities. *Advances in Colloid and Interface Science, 145*(1–2), 83–96.
5. Singh, P., Kim, Y. J., Zhang, D., & Yang, D. C. (2018). Biological synthesis of nanoparticles from plants and microorganisms. *Trends in Biotechnology, 36*(6), 588–602.
6. Kharissova, O. V., Dias, H. R., Kharisov, B. I., Pérez, B. O., & Pérez, V. M. J. (2013). The greener synthesis of nanoparticles. *Trends in Biotechnology, 31*(4), 240–248.
7. Mittal, A. K., Chisti, Y., & Banerjee, U. C. (2013). Biosynthesis of nanoparticles: A review. *Journal of Nanoparticles, 2013*, Article 1–20.
8. Raveendran, P., Fu, J., & Wallen, S. L. (2003). Completely "green" synthesis and stabilization of metal nanoparticles. *Journal of the American Chemical Society, 125*(46), 13940–13941.
9. Singh, J., Dutta, T., Kim, K.-H., Rawat, M., Samddar, P., & Kumar, P. (2018). Biological synthesis of nanoparticles from plants and microorganisms. *Trends in Biotechnology, 36*(6), 588–602.
10. Gawande, M. B., Pandey, R. K., & Jayaram, R. V. (2013). Green chemistry: A strategy for chemical sustainability. *Green Chemistry, 15*, 189–207.
11. Baruwati, B., Polshettiwar, V., & Varma, R. S. (2009). Green synthesis of silver nanoparticles using leaves of *Syzygium cumini* and their application in catalytic reduction of dyes. *ChemSusChem, 2*(10), 1041–1047.
12. Kuppusamy, P., Yusoff, M. M., Maniam, G. P., & Govindan, N. (2016). Biosynthesis of metallic nanoparticles using plant derivatives and their new avenues in pharmacological applications—An updated report. *Journal of Nanostructure in Chemistry, 6*(1), 1–13.
13. Kumar, A., Kumar, A., Sharma, S., & Pandey, L. M. (2021). Advances in green synthesis of nanoparticles: A review. *Biointerface Research in Applied Chemistry, 11*(3), 10952–10974.
14. Roy, A., Bulut, O., Some, S., Mandal, A. K., & Yilmaz, M. D. (2021). Recent advancements in green synthesis of metal nanoparticles. *Materials Today: Proceedings, 46*, 1286–1290.

15. Sosa, I. O., Noguez, C., & Barrera, R. G. (2003). Optical properties of metal nanoparticles with arbitrary shapes. *The Journal of Physical Chemistry B, 107*(26), 6269–6275.
16. Vigneshwaran, N., Nachane, R. P., Balasubramanya, R. H., & Varadarajan, P. V. (2006). Biological synthesis of silver nanoparticles using *Staphylococcus aureus* and their antimicrobial activity. *Biotechnology Letters, 28*, 1347–1352.
17. Ahmad, A., Senapati, S., Khan, M. I., Kumar, R., & Sastry, M. (2003). Intracellular synthesis of gold nanoparticles by a novel alkalotolerant actinomycete. *Nanotechnology, 14*(7), 824–828.
18. Mohanpuria, P., Rana, N. K., & Yadav, S. K. (2008). Biosynthesis of nanoparticles: Technological concepts and future applications. *Journal of Nanoparticle Research, 10*(3), 507–517.
19. Salata, O. V. (2004). Applications of nanoparticles in biology and medicine. *Journal of Nanobiotechnology, 2*(1), 3.
20. Jain, D., Daima, H. K., Kachhwaha, S., & Kothari, S. L. (2009). Green synthesis of silver nanoparticles using *Argemone mexicana* leaf extract and evaluation of their antimicrobial activities. *Digest Journal of Nanomaterials and Biostructures, 4*(3), 557–563.

THE BASICS OF PHYSICAL AND CHEMICAL SCIENCE: MATTER AND MOTION

Jagdish Chavan*, Rajendra Patil, Sudhakar Ujgare and Anil Beldar
Department of Chemistry,
Poojya Sane Guruji Vidya Prasarak Mandal's Sajan Isan Patil Arts,
Girdhar Barku Patel Science, and Shahada Taluka Kharedi Vikri Sangh Commerce College,
Shahada, Nandurbar, INDIA (425409)
*Corresponding author E-mail: chavanju@gmail.com

Abstrtact:

The concise overview of the foundational principles of matter and motion that unite physics and chemistry. It describes the nature and states of matter, the structure of atoms and subatomic particles, and the quantum mechanics that govern microscopic behaviour. Key laws Newton's laws of motion, conservation principles, and thermodynamics are outlined to show how energy, forces, and motion shape the universe at all scales. Chemical reactions, energy transfer, and phase changes are discussed to illustrate how matter transforms. Together, these concepts reveal the deep interconnectedness governing both daily life and scientific discovery.

Introduction:

Studying matter and motion is not just an academic exercise; it is an important journey that connects the physical and chemical sciences and helps us understand how the universe works in more detail. The many different things we see every day are possible because particles are always moving at the atomic and molecular levels. The laws of physics are what make everything work, from the smallest particles to the largest galaxies. These laws are based on the little movements and the forces that act on them. This ongoing exploration invites us to marvel at the complex dance of particles and forces, revealing the profound interconnectedness that underpins the fabric of the cosmos. We have already talked about the basic ideas of matter and motion in this chapter, like the laws of motion and atomic theory. This part will go into these ideas even more. We will examine the processes that result in the formation of matter, its behavior at the quantum level, and the functioning of forces across various scales. We will also look into how these interactions cause the many different things we see, from simple chemical reactions to the complex physical laws that govern celestial bodies. This will help us learn about the basic laws that govern the universe.

This chapter will give you a solid understanding of how the basic ideas of physics and chemistry affect the universe in both everyday situations and at the deepest levels of scientific research. As we start this journey of discovery through these hard subjects, we will learn about quantum mechanics, the strange nature of time and space, and the basic rules that govern everything in the universe. This will help us learn more about how the universe is put together.

The Essence of Matter

Matter is what makes up everything in the universe, even the things we can touch and see. It is the most basic part of all matter and energy, and it makes up the many different things in the universe. The air we breathe is made of gases, the oceans are made of liquid water, and the stars in the night sky are made of glowing gases and plasma. All of these things are types of matter. There are many different kinds of matter, like solids, liquids, gases, and plasma. Every kind has its own set of traits. By studying matter, we can learn about the universe and the laws of physics that explain how everything works.

The Building Blocks of Matter are Subatomic Particles

We need to know about the atomic and subatomic particles that make up everything in order to understand what matter is. Atoms, which are the smallest parts of matter, are made up of three basic parts: protons, neutrons, and electrons. Protons and neutrons are found in the nucleus, which is the center of the atom. Electrons, on the other hand, move around the nucleus at different energy levels. These tiny particles inside an atom determine how it acts and what it is like. They affect everything from how chemicals interact to how materials feel. The first step to understanding more complex structures and events in the universe is to understand these particles. This shows how important atomic science is for making progress in technology and learning.

The nucleus of an atom contains protons, which are particles with a positive charge. The atomic number tells you what element it is by telling you how many protons are in the atom's nucleus. This is a very important step in figuring out what an element is. For example, there are six protons in a carbon atom and one proton in a hydrogen atom. Protons also change how stable and chemically reactive an atom is by interacting with neutrons and electrons.

Neutrons are tiny particles that live in the nucleus of an atom. Neutrons are called uncharged particles because they don't have an electric charge like protons do. Neutrons are important for the stability of the atomic nucleus even though they don't have a charge. They help stop the nucleus from breaking apart by fighting against the positive repulsion between protons. Different isotopes can exist because the number of neutrons in atoms of the same element can change. For instance, carbon usually has six neutrons, but carbon-14 has eight neutrons. These changes can change the physical and chemical properties of an element. Neutrons are important parts of atomic structure that make isotopes different from each other and are important for nuclear reactions and stability.

Electrons are very small particles with a negative charge that quickly move around the nucleus of an atom. They are in certain areas called energy levels or orbitals. These particles are very important in chemistry because they make chemical bonds between atoms, which affects how substances react, combine, or interact with each other. The way electrons act affects how reactive atoms are, which is why they are so important to understanding chemical reactions and the properties of different elements. The variety of matter and the intricacy of chemical processes in nature and industry are due to their dynamic movement and interactions.

Quantum mechanics is a branch of physics that explains how matter behaves at the atomic and subatomic levels. This is how we know about these particles. Heisenberg's uncertainty principle posits that the precise position and momentum of a particle cannot be concurrently determined. This principle fundamentally contests classical mechanics and posits that particles lack precise positions, existing instead as probability distributions.

The Structure of Atoms and the Arrangement of Electrons

There are certain rules that govern how electrons are arranged in an atom. These rules help explain the chemical properties of an element. These electrons are in different energy levels or orbitals, which are like layers or areas around the nucleus where electrons are likely to be found. The Pauli exclusion principle, a basic idea in quantum mechanics, says that no two electrons in an atom can have the same quantum state. This means that they can't be in the same place at the same energy level. Hund's rule, on the other hand, helps us understand how electrons spread out in these orbitals. It says that electrons will fill empty orbitals one at a time as much as possible before pairing up, which usually means that there are more unpaired electrons. This arrangement affects how atoms react, bond, and behave chemically, showing how beautiful and complicated atomic structure is [1].

In chemistry, electron configuration is very important for understanding how atoms and molecules act. It tells you where electrons are in relation to the nucleus of an atom, which has a direct effect on how atoms bond with each other and take part in chemical reactions. The octet rule, which is one of the first things you learn in chemistry, says that atoms are most stable when their outermost electron shell has eight electrons in it. This tendency is what makes chemical bonds happen. Atoms will gain, lose, or share electrons to get to this stable state. These kinds of interactions are what make up a lot of chemical compounds, from simple molecules like water to more complex biological structures. The electron configuration elucidates bonding mechanisms and offers insights into the reactivity and stability of various elements within our universe [2].

Quantum Mechanics and the Essence of Matter

Quantum mechanics explains how particles that are so small that we can't see them with our eyes behave. One of the most interesting things about this field is the wave-particle duality principle, which says that particles like electrons can act like both waves and particles, depending on how they are looked at. Louis de Broglie, a physicist, came up with this groundbreaking idea. He thought that electrons, which were thought of as particles, also had wave-like properties. Experiments that showed how electrons diffract quickly confirmed this idea. These experiments showed that electrons could make interference patterns like waves. These discoveries changed the way we think about the microscopic universe and led to the development of quantum mechanics, which is an important part of modern physics that helps us understand things at the atomic and subatomic levels [3].

The Schrödinger equation is a mathematical way to describe how particles behave like waves, which is an important part of quantum mechanics. The solutions to this equation create orbitals, which are areas of space where an electron is likely to be found. These orbitals are not set paths; they are probabilistic clouds that show how complicated atomic and molecular structure is. They are the building blocks of chemical bonds and how molecules behave, which affects how atoms interact, bond, and make the molecules that make up everything around us. This knowledge has changed the way we study chemistry and physics, allowing scientists to guess and change the properties of materials at the atomic level [4].

The Different States of Matter

Matter exists in different states, and each state has its own set of properties that affect how it acts in different situations. At the molecular level, how particles are arranged and how much energy they have are very important for deciding what kind of matter it is. For instance, in a solid, the particles are very close together and only vibrate in place. This gives the solid a clear shape and volume. Particles in liquids are not as tightly bound together, which lets them flow and take the shape of their container while keeping their volume the same. Gases are made up of particles that are far apart and can move freely, completely filling their container. Plasma is often thought of as the fourth state. It is made up of ionized particles that are electrically charged and are found in places with very high energy, like stars or lightning. We can better understand these states by looking at how atoms move and how particles interact with each other. This helps us see how matter can change shape and how these changes happen in different situations, showing how dynamic the material universe is[5].

Solid: Particles in solids are tightly packed together in a regular pattern and vibrate in place. The particles in solids are held together by strong forces, which give them a definite shape and volume. Because the particles are tightly bound together, solids keep their shape unless an outside force is applied. This makes them stable and rigid.

Liquid: Particles in liquids are close together but can move past each other. Liquids have a set amount of space, but they take on the shape of the container they are in. Because the forces between particles are weaker than in solids, liquids can flow and change shape to fit their containers. This fluidity makes liquids useful in everyday life, like water in a glass or milk in a bottle.

Gas: The particles in gas are very far apart and move quickly in all directions. Gases don't have a set shape or volume, and they will fill any space they are in. The particles in a gas have a lot of energy, which lets them break free from the forces that would normally keep them together.

Because gases have a lot of energy, they can compress and expand. This is important in many natural and industrial processes, like breathing and engines.

Plasma: Plasma is a gas that has been ionized, which means that electrons have been taken away from atoms, leaving behind positively charged ions and free electrons. Plasmas can be found in stars, lightning, and some kinds of electrical discharges. They are often called the fourth state of matter because they have their own electrical conductivity and react to electromagnetic fields. This makes them useful in things like fluorescent lights, plasma TVs, and experimental fusion reactors.

Energy Transfer and Phase Changes

A basic idea in physical science is that matter can change states depending on how much energy is put into it. When you add energy to something, like heating a solid, its particles get more kinetic energy and may change state. For example, they may go from being a solid to a liquid (melting) or from being a liquid to a gas (boiling). You can see this happen in everyday life, like when ice melts on a warm day or water boils on the stove. On the other hand, taking away energy, like cooling a gas or liquid, can make the substance condense or freeze, turning it back into a solid or liquid. We can control and predict how materials will behave in different situations, from weather patterns to industrial processes, by understanding these changes in state.

The latent heat is the amount of heat needed to change a substance's phase without changing its temperature. Instead of raising the temperature, energy is absorbed or released during melting, boiling, or condensation to break or form intermolecular forces [6], [7].

The Nature of Movement

One of the most important things about the universe is motion. Understanding motion is important for understanding the physical world, whether it's the movement of atoms, the movement of planets, or the interaction of light and matter. Kinematics is the study of motion itself, and dynamics is the study of the forces that cause motion. People have always been interested in motion. From the first astronomers who mapped the paths of stars to today's physicists who study the tiny world, our desire to know how and why things move has led to many scientific discoveries. This quest has not only taught us more, but it has also led to technological advances that affect our daily lives. For example, knowing Newton's laws of motion helped us make transportation systems that work well, and learning about electromagnetic waves led to new ways to communicate[8].

The Laws of Motion

Newton's Three Laws of Motion help us understand how forces affect motion:

First Law (Inertia): An object will stay still or move at a constant speed unless something outside of it acts on it. This law shows that objects naturally resist changes in motion, which is called inertia. For instance, if you push a book across a table, it will stop moving because of friction unless something keeps it moving. This principle helps us figure out why things act the way they do in real life.

The Second Law (F = ma) says that the force acting on an object is equal to the object's mass times its acceleration. This equation tells us how things react to forces, and it's important for understanding everything from how cars move to how stars and planets move. For example, it takes more force to speed up a car with a lot of weight than one with less weight. It also tells us why astronauts feel more thrust when they launch a big spacecraft than when they launch a small drone.

Third Law (Action and Reaction): For every action, there is an equal and opposite reaction. This law tells us how objects interact with each other and how forces work. When a rocket's engines release gas, the gas pushes the rocket in the opposite direction, which lets it take off. You can feel a push back when you push against a wall for the same reason. This basic idea is what makes flying, moving, and even walking possible.

Work and Kinetic Energy

Kinetic energy is the energy of an object due to its motion and is given by the equation:

$$KE = \frac{1}{2}mv^2$$

Where:

- m is the mass of the object.
- v is the velocity of the object

When a force moves an object, it is said to be doing work. For instance, moving a box across the floor or lifting a weight are both examples of work. The work-energy theorem says that the work done on an object is the same as the change in its kinetic energy. This means that when energy is added to or taken away from an object, its motion changes in the same way. This relationship is important for figuring out how moving objects work, since it lets us guess how they will react to different forces and situations. It is a fundamental principle in physics that links the concepts of force, motion, and energy to elucidate numerous real-world phenomena [9].

Laws of Conservation

The conservation laws are basic rules that explain how matter and energy behave:

The total amount of energy in a system that is not connected to anything else stays the same. Energy cannot be created or destroyed; it can only be converted from one form to another, such as from potential to kinetic energy. This principle is very important in physics and helps us understand a lot of natural events, like how planets move and how we do things like run or heat water every day.

The total momentum of a system stays the same unless an outside force acts on it. An object's mass and speed are what give it momentum. This idea is very important for looking at collisions, whether they are car crashes, billiard balls hitting each other, or particles interacting at the quantum level. It reminds us that the overall motion of a system stays the same when there are no outside forces acting on it. This gives us a stable way to predict what will happen in different physical situations [10].

The Role of Matter in Motion and Chemical Reactions

Chemical reactions are the interesting processes that change one set of substances into another. They are what make up the material world around us. The complex and beautiful ways that atoms are rearranged and the forces that act on them cause these changes. Chemical kinetics looks at how fast reactions happen, and thermodynamics looks at the energy changes that happen during these reactions. Not only do these reactions help us understand the basic workings of nature, but they also help us make new materials, medicines, and technologies that make our lives better.

Different Kinds of Chemical Reactions

Synthesis Reactions: Two or more reactants come together to make one product. For instance, when hydrogen and oxygen come together, they make water:

$$2H_2 + O_2 \rightarrow 2H_2O$$

Decomposition Reactions: One reactant breaks down into two or more products. For instance, calcium carbonate breaks down into calcium oxide and carbon dioxide:

$$2H_2 + O_2 \rightarrow 2H_2O$$

Combustion Reactions: When a substance burns, it reacts with oxygen and gives off energy as heat and light. For instance, burning methane:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

Reactions that involve the transfer of electrons between substances are called redox reactions. A redox reaction is when hydrogen and oxygen react to make water, with hydrogen being oxidized and oxygen being reduced [11], [12].

Energy of Activation and Catalysis

Every chemical reaction needs an activation energy, which is the energy needed to break the bonds between the reactants and start the reaction. Think of it like the first push that gets a ball rolling down a hill. Catalysts are things that lower the activation energy, which makes the reaction go faster and often speeds up the process a lot. Enzymes are a special kind of biological catalyst that are very important for many biochemical processes that keep life going. They help cells react without being used up, acting like very efficient biological machines that make it possible for the body to do things like digest food, make energy, and copy DNA. Without enzymes, many of these important reactions would happen too slowly for life as we know it to happen.

Thermodynamics and the Cosmos

Thermodynamics is the study of how energy changes and how matter reacts to those changes. The laws of thermodynamics explain how energy moves through systems and control everything from how gases behave to how well engines work. This field is very important for understanding a lot of natural and man-made processes. Thermodynamics explains how refrigerators keep food cold, how engines turn fuel into motion, and even how our bodies make and use energy in everyday life. Thermodynamics helps scientists and engineers make machines that work better, come up with ways to get energy that don't run out, and learn more about the universe [13], [14].

The Rules of Thermodynamics

First Law (Conservation of Energy): Energy can't be made or destroyed; it can only change form. This principle is necessary for understanding how both chemical and mechanical processes work. Even though energy can change forms (for example, from potential to kinetic energy), the total energy of an isolated system stays the same.

Second Law (Entropy): Entropy tells you how random or disordered a system is. The second law says that when energy moves from one place to another, the total entropy of an isolated system tends to go up. This law explains why energy loses its usefulness over time: changes in energy often make things more chaotic.

Third Law (Absolute Zero): The closer a system gets to absolute zero, the less entropy it has. At absolute zero, molecular motion comes to a halt, and matter reaches its most ordered state.

Conclusion:

In conclusion, the study of matter and motion shows that there is a deep, interconnected web of rules that govern every part of life. Universal laws that can be explained through math and theory control the movement of all matter, from the smallest atoms to the biggest galaxies. These laws include quantum interactions, chemical reactions, and the movement of celestial bodies. These laws not only help us make sense of the universe, but they also make us curious and amazed by how complicated nature is. Scientists and other thinkers push the limits of what we know by constantly looking into these ideas. They remind us of how much we still have to learn and how powerful human curiosity can be in unlocking the mysteries of the universe.

Knowing about matter, motion, and energy is useful in everyday life, from making computers and engines to making medical advances and exploring space. As we learn more about these basic ideas, we open the door to even more important discoveries that will change the course of science and humanity.

References:

1. Atkins, P. & de Paula, J. (2018). *Atkins' Physical Chemistry*. 11th Edition, Oxford University Press.
2. Halliday, D., Resnick, R., & Walker, J. (2014). *Fundamentals of Physics*. 10th Edition, Wiley.
3. Levine, I. N. (2014). *Quantum Chemistry*. 7th Edition, Pearson.
4. Cotton, F. A., Wilkinson, G., Murillo, C. A., & Bochmann, M. (1999). *Advanced Inorganic Chemistry*. 6th Edition, Wiley-Interscience.

5. Zumdahl, S. S., & Zumdahl, S. A. (2020). *Chemistry: An Atoms First Approach*. 3rd Edition, Cengage Learning.
6. Silbey, R. J., Alberty, R. A., & Bawendi, M. G. (2004). *Physical Chemistry*. 4th Edition, Wiley.
7. Tipler, P. A., & Mosca, G. (2007). *Physics for Scientists and Engineers*. 6th Edition, W.H. Freeman.
8. Atkins, P. & Friedman, R. (2011). *Molecular Quantum Mechanics*. 5th Edition, Oxford University Press.
9. Laidler, K. J., Meiser, J. H., & Sanctuary, B. C. (2003). *Physical Chemistry*. 4th Edition, Houghton Mifflin.
10. Einstein, A. (1905). *On the Electrodynamics of Moving Bodies*. Annalen der Physik, 17, 891–921.
11. Callen, H. B. (1985). *Thermodynamics and an Introduction to Thermostatistics*. 2nd Edition, Wiley.
12. Arfken, G. B., Weber, H. J., & Harris, F. E. (2012). *Mathematical Methods for Physicists*. 7th Edition, Academic Press.
13. Heisenberg, W. (1927). *Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik*. Zeitschrift für Physik, 43, 172–198.
14. de Broglie, L. (1924). *Recherches sur la théorie des quanta*. Annales de Physique, 10, 22–128.

BEYOND BONDS: THE EVOLVING FRONTIER OF ORGANIC CHEMISTRY

Priyabrata Roy
Department of Chemistry,
Victoria Institution (College), 78B, A.P.C. Road, Kolkata 700009, India
Corresponding author E-mail: priyo_chem@yahoo.co.in

Abstract:

Organic chemistry has long been described as the chemistry of carbon compounds — but its scope today is far broader and more dynamic than that simple definition suggests. This chapter explores how organic chemistry shapes nearly every aspect of modern life, from the creation of synthetic dyes, plastics, and flavours to the discovery and manufacture of lifesaving pharmaceuticals and agrochemicals. It traces the field's origins in natural products like indigo and pyrethrins to today's vast petrochemical and pharmaceutical industries, which produce millions of tonnes of essential molecules each year. Along the way, the chapter highlights fascinating examples — including surprising molecules such as foscarnet that blur the lines between organic and inorganic chemistry — and explains how chemists work at the frontiers of disciplines once seen as separate. In doing so, this chapter shows how the ever-evolving practice of organic chemistry demonstrates the richness that comes from breaking traditional boundaries, revealing a science that continues to create, adapt, and impact society in ways both expected and unexpected.

Keywords: Organic Chemistry, Synthetic Molecules, Pharmaceuticals, Agrochemicals, Industrial Chemistry.

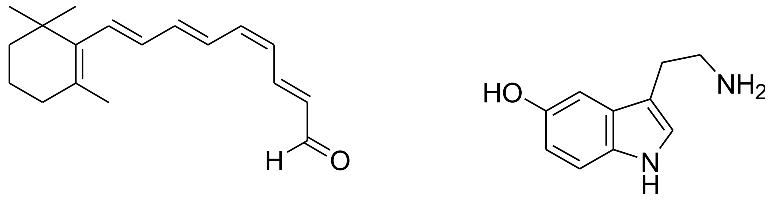
1. Introduction:

Chemistry, like every scientific discipline, holds a fundamental place in shaping our understanding of the universe. At its core, it is the science of molecules — their structures, transformations, and interactions. Chemists work hand in hand with physicists and mathematicians to reveal how molecules behave under various conditions and collaborate with biologists to uncover how molecular processes govern life itself [1].

Among the many branches of chemistry, organic chemistry stands out as an ever-evolving field. It does not merely study existing molecules but goes a step further — it imagines and constructs entirely new ones. This remarkable ability to design and synthesize novel compounds has revolutionized modern life. From life-saving pharmaceuticals and innovative polymers to vibrant dyes, fragrances, and advanced materials, organic chemistry continuously expands the limits of what is possible.

There are occasional concerns that such human-made compounds are somehow "unnatural" or inherently harmful. However, this perception overlooks a fundamental truth: these molecules are assembled by humans from building blocks already present in nature, guided by our knowledge and creativity. Just as birds instinctively weave nests and beavers build dams, humans transform nature's raw materials into things that support and enrich our lives — houses, medicines, textiles, and countless other essentials. For the organic chemist, drawing a line between natural and synthetic is, in many ways, irrelevant — both arise from the same fundamental elements and obey the same laws of nature.

In fact, every living human being is an intricate, living testament to organic chemistry. As you read these lines, your eyes rely on the organic molecule retinal to convert light into electrical signals that your brain can process. Each breath you take fuels metabolic reactions that convert glucose into usable energy, powering your muscles to turn the pages of this book. Even now, your thoughts and memories are being transmitted across billions of neurons by organic compounds called neurotransmitters, bridging the gaps between brain cells with astonishing precision [2].



11-*cis*-retinal
absorbs light when we see

serotonin
human neurotransmitter

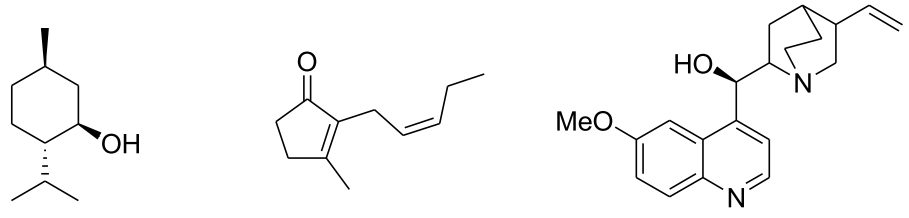
Figure 1

2. Organic Compounds

Organic chemistry began as the study of the substances that make up living organisms, at a time when many scientists believed that "living" and "non-living" matter obeyed separate chemical laws. This idea, called *vitalism*, dominated early thought until the 19th century, when Friedrich Wöhler famously synthesized urea — an organic compound — from inorganic ammonium cyanate, proving that life's molecules could be made in the laboratory [3]. This milestone marked the birth of modern organic chemistry as the study of carbon compounds, regardless of their origin.

In its early years, organic chemists mainly worked with substances extracted from plants and animals. Essential oils, for example, were distilled from flowers and leaves to produce fragrant compounds and flavorings. Well-known examples include *menthol*, the cooling agent found in spearmint oil, and *cis-jasmone*, an aromatic component distilled from jasmine blossoms [4]. Likewise, naturally occurring alkaloids — nitrogen-containing organic compounds — were extracted from plants such as poppies (morphine) or cinchona bark (quinine), laying the foundation for medicinal chemistry and natural product research [4].

Over time, the field grew far beyond these natural extracts. Today, organic chemists not only isolate and analyze natural compounds but also design entirely new molecules with tailored properties for medicine, agriculture, industry, and technology — continuing a journey that began with the simple distillation of plant oils and extraction of alkaloids [3].

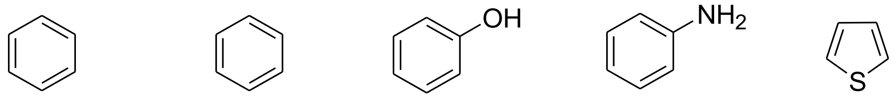


menthol *cis*-jasmone quinine

Figure 2

As early as the sixteenth and seventeenth centuries, organic compounds of natural origin were already being used to treat human diseases. One notable example is quinine, an alkaloid extracted from the bark of the South American *Cinchona* tree. Indigenous people used this bark to treat fevers long before European colonists learned of it. By the 17th century, Jesuit missionaries popularized the use of this "Jesuit's bark" across Europe, where it became the principal remedy for malaria [5]. Although those early healers had no idea of quinine's precise chemical structure, modern organic chemistry has since revealed and synthesized it, making it one of the first natural products to be understood and used on a large scale [5].

As the Industrial Revolution unfolded in the 19th century, chemists looked beyond plants for new chemical feedstocks. One of the largest reservoirs was coal. Coal gasification — the process of heating coal to produce gas for lighting and heating — also yielded a viscous byproduct known as coal tar. Though unpleasant to handle, coal tar proved a treasure trove of aromatic compounds, giving rise to the synthetic dye and pharmaceutical industries. From this black tar, chemists isolated foundational organic chemicals such as benzene, pyridine, phenol, aniline, and thiophene — compounds that continue to underpin countless materials and reactions in organic synthesis today [6].



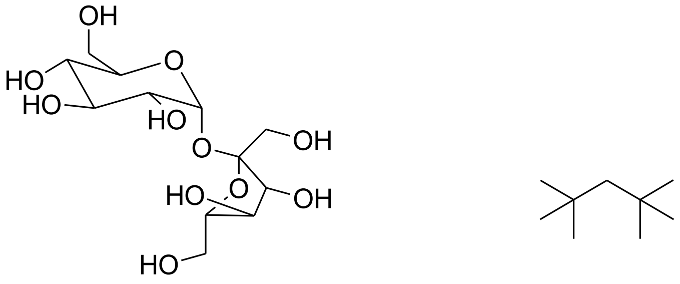
benzene pyridine phenol aniline thiophene

Figure 3

One of the earliest breakthroughs that highlighted the power of synthetic organic compounds was the medical use of phenol. In the late 19th century, Joseph Lister pioneered antiseptic surgery by using phenol (then called carbolic acid) to sterilize wounds and surgical instruments, drastically reducing infection rates and transforming medical practice [7]. Around the same time, aniline, another compound derived from coal tar, laid the foundation for the synthetic dye industry — a turning point that proved chemists could make entirely new, valuable substances rather than relying solely on what nature provided [7].

The success of these early synthetic compounds sparked an ever-growing search for new organic molecules. By the 20th century, the source of bulk organic chemicals shifted from coal to crude oil and natural gas, which offered abundant simple hydrocarbons like methane (CH_4) and propane (C_3H_8). These raw materials fueled the rise of the modern petrochemical industry, supplying feedstocks for plastics, fuels, and countless synthetic materials that define contemporary life [8].

Today, the catalog of known organic compounds continues to expand at an extraordinary rate. As of recent estimates, more than 16 million distinct organic compounds have been documented — with no theoretical limit in sight [8]. Their diversity is astonishing: they may appear as crystalline solids, oils, waxes, resins, polymers, flexible rubbers, volatile liquids, or gases. Everyday examples range from common table sugar — a crystalline natural compound refined from plants — to petrol (gasoline), a carefully blended mixture of lightweight hydrocarbons. A major component of high-octane petrol is isooctane, which gives its name to the "octane rating" that measures fuel performance in engines [8].



sucrose – ordinary sugar
isolated from sugar cane
white crystalline solid

isooctane (2,3,5-trimethylpentane)
a major constiuent of petrol
volatile inflammable liquid

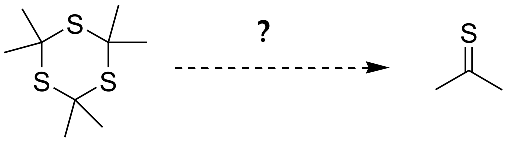
Figure 4

Not all organic compounds are pleasant or useful in obvious ways — some are famously foul-smelling. A striking example comes from the skunk, which defends itself by spraying a potent mixture of volatile sulfur compounds called thiols (or mercaptans). These compounds, which contain an –SH (sulfhydryl) functional group, are responsible for the skunk's notorious, persistent odor. Even at extremely low concentrations, thiols can be detected by the human nose and are among the strongest-smelling organic molecules known [9]. Interestingly, the same class of compounds is used in trace amounts to add a warning smell to otherwise odorless natural gas, helping prevent accidental leaks [9].

Perhaps one of the most infamous examples of foul-smelling organic chemistry occurred in Freiburg, Germany, in 1889, during an attempt to synthesize thioacetone. Thioacetone, a sulfur-containing ketone, is notorious for its almost unbearable stench. Early chemists prepared it by cracking trithioacetone, but the experiment quickly turned into a disaster. According to historical accounts, the resulting vapors spread rapidly through the city, causing widespread nausea, vomiting, and even fainting among local residents. The odor was so overpowering that parts of Freiburg had to be evacuated, and the experiment was swiftly abandoned [10].

Figure 5

To this day, thioacetone retains a legendary status among chemists as one of the most revolting-smelling substances ever produced. Modern chemical safety manuals still cite it as a reminder that even small amounts of certain volatile sulfur compounds can have dramatic and unexpected consequences far beyond the laboratory walls [10].



trithioacetone;
Freiburg was evacuated
because of a smell from
the distillation this compound

thioacetone

Figure 6

To this day, the precise chemical culprit behind the infamous Freiburg stench remains debated among chemists. Two main candidates have been proposed. One is propane-2,2-dithiol, also known as acetone gem-dithiol, a compound with two sulfhydryl (–SH) groups attached to the same carbon atom. The other possibility is 4-methyl-4-sulfanylpentan-2-one, a sulfur-containing ketone believed to form as a byproduct under certain cracking conditions [11].

Both candidates are extraordinarily malodorous, and given the legendary severity of the smell — strong enough to empty an entire city — it is unlikely that modern chemists will risk reproducing the original conditions just to resolve the controversy. For most, the tale of thioacetone remains a vivid reminder that sometimes even the smallest molecules can make the biggest impact — for better or worse [11].

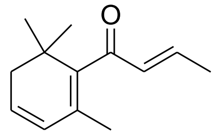
propane dithiol

4-methyl-4-sulfanylpentan-2-one

Figure 7

Not all surprising aromas in organic chemistry are unpleasant — some famous fragrance compounds reveal their true beauty only under special conditions. A classic example is the damascenones, a family of aromatic compounds that contribute significantly to the characteristic scent of roses. Interestingly, a single drop of pure damascenone may not smell floral at all at first; instead, it can give off a sharp, pungent odor reminiscent of turpentine or camphor. However, when diluted or exposed to air over time, the powerful rose-like fragrance emerges, often clinging to clothing and lingering for hours or even days [12].

This unusual behavior — where a pleasant smell develops only at very low concentrations — is not unique to damascenones. It is similar to the phenomenon observed with certain volatile sulfur compounds like those derived from trithioacetone, where dilution transforms an initially harsh or overpowering odor into something quite different [12]. Such effects remind us that the perceived scent of an organic compound often depends on its concentration, volatility, and interactions with our sense receptors, making fragrance chemistry a subtle art as much as a science.

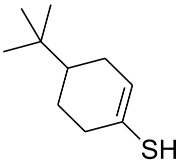


damascenone - the smell of roses

Figure 8

Smell and taste are deeply linked, and organic chemistry plays a key role in both senses. Take the grapefruit, for example. Its distinctive, slightly bitter yet fresh flavor comes mainly from a powerful sulfur-containing compound called 1-p-menthene-8-thiol (also known as grapefruit mercaptan) [13]. This molecule is so potent that humans can detect it at astonishingly low concentrations — as little as 2×10^{-5} parts per billion. To put this in perspective, that's about 0.0001 milligrams per metric tonne, or roughly one drop dispersed in an entire large lake [13].

This extreme sensitivity is remarkable, especially considering that not all animals share it to the same degree. Why evolution has left humans unusually attuned to this faint sulfur note in grapefruit is still an open question — perhaps a quirk of our shared chemical senses that link survival instincts, flavor preference, and even mild bitterness detection into one remarkable sensory experience.



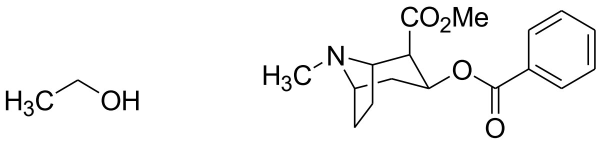
flavouring principle of grapefruit

Figure 9

Organic compounds can have some of the most profound — and sometimes dangerous — effects on the human mind and body. Many substances that we commonly call drugs are simply organic molecules that interact with our nervous system in complex ways. For example, ethanol (alcohol) is a simple organic compound that has been used for centuries to relax social inhibitions and produce feelings of temporary euphoria. However, its misuse is also responsible for significant personal and societal harm — including addiction, disease, and social problems [14].

Similarly, cocaine, another naturally derived organic compound obtained from the leaves of the coca plant (*Erythroxylum coca*), acts as a powerful stimulant. While it can briefly elevate mood and energy, cocaine is highly addictive and can trap users in a cycle of dependence that is extremely difficult to break [14].

These examples remind us that the same discipline that creates life-saving medicines and pleasant fragrances also deals with substances that demand great care and responsibility. The power of organic chemistry lies not just in the molecules themselves, but in how wisely we choose to use them.



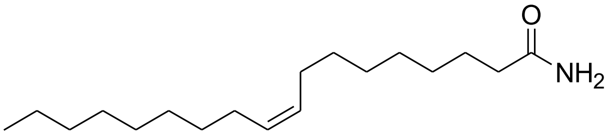
alcohol
(ethanol)

cocaine - an addictive alkaloid

Figure 10

Organic compounds do not just influence humans — they can profoundly affect other animals too. Take cats, for example, which seem to possess an uncanny ability to drift off to sleep at any moment. Scientists studying this phenomenon discovered that a simple organic compound present in the cerebrospinal fluid of sleeping cats could induce sleep when injected into other animals, such as rats — and even humans in experimental settings [15].

This compound, later identified as muramyl peptide, is surprisingly small and structurally simple, yet it plays a powerful role in regulating sleep. Its discovery highlighted how even basic organic molecules can have complex physiological effects, deepen our understanding of sleep regulation and open new pathways for sleep medicine research [15].

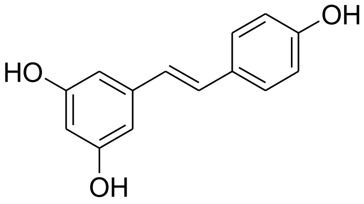


a sleep-inducing fatty acid derivative
cis-9,10-octadecenoamide

Figure 11

Another well-known example of how organic compounds can influence human health is resveratrol, a natural molecule that has attracted widespread attention in recent decades. Resveratrol is a polyphenolic compound found in the skins of red grapes — and therefore present in red wine — and is thought to contribute to the so-called “French Paradox”: the observation that populations with moderate red wine consumption often have relatively low rates of heart disease despite diets rich in saturated fats [16].

Chemically, resveratrol is quite different from the other molecules mentioned here. Its structure features two benzene rings connected by a short carbon bridge, classifying it as a stilbene derivative. Research suggests that resveratrol acts as an antioxidant and may help protect cardiovascular health by reducing inflammation and preventing the oxidation of low-density lipoprotein (LDL) cholesterol [16]. Although its exact benefits and optimal dosage are still debated, resveratrol remains a striking example of how even simple plant-derived organic compounds can have a measurable impact on human health and lifestyle.



resveratrole from the skins of grapes
is this the compound in red wine
which helps to prevent heart disease?

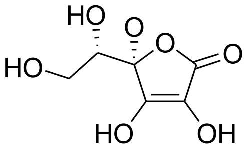
Figure 12

3. Organic Chemistry and Industry

For our first example of an edible organic molecule, consider vitamin C, also known as ascorbic acid. This compound is essential for human health — the very reason it is classified as a vitamin. A deficiency of vitamin C causes scurvy, a disease historically dreaded by sailors on long voyages, including those during the era of Columbus. Scurvy leads to the degeneration of soft tissues, particularly in the gums and mouth, resulting in bleeding, tooth loss, and severe fatigue [17].

Beyond preventing scurvy, vitamin C plays a broader role as one of the body's most important antioxidants. It helps neutralize reactive oxygen species — so-called free radicals — that can damage cells and DNA, potentially reducing the risk of certain cancers and other degenerative diseases [17]. There has also long been debate about whether large supplemental doses of vitamin C can prevent or shorten the duration of the common cold. Although some studies suggest a modest benefit for certain groups, the evidence overall remains inconclusive [17].

Nevertheless, vitamin C remains one of the most widely consumed and researched dietary compounds — a clear reminder of how simple organic molecules can have vital roles in everyday health.



vitamin C (ascorbic acid)

Figure 13

Vitamin C is a prime example of how organic chemistry meets real-world demand on an industrial scale. This essential compound is produced in vast quantities — one of the largest manufacturers is Roche, the Swiss multinational that has long dominated the global vitamin C market [18]. More broadly, countless chemistry-based industries worldwide manufacture organic molecules ranging from high-value pharmaceuticals and specialty chemicals to bulk commodities like solvents and fuels. Some facilities produce only a few kilograms of rare compounds each year; others turn out thousands of tonnes annually [18].

This vast industrial network is good news for students and professionals in organic chemistry. It means there is a steady global job market, with opportunities spanning research, production, quality control, green chemistry, and sustainable materials. Many organic compounds can be made from either petrochemical or biological feedstocks. For example, ethanol — an important industrial starting material — is typically produced by the catalytic hydration of ethylene, a hydrocarbon derived from crude oil [19]. However, ethanol can also be made by fermenting plant biomass.

A leading example is Brazil, where ethanol fuel is produced on a massive scale by fermenting sugarcane residues. This renewable bioethanol industry helps reduce oil imports and cuts urban air pollution, especially in major cities like Rio de Janeiro and São Paulo [19]. Such examples show how organic chemistry not only drives industrial innovation but also contributes to more sustainable energy solutions for the future.

3.1. Plastics and Polymers

A significant share of the modern petrochemical industry is devoted to producing plastics and polymers, which are built from small reactive molecules known as monomers. Key monomers include styrene, used to make polystyrene for packaging and insulation; acrylates, used in paints, adhesives, and textiles; and vinyl chloride, the building block for PVC (polyvinyl chloride), one of the world's most widely used plastics [20].

The scale of this industry is enormous. It supplies virtually everything made from plastic — from rigid household items and furniture to lightweight foams for protective packaging. Synthetic fibres derived from polymers, such as polyester and nylon, account for tens of millions of tonnes annually, supplying textiles for clothing, upholstery, and industrial fabrics [20]. Flexible, durable elastomers like synthetic rubber are essential for products such as car tyres, while high-performance plastics meet demands in electronics, medicine, and aerospace.

Major international chemical companies, including BASF, DuPont, Amoco, Monsanto, Laporte, Hoechst, and ICI, have long been global leaders in this field, driving research, production, and innovation in polymer chemistry. The scale and versatility of this industry make it one of the cornerstones of modern material science — and a key employer for chemists worldwide [20].

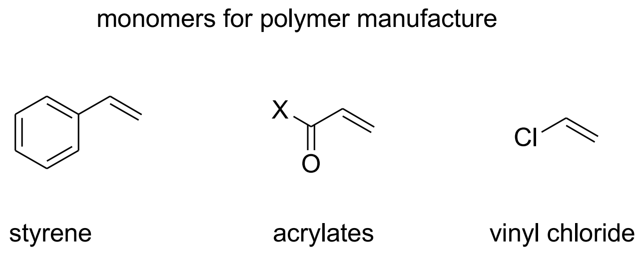


Figure 14

3.2. Dyes

There is a vast and continually growing market for intensely coloured organic compounds used in dyes and pigments. These bright molecules bring colour to everything from textiles and plastics to packaging, printed paper, and painted surfaces. One of the most famous dyes in history is indigo, a deep blue dye originally extracted from the leaves of plants in the genus *Indigofera*. For centuries, natural indigo was highly prized for dyeing fabrics. Today, it is produced synthetically on an industrial scale and is best known as the iconic colour of blue jeans [21].

Modern advances in dye chemistry have led to new classes of synthetic dyestuffs that offer bright, durable colours for a wide range of synthetic fabrics. For instance, benzodifuranones, developed by companies like ICI, provide fashionable, vibrant reds that adhere well to synthetic fibres such as polyester [21].

In addition to dyes, everyday pigments — used in plastics, coatings, and inks — often come from a family of robust metal complexes called phthalocyanines. These versatile compounds feature a metal atom (commonly copper or iron) at the centre of a large, planar ring structure. By swapping out the central metal or modifying the halogen atoms around the ring, chemists can fine-tune the pigment's colour, although blues and greens remain the most common shades [21].

These examples highlight how organic chemistry continues to shape the colours that surround us, combining molecular design with practical manufacturing on a global scale.

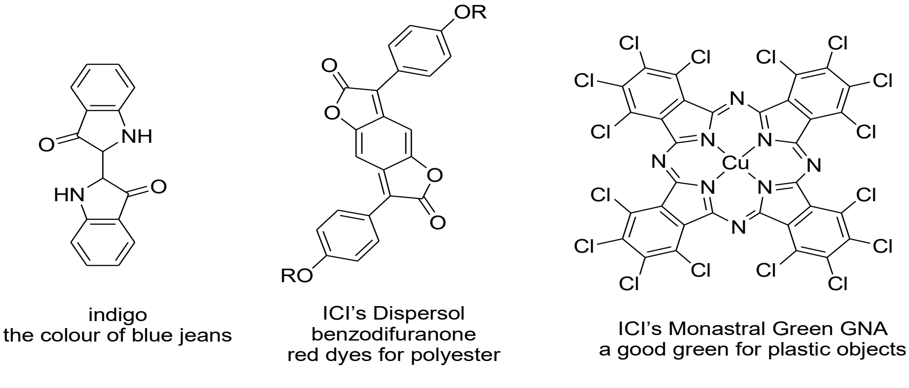


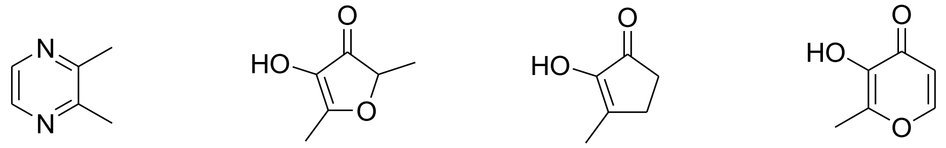
Figure 15

3.3. Food and Perfumery

Chemists don't just create colours and materials — they also design many of the synthetic flavourings that make our food taste appealing. A huge variety of flavour compounds are made and blended to mimic the complex aromas of natural foods. For example, the characteristic 'smoky bacon' flavour found in snack foods and seasonings can be recreated using simple heterocyclic organic molecules called alkyl pyrazines. These same compounds occur naturally in roasted coffee, baked bread, and grilled meats, where they form during the Maillard reaction as food is cooked [22].

Another group of flavour chemicals includes furonol, a compound originally identified in pineapples, which lends fruity or roasted notes when blended into artificial flavours. Similarly, molecules such as corylone and maltol contribute caramel-like and meaty flavours — they add depth to processed foods, soups, sauces, and confectionery by enhancing the sweet, roasted notes that make these products so appealing [22].

Such flavour chemistry is a thriving branch of modern organic synthesis, combining food science, sensory research, and creative molecule design to make everyday foods taste familiar and satisfying.



an alkyl pyrazine
from coffee and
roast meat

furonol
roast meat

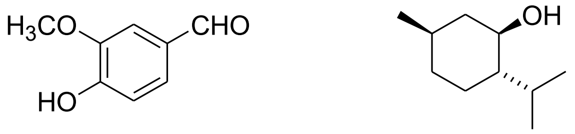
corylone
caramel
roasted taste

maltol
E-636 for cakes
and biscuits

Figure 16

Interestingly, some compounds that we use as flavourings are also valued as fragrances and as intermediates in the production of other chemicals. This versatility means that certain aroma compounds are produced on a huge industrial scale. A classic example is vanillin, the molecule responsible for the sweet, creamy flavour of vanilla — found in countless foods, especially ice cream, baked goods, and confectionery. Although natural vanilla is still extracted from vanilla orchid pods, the vast majority of the world's vanillin is now made synthetically from lignin (a by-product of the wood and paper industries) or from guaiacol, an organic intermediate [23].

Another important example is menthol, the cooling compound that gives mint its familiar fresh taste and aroma. Menthol is used not only to flavour chewing gum, toothpaste, and confectionery but also in perfumes, cosmetics, and medicinal products like cough drops and topical ointments. Its refreshing effect comes from its ability to activate cold-sensitive receptors in the skin and mouth, adding a sensory dimension beyond taste alone [23]. Together, these molecules illustrate how organic compounds can cross the boundaries between flavour, fragrance, and industrial feedstock, making them cornerstones of the modern flavour and fragrance industry.



vanillin
found in vanilla pods;
manufactured
on a large scale

menthol
extracted from mint;
25% of the world's supply
manufactured

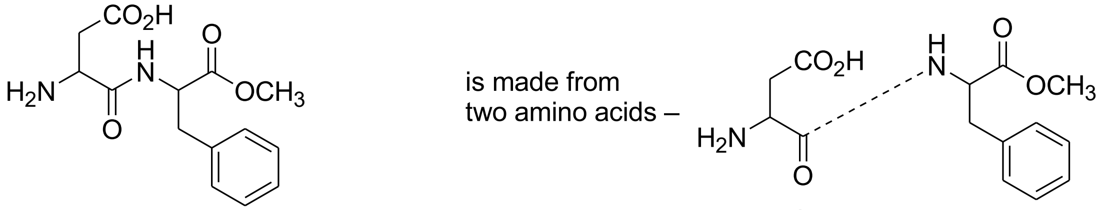
Figure 17

Food chemistry also includes much larger-scale organic compounds than just flavours and aromas. Sweeteners are a prime example, with ordinary sugar (sucrose) still being one of the most widely produced organic chemicals in the world, extracted from plants like sugarcane and sugar beet in massive quantities every year [24].

Beyond natural sugars, chemists have developed artificial sweeteners that deliver intense sweetness with little or no caloric content. Saccharin, the first widely used artificial sweetener, was discovered back in 1879 and quickly found a market for people seeking sugar substitutes, especially during wartime and rationing periods. Another major milestone came with aspartame, discovered in 1965, which remains one of the most popular low-calorie sweeteners used today [24].

Chemically, aspartame is interesting because it is a dipeptide, formed from two natural amino acids — aspartic acid and phenylalanine — both of which occur naturally in all living things. Modern production of aspartame is done on a large industrial scale; for example, the company Monsanto has produced over 10,000 tonnes per year for the global market, where it is widely used in soft drinks, desserts, and sugar-free products [24].

These examples show how food chemistry combines natural and synthetic pathways to meet huge consumer demand — and how simple organic compounds shape everyday life in ways we often take for granted.



aspartame ('NutraSweet')
200 ´ sweeter than sugar

aspartic
acid

methyl ester of
phenylalanine

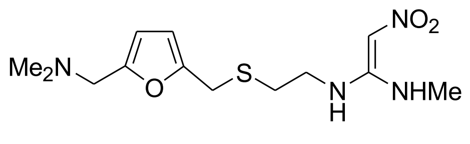
Figure 18

3.4. Drugs

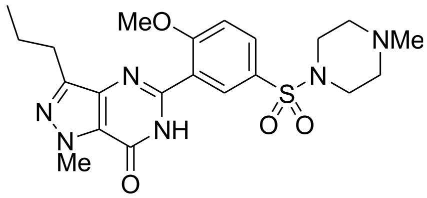
The pharmaceutical industry is one of the largest and most important sectors of applied organic chemistry, producing a vast range of drugs and medicinal products to treat, manage, and prevent diseases. One of the great revolutions of the modern era has been the widespread expectation that many once-deadly illnesses can be controlled or cured by medicines precisely designed to target them [25].

Among the landmark examples of pharmaceutical success is ranitidine, marketed as Zantac, which was developed by Glaxo–Wellcome in the late 1970s. Ranitidine became one of the world's top-selling prescription drugs for treating gastric ulcers and acid reflux, revolutionising treatment for millions [25]. Another major pharmaceutical success story is sildenafil, famously sold as Viagra by Pfizer. Launched in the late 1990s, sildenafil quickly became one of the fastest-growing blockbuster drugs in history, transforming the treatment of erectile dysfunction and symbolising how a single small organic molecule can dramatically change lives — and generate enormous economic returns [25].

These examples illustrate that 'success' in pharmaceuticals often means a win both for human health and for industry profit, showing how organic chemistry lies at the heart of modern medicine and global health care.



Glaxo-Wellcome's ranitidine
the most successful drug to date
world wide sales peaked >£1,000,000,000 per annum

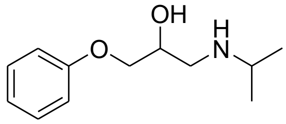


Pfizer's sildenafil (Viagra)
three million satisfied customers in 1998

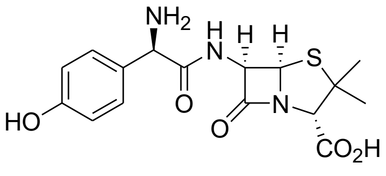
Figure 19

Many people — especially older adults — are prescribed β-blockers, a widely used class of organic compounds that help manage heart disease and related cardiovascular conditions. β-blockers work by blocking the effects of adrenaline (also known as epinephrine) on the heart and blood vessels. By doing so, they lower heart rate and blood pressure, reduce the heart's workload, and help prevent complications such as heart attacks and arrhythmias [26].

One of the best-known β-blockers is atenolol, marketed under the brand name Tenormin by Zeneca (now part of AstraZeneca). Atenolol has been a cornerstone of cardiovascular therapy for decades due to its effectiveness, predictable action, and generally favourable side-effect profile. It remains a clear example of how targeted organic molecules can help millions live longer and healthier lives by managing chronic diseases that were once far more deadly [26].



Zeneca's tenormin
cardioselective b-blocker
for treatment and prevention
of heart disease



SmithKline Beecham's amoxycillin
b-lactam antibiotic
for treatment of bacterial infections

Figure 20

3.5. Agrochemicals

Feeding the world's growing population — while protecting crops from damage and competition — remains one of the great challenges of modern chemistry. In the developed world, a secure food supply depends on preserving yields against pests, fungi, and weeds, while in the developing world, agrochemicals help fight malnutrition by increasing agricultural productivity [27].

The global agrochemicals market is enormous, valued at over £10 billion per year, and is divided roughly equally between herbicides, fungicides, and insecticides. Many modern insecticides are inspired by natural compounds. For example, some of the safest and most effective insecticides today are modelled on pyrethrins, natural chemicals produced by certain chrysanthemum flowers. Synthetic versions — known as pyrethroids — have been chemically modified to resist degradation by sunlight and to target specific pests more precisely [27].

A striking example is decamethrin (also called deltamethrin), which works with remarkable selectivity: it is over 10,000 times more toxic to certain insect pests, such as mustard beetles, than to mammals. This high safety margin allows it to be applied in very small quantities — around 10 grams per hectare, which is roughly one tablespoon spread across an entire football field. Thanks to careful design and biological testing, decamethrin leaves minimal environmental residues while providing reliable pest control in cooperation with crop scientists and ecologists [27].

These advances show how organic chemistry, working hand in hand with biology and agriculture, remains vital for global food security.

a natural pyrethin
from pyrethrum - daisy-like flowers from East Africa

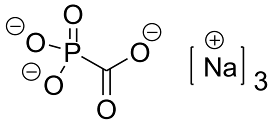
decamethrin
a modified pyrethrin - more active and stable in sunlight

Figure 21

All of the compounds we have discussed so far are built upon hydrocarbon skeletons, meaning they contain frameworks of carbon and hydrogen atoms. Most also include other key elements such as oxygen and nitrogen, while some contain sulfur or phosphorus. Together, these elements form the backbone of organic chemistry, the branch of science that studies carbon-based molecules and their countless transformations.

But where do we draw the line between organic and inorganic compounds? Consider foscarnet sodium, an antiviral medication used especially for treating CMV retinitis in patients with weakened immune systems. Its chemical formula is CPO_5Na_3, which looks unusual for an organic molecule: it contains carbon and phosphorus, but no C–H bonds, the hallmark of most organic compounds.

So is foscarnet truly organic? Many chemists would say yes, because it is carbon-based and its biological action places it firmly in the realm of medicinal organic chemistry. Others might argue that its lack of carbon–hydrogen bonds and its mineral-like structure make it more inorganic in character. This subtle boundary shows how the definition of 'organic' is flexible — but in practical terms, anything that is carbon-based and biologically active often ends up in the hands of organic chemists, regardless of its formal classification.



foscarnet – antiviral agent

Figure 22

So, is foscarnet truly organic or inorganic? The honest answer is that, in practice, we don't really know — and we don't really care. What matters more today is the recognition that rigid boundaries between traditional scientific disciplines are often unnecessary and outdated. Chemistry, like nature, does not respect neat labels.

In reality, modern research crosses freely over the old borders between organic chemistry and inorganic chemistry, and between organic chemistry and biochemistry. The blurred edges make the science stronger, not weaker, because they allow chemists to tackle real-world problems from multiple directions, using the best ideas and tools available.

Whether it has C–H bonds or not, the molecule CPO_5Na_3 — foscarnet — belongs to chemistry, full stop. And we should be glad that the field remains flexible, creative, and open, because it means that our ability to understand and shape the molecular world is richer than ever.

Conclusion:

Organic chemistry has evolved far beyond its early definition as the chemistry of carbon compounds with C–H bonds. From ancient natural dyes like indigo to modern synthetic medicines, agrochemicals, plastics, and everyday flavours and fragrances, organic chemistry has continually transformed how we live, what we eat, how we stay healthy, and how we shape our environment.

As this chapter has shown, the boundaries that once separated organic chemistry from inorganic chemistry and biochemistry are now fluid and increasingly irrelevant. Molecules like foscarnet remind us that chemistry's power comes not from rigid categories but from a deep understanding of how atoms can be arranged to solve real-world problems.

Today, chemists work hand in hand with physicists, biologists, engineers, and environmental scientists to design molecules that improve quality of life while meeting the challenges of sustainability, health, and technological innovation. The field's openness and adaptability ensure that organic chemistry remains a vital, creative force in science — a discipline that keeps pushing the limits of what is possible, molecule by molecule.

References:

1. Clayden, J., Greeves, N., Warren, S., & Wothers, P. (2001). *Organic Chemistry*. Oxford University Press.
2. Voet, D., & Voet, J.G. (2011). *Biochemistry* (4th ed.). John Wiley & Sons.
3. Anslyn, E. V., & Dougherty, D. A. (2006). *Modern Physical Organic Chemistry*. University Science Books.
4. Dewick, P. M. (2009). *Medicinal Natural Products: A Biosynthetic Approach* (3rd ed.). Wiley.
5. Sneader, W. (2005). *Drug Discovery: A History*. John Wiley & Sons.
6. Travis, A. S. (1993). *The Rainbow Makers: The Origins of the Synthetic Dyestuffs Industry in Western Europe*. Lehigh University Press.
7. Bud, R. (1999). The uses of life: A history of biotechnology. *Cambridge University Press*. (*Discusses Lister's antisepsis and the early dye industry.*) Rahimi, A., & García, J. M. (2017). Chemical recycling of waste plastics for new materials production. *Nature Reviews Chemistry*, 1(6), 0046. doi:10.1038/s41570-017-0046. (*Provides updated insights into petrochemical feedstocks and synthetic organic compounds.*)
8. Wood, W. F. (1999). The history of chemical defense in skunks: how chemical ecology uncovered the secrets of the skunk's spray. *Chemical Educator*, 4(2), 44–50.
9. Foulkes, F. R. (1990). The odour of thioacetone: Chemical curiosity or chemical horror? *Journal of Chemical Education*, 67(11), 933–935.
10. Stahmann, M. A., & Shriner, R. L. (1945). Thioacetone and related compounds. *Journal of the American Chemical Society*, 67(3), 429–431.
11. Ohloff, G., Pickenhagen, W., & Kraft, P. (2012). *Scent and Chemistry: The Molecular World of Odors*. Wiley-VCH.
12. Acree, T. E., & Barnard, J. (1984). Odor thresholds for chemicals with intense odors. *Flavor Chemistry*, 20(3), 1–20.
13. Pappenheimer, J. R., Koski, G., Fencl, V., Karnovsky, M. L., & Krueger, J. M. (1975). Extraction of sleep-promoting factor S from cerebrospinal fluid and from brains of sleep-deprived animals. *Journal of Neurophysiology*, 38(6), 1299–1311.
14. Baur, J. A., & Sinclair, D. A. (2006). Therapeutic potential of resveratrol: The in vivo evidence. *Nature Reviews Drug Discovery*, 5(6), 493–506.
15. Carr, A. C., & Maggini, S. (2017). Vitamin C and immune function. *Nutrients*, 9(11), 1211.
16. Geyer, R., Jambeck, J. R., & Law, K. L. (2017). Production, use, and fate of all plastics ever made. *Science Advances*, 3(7), e1700782. doi:10.1126/sciadv.1700782.
17. Zollinger, H. (2003). *Color Chemistry: Syntheses, Properties, and Applications of Organic Dyes and Pigments* (3rd ed.). Wiley-VCH.

18. Reineccius, G. (2006). *Flavor Chemistry and Technology* (2nd ed.). CRC Press.
19. Havkin-Frenkel, D., & Belanger, F. C. (2010). *Handbook of Vanilla Science and Technology*. Wiley-Blackwell.
20. Magnuson, B. A., Burdock, G. A., Doull, J., Kroes, R. M., Marsh, G. M., Pariza, M. W., Spencer, P. S., Waddell, W. J., Walker, R., & Williams, G. M. (2007). Aspartame: A safety evaluation based on current use levels, regulations, and toxicological and epidemiological studies. *Critical Reviews in Toxicology*, 37(8), 629–727.
21. Sneader, W. (2005). *Drug Discovery: A History*. Wiley.
22. Frishman, W. H. (1983). Atenolol: A new beta-adrenergic blocking agent. *Annals of Internal Medicine*, 98(2), 226–231.
23. Casida, J. E., & Durkin, K. A. (2013). Pesticide chemical research in toxicology: Lessons from nature. *Chemical Research in Toxicology*, 26(4), 643–651.

METAL CHALCOGENIDE NANOPARTICLES: SYNTHESIS, CHARATERIZATION AND APPLICATIONS

Arunendera Kumar Tiwari
Shahid Domeshwar Sahu Govt. College,
Jamgaon-R Bharar, Durg (C.G.) 491223
Corresponding author E-mail: arunendra.710@gmail.com

Abstract:

Metal chalcogenide nanoparticles represent an important group of efficient materials, in which the subtle variations in shape, size and phase of nano-powders resulted in physical properties (*e.g.*, electronic and optical) differing from their bulk counterparts, which makes them useful materials for various technological devices. In the last couple of decades, facile routes for their synthesis and strategies for controlling the size, shape and morphology have been reported. Numerous synthetic routes such as template directed method, vapor phase approach, vapor liquid solid growth, sol-gel technique, solvothermal synthesis, solution phase growth based on capping agents, sonochemical, radiolytic method for synthesis nanoparticles. Nanoparticles and self-assemblies of CdSe, CdTe, HgTe and ZnSe are synthesized using new and facile single molecular precursor based noble route that uses non-pyrophoric, low temperature and non-toxic chemicals is reviewed. In this paper, chemistry of chalcogens, metal chalcogenide nano particles and Synthetic route, characterization techniques like PXRD, SEM/TEM, EDAX, UV-Visible, Raman spectroscopy and some recent applications of metal chalcogenides NPs in the fields of solar cell, optoelectronic, biosensing, photocatalysts and bo-imaging etc. are discussed.

Keywords: Metal Chalcogenide Nanoparticles, Single Molecular Precursors, Solvothermal Process, X-ray Diffraction, Solar cell, Optoelectronic.

1. Introduction:

1.1 Chalcogen and its Chemistry

Oxygen, sulphur, selenium and tellurium are members of sixteenth group in the periodic table. These elements are known as ‘chalcogen’ or ‘ore forming’ elements, because a large number of metal ores are oxides or sulphides. The elements show usual increase in metallic character on descending the group. Oxygen and sulphur are totally non metallic; the non metallic character is weaker in selenium and tellurium. All the compounds of selenium and tellurium are potentially toxic and should be handled with care (Lee *et al.,* 1981).

The chemistry of selenium and tellurium compounds has grown considerably during the last few decades (Levason, 2002; Kanatzidis, 1994). Hybrid ligands containing soft donor atoms such as selenium/tellurium with hard donor atoms such as nitrogen and oxygen are creating greater interest to chemists, because it stabilizes metals in both oxidation states, i.e. low oxidation state and high oxidation states. They provide multi metallic systems and compel the metal ions to adopt remarkable coordination geometry and structural features. It is largely motivated by various applications exhibited by chalcogen compounds such as (i) Inorganic synthesis (Nishibyashi, 1996) (ii) Unusual structures and novel reactivity patterns (iii) Single source precursors for generating new high tech materials by MOCVD processes (Trindade, 1997) (iv) In developing metal clusters having potential use in catalysis (Schmidt, 1994) etc.

1.2 Semiconductor Nanomaterial

As a rapidly growing multidisciplinary research area, semiconductor nanomaterial research has received great attention from a wide range of scientists, including physicists, chemists, material scientists, engineers, and biologists. This extensive interest arises from the unique optical and electronic properties of semiconductor nanocrystals that dramatically distinguish them from their bulk counterparts (Trindade *et al.,* 2001).

In a bulk semiconductor, there are a large number of atomic orbitals available and overlaps to form continuous energy level leading to generation of valence band and conduction band (West, 1999). In distinction to metallic materials, intrinsic semiconductors posses an entirely separated valence band and conduction with a constant band gap (HOMO-LUMO separation) in the range of 0.3 to 3.8 eV on the basis of identity of the material (Trindade *et al.,* 2001; West *et al.,* 1999). In case of semiconducting metal chalcogenide nanomaterial band gap energy increases as the physical size of nanomaterial decreases within critical range especially the size of the particle decreases below the bulk Bohr exciton radius. There are not a sufficient number of atoms to form continuous energy levels. In this case, nanocrystallites confines electron and holes in three dimensions. Consequently, continuous energy bands are collapsed in to discrete atomic like energy states as shown in Figure 1 (Klimov, 2004). On the basis of characteristics of the semiconductor (III-V, IV, IV-VI or II-VI group), the critical radius can be widely different, ranging from 2 nm to 60 nm. As previously mentioned, blue shift in first excitonic absorption peak occurs due to quantum confinement by nano crystallite as compared to corresponding bulk substance. By means of an effective mass approximation model, Brus has revealed that the amount of the blue shift of the energy band gap is approximately inversely proportional to the size of the semiconducting nanomaterial (Steigerwald *et al.,* 1990; Brus, 1983; Brus, 1984). The blue shift of the energy band gap can be calculated by

$$\Delta \mathrm{Eg} = (h^2/8R^2)(1/m_\mathrm{e} + 1/m_\mathrm{h}) - 1.8\mathrm{e}^2/4\pi\varepsilon_0\varepsilon R \qquad (1.1)$$

Where R is the radius of nanocrystals, m_e represents effective mass of the electron, m_h represents effective mass of the hole, ε is the dielectric constant of the semiconducting material and ε_0 is the permittivity of a space in the semiconductor (Brus *et al.,* 1983; Brus *et al.,* 1984). The capacity to tune optical absorption and emission characteristics by changeable particle size make possible the function of nanocrystals for a variety of uses, including light emitting diodes (LED), photovoltaic, sensors, biomedical labels and so on (Trindade *et al.,* 2001; Klimov, 2004).

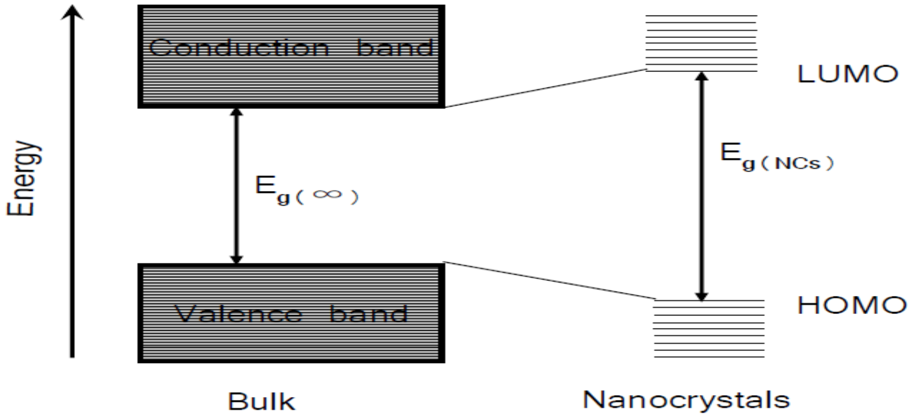


Figure 1: A diagrammatic illustration of the electronic states in bulk and semiconducting nanocrystalline (adapted from Steigerwald and Brus 1983)

Along with size-dependent optoelectronic properties, a second significant characteristic of semiconducting nanomaterial is the increase in surface to volume ratio with decreasing particle size; such that a 2.8 nm diameter CdSe particle has 37% of its atoms on the surface, which drops to < 1 % in its bulk form. As a result, the surface composition and structure strongly influence both the physical and chemical properties of semiconducting nanocrystals. For example, depending upon the inactiveness of the nanocrystals surface, the photoluminescence properties can be considerably different from bulk. In general, the nanocrystals surface often contains trap states caused by vacancies or local lattice mismatche defects, surface ligands, unsaturated bonds (floppy bonds) or other adsorbents on the surface (Figure 2). These energy states are able to trap excited electron or hole by this means, circumventing band-edge to band-edge radiative recombination yielding reduced band-edge luminescence (Toor *et al.,* 2014). These trapped electrons and holes recombine, direct to trap-state luminescence that emerge as typical broad emission band at a lower energy than the band-edge luminescence (Klimov, 2004). A fine passivated surface is required to attain improved band-edge luminescence. Secondary inorganic phase (shell) or organic ligands over coat the surface of nanocrystals. In this way surface gets de passivated (Klimov, 2004). It has been well recognized that definite coordinating ligands (Alkyl phosphine oxides, alkyl amines (Peng *et al.,* 2001) and fatty acids (Qu *et al.,* 2001; Yu *et al.,* 2003) can provide efficient passivation of the nanocrystal surface. The second semiconducting phase with a wider band gap grown on the nanocrystal core has proven to be even more effective at passivation (Klimov, 2004). ZnS is one of the most widely used shell materials for CdSe nanocrystals owed to its broad band gap (3.6 eV).

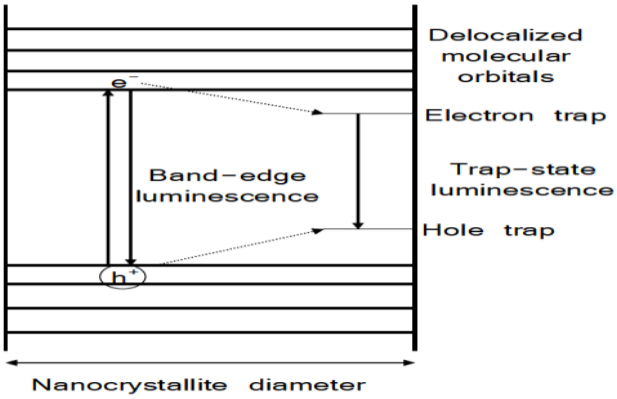


Figure 2.: Relationship illustration for a nanocrystalline semiconductor for spatial electronic state (Adapted from Chestnoy and Brus, 1986).

1.3 Metal Chalcogenide as Semiconducting Nanomaterials

Nanocrystalline II-VI and IV-VI semiconducting metal chalcogenide are special group of materials that display band gap energies straddling from the mid-to-near infrared (e.g. PbS, PbSe, PbTe) to the visible region (e.g. CdS, CdSe, CdTe) and into the ultraviolet (ZnS, ZnSe) region. Especially cadmium based chalcogenide (CdE; E = S, Se, Te) nanomaterials with their core shell structure (e.g. CdSe/ZnS) have given huge attention to physicists, chemists. Because, of their ease to synthesis and ability to produce high quality nanocrystals, reference to their particle size and shape. The produced nanocrystals have linked capacity to tune absorption and emission all over the visible region. These metal chalcogenide nanomaterials are considered to be potential material for biological imaging (Somers, 2007), contrast to traditional fluorophores (e.g. organic dyes). Nanocrystalline metalchalcogenide possess numerous advantages as fluorescent labels. Besides, comparatively long fluorescence life span (hundreds of nanoseconds), these are photo-chemically stable and demonstrate a tunable, narrow, symmetric emission spectrum (Alivisatos, 1998). However, the efficacy of nanocrystals in fluorescence imaging was originally prohibited by their insolubility in aqueous media due to the hydrophobic surface of nanocrystals (as dictated by the surface capping groups). The insolubility problem has been overcome by modification of the nanocrystals surface with phospholipids (Dubertret, 2002), amphiphilic polymers (Wu *et al.,* 2003), dendrimers (Guo *et al.,* 2003) and oligomeric phosphines (Kim, 2003). Conjunction of nanocrystalline material with protein and polypeptide facilitate their usefulness in biological field (e.g. imaging and bio-sensing).

2.0 Methods for Synthesis of Metal Chalcogenide Nanomaterials

Fundamental properties of nanocrystalline material are largely dependent on equality, size and shape of material that’s why, preparation of nanomaterials with uniform size and shape is very essential for basic studies as well as for their probable applications.

It is remarkable to point out here that the synthesis of nanocrystalline material with regular size and shape is one of the most difficult tasks in the area of nanotechnology. A large number of synthetic strategies including physical and chemical methods have been introduced to attain these requirements. The physical methods such as metal-organic-chemical-vapor-deposition (MOCVD) and molecular-beam-epitaxy (MBE) or nano wires (Hu *et al.,* 1999) through vapor-liquid-solid (VLS) growth require higher temperature to produce nanocrystalline materials (Yoffe, 1996). Chemical methods take account of template directed method, sol-gel technique, solvothermal synthesis, vapor phase approach, sonochemical, solution phase growth based on capping agents, radiolytic method in the center of others methods reported. Alternatively, synthesis of nanomaterial by solvothermal chemical routes requires only little amount of energy to produce nanocrystals from molecular stage and does not any special glassware or instruments. That's why solvothermal chemical synthetic routes stand for the most extensively utilized process to prepare semiconducting nanocrystals. The advancements have been employed in synthetic approach to achieve nanomaterials with desired shape and size. The basic thought process for this purpose is to control reaction to start nucleation and growth of nuclei (Sahay *et al.,* 2007). However, every process has its merits and restrictions. Therefore, productions of functionalized and restricted nanoparticles and assemblies yet have a great challenge.

Efficiency of metal chalcogenide nanomaterials are largely depending on their physical and chemical characteristics of materials. The characteristics may turn around, composition, crystal structure, size, shape, defects of nanomaterials. These phenomenons are regulated through thermodynamic and kinetic aspects of synthetic strategies. The nanomaterial can be attained by attrition of bulk material to material at nano scale by using top down process. Alternatively, aggregation of atoms or particles to material at nano scale using bottom up process (Herron *et al.,* 1996) can also be adopted.

A suitable solvothermal method has been effectively functional to produce hexagonal CdSe and cubic CdTe nanoparticles from fresh air stable, non pyroforic, non toxic, single source molecular precursors i.e. Cd(II)bis-(aminopropyl)selenide and Cd(II)bis-(aminoethyl)telluride. Precursors are added in to hot quinoline used as coordinating solvent as well as decomposition solvent nearly at 200°C. The average particle size was estimated CdSe $\approx$ 3 nm, CdTe $\approx$ 29 nm from X-ray diffraction pattern of synthesized nanoparticles. The synthesized nanoparticles posses optical properties and calculated energy band gap of nanoparticles are CdTe = 3.78 and CdSe = 4.05 eV from UV-visible spectra. Approximately spherical shape nanoparticles with average diameter 300 nm for CdSe and rod shape development of particles with diameter of 1.15 μm for CdTe nanoparticles was observed from microscopic characterization, The tendency of agglomeration was seen in both cases since particles were not fine sealed by quinoline. Hence, the economical, harmless single source molecular method may be a striking technique to fabricate metal chalcogenide nanoparticles (Tiwari *et al.,* 2013, Tiwari *et al.,* 2014, Tiwari *et al.,* 2014, Bajpai *et al.,* 2015, Tiwari *et al.,* 2016.)

3.0 Characterization Techniques

Metal chalcogenide semiconducting nanomaterials are characterized by various physicochemical techniques such as energy dispersive X- ray analysis (EDAX), powder X-ray diffraction (PXRD), scanning electron microscope (SEM), transmission electron microscope (TEM), UV–visible spectrophotometer, Raman spectroscopy etc.

3.1 Powder X-Ray Diffraction Technique

Powder X-ray diffraction (PXRD) is a commonly used diffraction technique in materials science that can offer knowledge about phase, structure and average size of crystallite. From all available solid materials 95% solids are termed as crystalline, crystalline phase of material interacted with X- ray. Interaction of incident X-ray with atomic arrangement of solid produces of X- ray diffraction pattern of material. Every crystalline solid have exclusive arrangement atom hence provide characteristic Powder X- ray diffraction pattern. This unique pattern of X- ray can utilized as characteristics “finger pattern” for identification of nanomaterials. When the material is identified, with the application of X- ray crystallography, phase, crystallinity, size and unit cell shape of nanomaterial can be established. The size of crystallite is determined by the Debye-Scherer equation

$$\tau = \frac{k\lambda}{\beta cos\theta}$$

and is related to the broadness of the peak.

In above equation, τ represent the mean size of crystallite domain; *K* is the shape factor, for dimensionless shape factor it has characteristic value 0.9; λ is wavelength of incident X- ray (0.154 nm); B is the full width half maxima intensity at diffraction peaks, θ is diffraction angle termed as Bragg angle of diffraction (Yao, 2010).

3.2 Electron Microscopic Technique

Electron microscopy (EM) is one of the regularly used methods in materials science. In similarity to optical microscopes that use light, electron microscopes make use of electron beams to picture the sample.

3.2.1 Scanning Electron Microscope (SEM)

SEM is a prevailing instrument for assessment and explanation of nano structured and is broadly applicable in the area of material science. Strike of incident of electron beam on the solid surface is underlying theory of scanning electron microscope. In SEM, attack of electron can create an extensive range of emissions from the sample, together with Auger electrons, backscattered electrons, visible photons, secondary electrons, X-rays etc. the instrument brings live images of the selected are of sample by the collection of back scattered electrons and emitted secondary electrons from the plane of the sample.

Therefore, SEM is mainly helpful to get information about topological and surface feature of material. The basic requirement for scanning electron microscope sample must be semiconductor or conductor. Non-conductor (e.g. polymers) samples require to be sputtered on a thin layer of conducting material (e.g. gold) (Flewitt *et al.,* 1994) Previous to SEM analysis.

3.2.2Transmission Electron Microscopy (TEM)

Transmission electron microscopy is another very dominant investigative tool in the material science, which has been broadly applicable in the categorization of nanomaterials. It has capability to inspect the constitution of nanomaterial for instance size and shape of particle, crystallinity, chemical distinction and imaging of pictures at nano-scale.

In TEM, two basic operational modes are performed to imager the selected area of samples: Dark field and bright field mode. Bright field mode is the most familiar imaging technique in TEM. Under this situation, TEM assemble both the beams i.e. directly transmitted and diffracted beam or only the incident beam. In dark areas of sample images are the section with large atomic numbers or with ticker samples, while the bright areas of the imagers are the area with no sample or thin sample. The dark area mode functions under diffraction distinction situation where only preferred diffraction beams are composed to produce an image. In this method, the diffracted electron beam in the ideal direction can be selected by using objective orifice, therefore only that sample region that cause that favored direction diffraction will be pictured.

The rest regions of the samples, where no sample or the area of sample cannot produce specific diffraction will appear dark.

Consequently, the bright field regions of image commonly provide information about particle size and shape while dark field region of images produces crystallographic information (Flewitt, 1994).

The investigation ability of TEM has been appreciably improved by incorporation of a number of superior techniques into the apparatus. These techniques include spectrometers, such as electron energy loss spectroscopy (EELS) and energy dispersive X-ray analysis (EDAX).

3.2.3 Energy Dispersive X –Ray Analysis (EDAX)

Energy dispersive X-ray analysis (EDAX) spectroscopy is an investigative tool mainly used for chemical characterization. Moreover, class of electron microscopy it also depends on interaction of light on nanomaterial to elucidate the chemical formulation nanomaterial. Strikes of high energetic electron beams (SEM/TEM) on the surface of nano sample resulted emission of X-ray. The emitted X-rays are utilized to recognize as well as examine the elemental ratio of the sample plane. Each element in the periodic table posse's exclusive electronic structure and it gave unique response to electromagnetic wave during interaction with this, is fundamental principle of EDAX.

Elemental composition of nanocrystals is calculated by using an in-situ energy dispersive spectroscopy unit (EDAX Inc.) within SEM/EDAX or TEM/EDAX instruments, incident electron beam and the sample.

3.3 UV-Visible Spectroscopy (UV-Vis)

UV-visible spectroscopy is a broadly used spectroscopic technique to examine the absorption characteristics of materials in UV-Visible region (200 ~ 800 nm).

In semiconducting materials, the absorption of light from UV- visible region may cause excitation of electron from valence band to the conduction band consequently an absorption edge is obtained in optical spectra. The energy is equal to the gap between valence band and conduction band i.e. band gap energy of the semiconducting material.

The absorption spectra of the nanoparticles were measured excluding the reflection losses. From the Tauc law, the absorption coefficient $\alpha(\nu)$ due to inter-band transitions near the band edge has been related to the incident photon energy by

$$\alpha(\nu)h\nu = B(h\nu - E_g)^n$$

Where $\alpha(\nu)$ is absorption coefficient, B is constant and $h\nu$ is incident photon energy; n is index which receives diverse values for unlike types of semiconductors and n = 1/2 for direct band gap semiconductors.

3.4 Photoluminescence Spectroscopy (PL)

Photoluminescence spectroscopy is widely applicable spectroscopic examination tool to analyze the emission characteristics of semiconducting nanomaterials. PL can be divided into two classes: fluorescence phosphorescence. Fluorescence and happen when electrons fall away from singlet excited states to singlet ground states and surplus energy is emitted as photons. Phosphorescence takes place when electrons relax from triplet excited states to singlet ground states via a radiation pathway. Fluorescence has a little life time (10-5 - 10-8 s) but tall intensity due to its high prospect of occurrence, whereas phosphorescence has an extended life time (10 - 4 – 104 s) but is usually weak because it is less feasible. Semiconducting nanomaterials display size-dependent photoluminescence characteristics. When an excitation light source shines on the material absorption occurs promoting an electron to the conduction band, and then excited electrons in the conduction band relax to the valence band via emission processes (Yao, 2010).

3.5 Raman Spectroscopy

Raman spectroscopy is one of the most important techniques utilized in material physics and chemistry to know the vibrational, rotational and other low-frequency form in a system. Raman spectroscopy arises due scattering of monochromatic light which is inelastic or Raman scattering. It usually occurs in form laser in ultra violet, visible, near infra red region. The inelastic scattering of photons by a solid, liquid or gas occurs Raman spectra. This effect is experiential as a shift in the frequency of the scattered light comparative to the excitation frequency. Molecular vibrations occur these energy transitions. Molecule contains certain functional groups interaction of light with functional groups results transitions, when these energized transitions are plotted as spectrum. This spectrum can be utilized for detection of molecule. This effect was observed by Smekal in 1923 (Smekal *et al.,* 1923). Raman and Krishnan verified experimentally in1928. Raman spectroscopy is widely applicable in chemistry since knowledge of vibration transition of functional groups is extremely precise for chemical bonds of molecule. The important benefits of Raman spectroscopy be its high in sequence content, compatibility with aqueous systems, not have sample preparation and non-destructive nature (Raman *et al.,* 1928).

4.0 Applications of Metal Chalcogenide Nanoparticles

Metal chalcogenide nanoparticles compounds containing a metal and a chalcogen (like sulfur, selenium, or tellurium), have a wide range of applications due to their tunable properties. Nanomaterials are composed of several atoms or molecules, which may be of various sizes and morphologies. Manmade nanomaterials are specially produced to take advantage of the unique properties of nanoscale. There are many metal chalcogenides with different structures and compositions such as CdSe, InAs, CdS, GaN, InGeAs, CdTe, PbS, PbSe, ZnS, Na_2S, CaTe, Ti_2S, and Cu_2Se These applications stem from their unique optical, electronic, and catalytic characteristics, which are enhanced at the nano-scale. They are particularly promising in areas like solar energy, optoelectronics, photo catalysis, and biomedicine.

There is some key application of metal chalcogenide nanoparticles (from web):

4.1 Solar Energy

Chalcogenide nanoparticles, particularly quantum dots, can be used in quantum dot-sensitized solar cells (QDSCs) to improve photoconversion efficiency by enhancing light absorption and electron injection. Binary metal chalcogenides like Ag_2S, Ag_2Se, CdS, CdSe, CdTe, ZnSe, and PbS are employed as sensitizers, Alloyed QDs offer tunability and higher stability.

4.2 Optoelectronics

Light-Emitting Diodes (LEDs): Their tunable optical properties make them suitable for creating LEDs with specific wavelengths.

Photodetectors: Metal chalcogenide nanoparticles can be used in photodetectors for detecting light in various wavelengths.

Photocatalysis: They can be used to split water to produce hydrogen using visible light, a process known as photolysis.

Optical Devices: Their tunable optical properties also make them suitable for various other optical devices.

4.3 Catalysis

Photocatalysis: Metal chalcogenide nanoparticles can act as photo-catalysts for various reactions, including water splitting.

Electrochemical Energy Storage: They can be used as electrode materials in batteries and super capacitors due to their high surface area and conductivity.

4.4 Biomedicine:

Antimicrobial Agents: Some metal chalcogenides, like silver nanoparticles, exhibit strong antimicrobial properties.

Drug Delivery: Their biocompatibility and tunable properties make them suitable for targeted drug delivery systems.

Biosensors: They can be used in biosensors for detecting various biomolecules.

Bioimaging: Ag_2X nanoparticles (silver chalcogenides, with X = S, Se, or Te) are crucial for near-infrared (NIR) fluorescence imaging, offering deep tissue penetration due to low tissue absorption, scattering, and auto fluorescence in the NIR region. Ag2X nanoparticles are used in NIR-I and NIR-II imaging for cancer detection, imaging blood flow, and angiogenesis.

4.5. Other Applications:

Infrared Optics: Chalcogenide glasses, which are amorphous metal chalcogenides, are used in infrared detectors, lenses, and optical fibers due to their infrared transparency.

Environmental Remediation: Metal chalcogenide nanoparticles can be used to remove pollutants from water and air.

Agriculture: They can be used to improve seed germination and plant growth.

Among the II-VI metalchalcogenide nanoparticles, CdSe and CdTe nanoparticles are largely synthesized due to their size dependent absorption and photoluminescence properties absorption (Ramalingam G and Madhavan J, 2011). Cadmium selenide [CdSe] nanoparticles is a promising material for various industrial applications, it is used as additive in preparation of Cosmetics, Rubber, Catalysts, optoelectronic devices and solar Cells (Sanjay *et al.,* 2018). Metal chalcogenide nanoparticles are widely received attention of researchers to synthesized Polymer based Light emitting diode due to Cheap, ease of preparation and assembly. Their limited commercial application is overcome by synthesized by quantum dot based polymer Light emitting diode these are supposed to brighter colour and longer life (Burroughes et al.1999, Ginger *et al.,* 2008). ZnO, CdSe and MEH-PPV Nanowire-QD-polymer, CdSe, ZnS.Cu and PIB Inkjet printer QD-polymer AC-driven Electroluminescence, CdSe/CdS/ZnS, PEDOT:PSS, TFB and TiO2, light emitting diodes A characteristics example of Hybrid Polymer light emitting diode. It is much closer to hybrid solar cell except mode of operation as it requires external AC source to excite electroluminescence layer.

Metal chalcogenide nanoparticles have remarkable application for degradation of organic pollutants, thermoelectric materials and self cleansing agent for chalcogenide glasses (Mehmet ates *et al.,* 2021)

Conclusions:

Metal chalcogenide nanoparticles prepared from various synthetic routes have functional applications. Properties and applications of nanoparticles largely depend on synthetic strategies and particle size. This Paper reviewed the synthetic methodologies to prepare metal chalcogenide nanoparticles especially single source molecular precursors route. Solvothermal and pyrolytic decomposition of single source molecular precursor yield metal chalcogenide nanoparticles of various shapes and sizes. Various characterization techniques such as powder X- ray diffraction technique (PXRD), electron microscopic techniques e.g. Scanning electron microscope (SEM) and transmission electron microscope (TEM), energy dispersive X-ray analysis (EDAX), NMR spectroscopy, UV-visible spectroscopy (UV- Vis) and Raman spectroscopy utilizes to know surface morphology and Topology discussed in length. This paper also the analyzed the functional applications of metalchalcogenide nanoparticles like CdSe and CdTe in field of solar energy, optoelectronics, photo catalysis, and biomedicine.

References:

1. Lee, J. D., Murray, S. C., & Hartley, F. R. (1981). *Concise inorganic chemistry* (5th ed.). Wiley India Edition.
2. Levason, W., Orchard, S. D., & Reid, G. (2002). Recent developments in the chemistry of selenoethers and telluroethers. *Coordination Chemistry Reviews, 225*(1–2), 159–199.
3. Kanatzidis, M. G., & Huang, S.-P. (1994). Coordination chemistry of heavy polychalcogenide ligands. *Coordination Chemistry Reviews, 130*(1–2), 509–621.
4. Nishibayashi, Y., Singh, J. D., Fukuzawa, S., & Uemura, S. (1996). Novel chiral ligands, diferrocenyl dichalcogenides and their derivatives, for rhodium- and iridium-catalyzed asymmetric hydrosilylation. *Organometallics, 15*(1), 370–379.
5. Trindade, T., Brine, P. O., & Zheng, X. M. (1997). Synthesis of CdS and CdSe nanocrystallites using a novel single-molecule precursors approach. *Chemistry of Materials, 9*(2), 523–530.
6. Hirpo, W. S., Dhingra, S., Sutrik, A. C., & Kanatzidis, M. G. (1993). Synthesis of mixed copper-indium chalcogenolates. Single source precursors for the photovoltaic materials CuInQ (Q = S, Se). *Journal of the American Chemical Society, 115*, 1597–1599.
7. Schmidt, G. (Ed.). (1994). *Clusters and colloids: From theory to applications*. Weinheim: VCH Verlagsgesellschaft mbH.
8. Trindade, T., O'Brien, P., & Pickett, N. L. (2001). Nanocrystalline semiconductors: Synthesis, properties, and perspectives. *Chemistry of Materials, 13*(11), 3843–3858.

9. West, A. R. (1999). *Basic solid state chemistry* (2nd ed.). John Wiley & Sons.
10. Klimov, V. I. (2004). *Semiconductor and metal nanocrystals*. Marcel Dekker.
11. Alivisatos, A. P. (1996). Semiconductor clusters, nanocrystals and quantum dots. *Science, 271*, 933–937.
12. Steigerwald, M. L., & Brus, L. E. (1990). Semiconductor crystallites: A class of large molecules. *Accounts of Chemical Research, 23*(6), 183–188.
13. Brus, L. E. (1983). A simple model for the ionization potential, electron affinity, and aqueous redox potentials of small semiconductor crystallites. *Journal of Chemical Physics, 79*, 5566.
14. Brus, L. E. (1984). Electron–electron and electron-hole interactions in small semiconductor crystallites: The size dependence of the lowest excited electronic state. *Journal of Chemical Physics, 80*, 4403–4407.
15. Murray, C. B., Norris, D. J., & Bawendi, M. G. (1993). Synthesis and characterization of nearly monodisperse CdE (E = sulfur, selenium, tellurium) semiconductor nanocrystallites. *Journal of the American Chemical Society, 115*(19), 8706–8715.
16. Toor, I. H., & Khan, S. (2014). Optical and structural properties of metal chalcogenide semiconductor nanostructures. In *Metal chalcogenide nanostructures for renewable energy applications*.
17. Peng, Z. A., & Peng, X. (2001). Formation of high-quality CdTe, CdSe, and CdS nanocrystals using CdO as precursor. *Journal of the American Chemical Society, 123*, 183–184.
18. Qu, L., Peng, Z. A., & Peng, X. (2001). Alternative routes toward high quality CdSe nanocrystals. *Nano Letters, 1*(6), 333–337.
19. Yu, W. W., Wang, Y. A., & Peng, X. (2003). Formation and stability of size-, shape-, and structure-controlled CdTe nanocrystals: Ligand effects on monomers and nanocrystals. *Chemistry of Materials, 15*(22), 4300–4308.
20. Chestnoy, N., Harris, T. D., Hull, R., & Brus, L. E. (1986). Luminescence and photophysics of cadmium sulfide semiconductor clusters: The nature of the emitting electronic state. *Journal of Physical Chemistry, 90*(15), 3393–3399.
21. Somers, R. C., Bawendi, M. G., & Nocera, D. G. (2007). CdSe nanocrystal-based chem-/bio-sensors. *Chemical Society Reviews, 36*, 579–591.
22. Bruchez, M., Jr., Moronne, M., Gin, P., Weiss, S., & Alivisatos, A. P. (1998). Semiconductor nanocrystals as fluorescent biological labels. *Science, 281*(5385), 2013–2016.
23. Dubertret, B., Skourides, P., Norris, D. J., Noireaux, V., Brivanlou, A. H., & Libchaber, A. (2002). In vivo imaging of quantum dots encapsulated in phospholipid micelles. *Science, 298*(5599), 1759–1762.

24. Wu, X., Liu, H., Liu, J., Haley, K. N., Treadway, J. A., Larson, J. P., Ge, N., Peale, F., & Bruchez, M. P. (2003). Immunofluorescent labeling of cancer marker HER2 and other cellular targets with semiconductor quantum dots. *Nature Biotechnology, 21*(1), 41–46.
25. Guo, W., Li, J. J., Wang, Y. A., & Peng, X. (2003). Conjugation chemistry and bioapplication of semiconductor box nanocrystals prepared by dendrimer. *Chemistry of Materials, 15*(16), 3125–3133.
26. Kim, S., & Bawendi, M. G. (2003). Oligomeric ligands for luminescent and stable nanocrystal quantum dots. *Journal of the American Chemical Society, 125*, 14652–14653.
27. Yoffe, A. D. (2001). Semiconductor quantum dots and related systems: Electronic, optical, luminescence and related properties of low dimensional systems. *Advances in Physics, 50*, 1–208.
28. Hu, J., Odom, T. W., & Lieber, C. M. (1999). Chemistry and physics in one dimension: Synthesis and properties of nanowires and nanotubes. *Accounts of Chemical Research, 32*(5), 435–445.
29. Sahay, P. P., Nath, R. K., & Tewari, S. (2007). Optical properties of thermally evaporated CdS thin films. *Crystal Research and Technology, 42*, 275–280.
30. Herron, N., & Wang, Y. (1990). Synthesis and characterization of surface-capped, size-quantized CdS clusters: Chemical control of cluster size. *Journal of the American Chemical Society, 112*, 1322–1326.
31. Chen, W., Liu, Z., & Wang, Z. (1996). Some new observations on the formation and optical properties of CdS clusters in zeolite-Y. *Solid State Communications, 100*, 101–104.
32. Tiwari, A. K., Verma, V. K., Jain, T. A., & Bajpai, P. K. (2013). Conclusive growth of CdTe nanorods by solvothermal decomposition using single source precursors. *Soft Nanoscience Letters, 3*, 52–57.
33. Tiwari, A. K., Jain, T., Verma, V. K., Choubey, S., & Bajpai, P. K. (2014). A facile route for CdSe nanoparticles: Synthesis and structural characterization. *Nanomaterials and Energy, 3*(5), 160–166.
34. Tiwari, A. K., Jain, T. A., Verma, V. K., Choubey, S., & Bajpai, P. K. (2014). Synthesis and characterization of HgTe nanorods via solvothermal route. *Archives of Applied Science Research, 6*(2), 37–41.
35. Bajpai, P. K., Yadav, S., Tiwari, A. K., & Virk, H. S. (2015). Recent advances in the synthesis and characterization of chalcogenide nanoparticles. *Solid State Phenomena, 222*, 187–233.
36. Tiwari, A. K., Jain, T., Choubey, S., & Bajpai, P. K. (2016, August). Synthesis and characterization of cadmium chalcogenide nanomaterial (CdE, E = Se/Te) from novel single source molecular precursor. *Current Nanoscience.*

37. Yao, Q. (2010). *Metal chalcogenide nanocrystal assembly: From synthesis to application* (Doctoral dissertation, Wayne State University, Detroit, MI).
38. Flewitt, P. E. J., & Wild, R. K. (1994). *Physical methods for materials characterisation*. Institute of Physics Publishing.
39. Smekal, A. (1923). Zur Quantentheorie der Dispersion. *Die Naturwissenschaften, 11*(43), 873–875.
40. Raman, C. V., & Krishnan, K. S. (1928). A new type of secondary radiation. *Nature, 121*, 501.
41. Ramalingam, G., & Madhavan, J. (2011). Investigation on the structural and morphological behaviour of CdSe nanoparticles by hydrothermal method. *Archives of Applied Science Research, 3*(3), 217–224.
42. Sanjay, P., Deepa, K., Madhavan, J., & Senthil, S. (2018). *Materials Science and Engineering, 360*, 012010.
43. Ates, M., Yılmaz, E., & Tanaydın, M. K. (2021). Challenges, novel applications, and future prospects of chalcogenides and chalcogenide-based nanomaterials for photocatalysis. In *Chalcogenide-based nanomaterials as photocatalysts* (Micro and Nano Technologies, pp. 307–337).

RECOVERY OF METALS FROM ELECTRONIC WASTE: CHEMISTRY PERSPECTIVE

Prajakta More
Department of Chemistry,
Smt. Chandibai Himathmal Mansukhani College, Ulhasnagar 421 003 (Maharashtra) India
Corresponding author E-mail: prajaktasandeep@gmail.com

Introduction:

Nowadays, it is impossible to imagine life without use of electronic gadgets. The online world is dominating the offline world, due to innovations in science and technology. Accordingly, E-waste (electronic waste) is becoming the most concerned segment of this era. In India the Central Pollution Control Board (CPCB) guides the formal E-waste recycling sectors. In such sectors educated and trained employs can do E-waste recycling in a scientific way. However, some unauthorized and unregistered sectors, make their lives by retrieving metals using dangerous techniques which can pollute the environment and endangering themselves under occupational health risk. E-waste can become the potential source for the huge business opportunities as it is the secondary resource of many metals and nonmetals. Properly treated E-waste can give the worldwide precious output in the form of valuable rare elements. Knowledge of chemistry plays vital role here to do so.

E-Waste Generation Scenario in India:

As per the complied study presented in Waste Management Bulletin on E-waste generation and management scenario of India, India contributes 1.7 million metric tons of E-waste which accounts for Asia’s 10.62% of E-waste production (year 2014). Further, the percentage contribution of E-waste generation increased to 11.11% in the year 2016. Moreover, since 2018, generation of E-waste in India has been increased to 2 million tones and also imported massive E-wastes from other countries. In the series of United states, China, Japan then Germany, India stood fifth in the world’s largest E waste producing countries (Bagwan, 2024).

Table 1: E-waste generation Global and India (Source: Sahdev *et al.*, 2024)

Year	Global	India
2015	46.4	1.97
2016	48.2	2.22
2017	50.0	2.53
2018	51.8	2.86
2019	53.6	3.23
2020	55.5	4.12

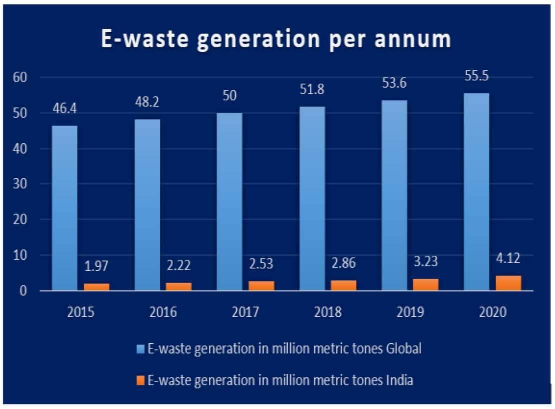


Figure 1: E-waste generation per annnum Global and India

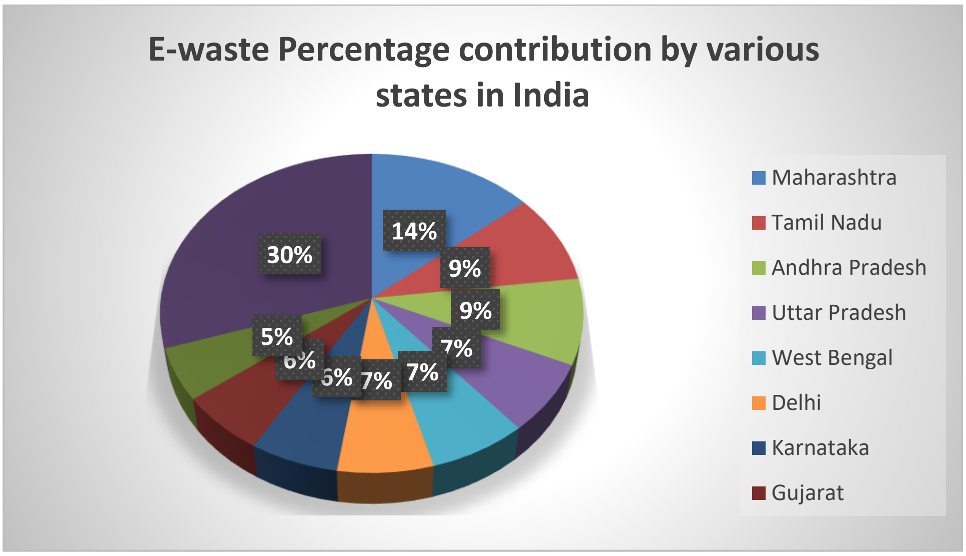


Figure 2: Percentage contribution by various states to e-waste generation per annum (Source: Sahdev, 2024)

E-Waste Monitoring Scenario in India:

India is the only country in south Asia, where dedicated E-waste management and handling rules are in effect since 2011. The E-waste rules explain the requirements for waste material transportation, storage and recycling. E-waste can be collected only by authorized dismantlers and recyclers. E-waste must be treated in a proper scientific way which can save environment and human health from the ill effects that can arise from it. The toxic heavy metals like mercury, lead, cadmium present in the E-waste are risky to the soil and water ecosystem if such E-wastes are improperly disposed. Proper E-waste management requires efficient metal extraction process and careful dismantling based on the understanding of the chemical properties of the metals. The compiled data given in Waste Management Bulletin based on the estimations given by Central Pollution Control Board, India can give the complete understanding of the current scenario of the E-waste management in India.

Table 2: E-waste generation and recycled or processed data in India (Bagwan, 2024)

	E-waste generation Metric Tones	E-waste recycled or processed Metric Tones	Hazardous waste recycling indicator %
2017-18	708445	69413.61	9.80
2018-19	771215	164.663	21.35
2019-20	1014961	224041	22.07
2020-21	1346496	354540.7	26.33

Hazardous waste indicator value in % = (Quantity of Hazardous waste recycled or processed in Metric Tons / Total quantity of Hazardous waste generated in Metric Ton)× 100

E-Waste Types:

E-waste stands for waste generated from electrical and electronic equipment (WEEE). It is one of the complicated wastes produced by the society. All this equipment requires electricity for their functioning. They include refrigerators, telephone, vacuum cleaners, heaters, dish washers, television, laptops, desk tops, cellphone, calculators, watches, portable audio etc. Due to its heterogeneous and complex composition, its treatment and recycling becoming a big challenge. Printed circuit board (PCB) is the important component of all the electrical and electronic gadgets which make up 3% of total mass of worldwide WEEE and 8% of the mass collected from the small appliances (E. Hsu et al (2019). One metric ton of printed circuit board contains about 160-210Kg of copper which is 30-40 times the amount that can be obtained by processing the ore recently in the United States. Similarly, the gold content found is 80-1500g which is 40 to 800 times bigger than that can be obtained by mining process (AB Obukohwo, 2023).

Conductive circuit lines are either printed or etched on the insulated flexible or inflexible substrate composed of glass fiber reinforce polymers such as epoxy resins, plastics etc. The circuit boards can be single sided, double sided or multi layered. Mainly copper foils are used for printing or etching the conductive circuits on the board or substrate and the metals such as gold, nickel and tin are used to protect the copper. Generally, the printed circuit boards consist of 40% metallic part, 30% organic part and 30% refractory material. The organic part mainly comprises polymers such as acrylonitrile butadiene styrene, polyvinyl chloride, polycarbonate, polyethylene, polytetrafluoro ethylene, polypropylene etc. Refractory material comprises aluminates, silicates, titanates, and alkaline oxides (Hsu *et al.,* 2019). Particularly the organic polymers embedded in the printed circuit boards are the hurdle in the treatment, characterization and recycling processes of it to get metal values.

Table 3: The metal composition by weight in various electrical electronic equipment scrap (Source: Hsu *et al.,* 2019)

Electrical electronic equipment	Precious metals Weight (ppm)			Base metals Weight (%)				
	Ag	Au	Pd	Cu	Fe	Al	Ni	Pb
Printed circuit boards	1000	250	90	20	6	4	1	2.5
Mobile phone	1380	350	210	13	5	1	0.1	0.3
TV board	280	20	10	10	28	10	0.3	1
Portable audio	150	10	4	21	23	1	0.03	0.14
DVD player	115	15	4	5	62	2	0.05	0.3
calculator	260	50	5	3	4	5	0.5	0.1

The type and durability of the electronic gadget depend on its chemical composition as well as plastics, glass and ceramic materials used for it coating. Thus, after end use of such gadget, it becomes complex waste to dismantle and recycle. Neglecting the metal values present in the E waste and disposing it into the landfills and water can have serious effects not only on the environment but also on the human health. Many toxic heavy metals are present in the E waste at the same time contains many precious rare metals also. Proper research and study should be carried out to make the recycling process of WEEE more profitable and ecofriendly.

General Methods for Recovery of Metals from E-Waste:

The base metals and precious metals can be extracted by various methods and techniques. The important metal values can be recovered by physical, mechanical, chemical and biological processes. Metallurgy deals with the extractive recovery of the metal from its ores or the matrix in a scientific and profitable way. Broadly, there are three types of metallurgy processes namely, hydrometallurgy, bio- hydrometallurgy, pyro-metallurgy. Hydrometallurgy uses the chemical reactions which are capable to extract the metal under study from its aqueous solution. Pyro-metallurgy is based on the proper temperature conditionings to extract the metal and involve the processes like leaching, roasting, smelting, calcination, oxidation, chlorination, sulphatization etc. Biohydro-metallurgy involves the use of microorganism in the recovery metal from the complex metal matrix (Manikandan *et al.,* 2023).

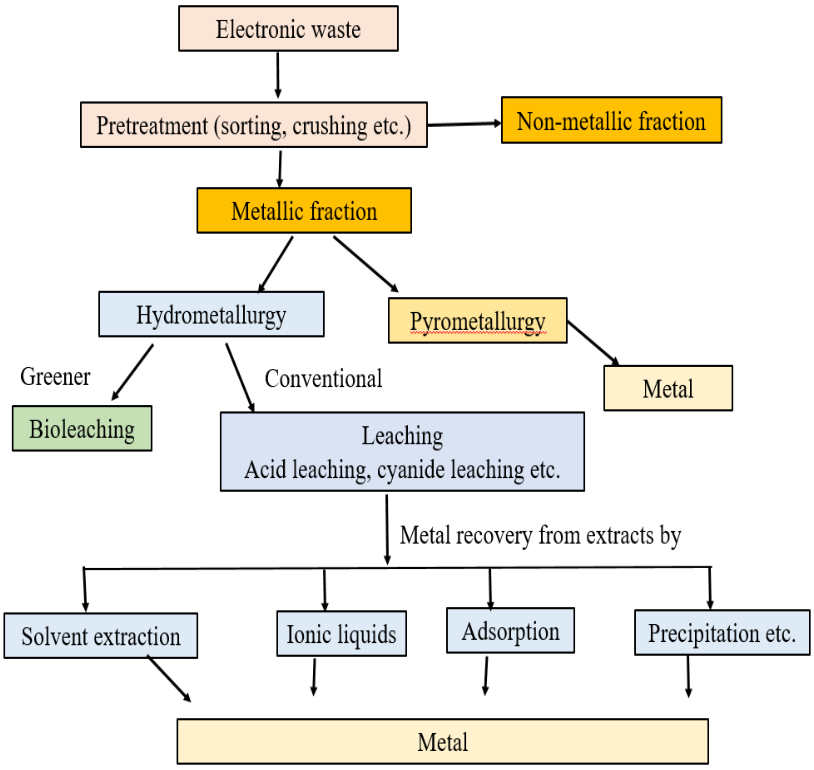


Figure 3: Outline of metal separation from electronic waste

Hydrometallurgy:

Hydrometallurgy requires dissolution of the metal under interest from the crushed electronic waste into the specific aqueous phase (leaching process). This is followed by separation and purification techniques such as solvent extraction, ion exchange, cementation, adsorption to isolate the metal from leached solution. A series of acid and caustic solutions can be used for the leaching process. Cyanidation method and Bayer method were the two fundamental methods invented for the extraction of alumina and gold from their ores. Precious metals are first dissolved in the proper leaching agent and then extracted by precipitation. The acidic or alkaline leaching may be carried out in presence of oxygen, hydrogen peroxide, chlorine, bromine or iodine. Usually, the temperature below 200°C should bring about the leaching process (Manikandan *et al.,* 2023).

Acid Leaching:

Common acids reported for the leaching process are nitric acid, hydrochloric acid, sulphuric acid and aqua regia. Nitric acid is very commonly studied solvent for the leaching process of the base metals like copper, lead and tin (solder removal) from waste printed circuit boards. Researchers Investigated the extraction of precious metal like gold from nitric acid to aqua regia leaches. The amount of the metal extracted depends upon the concentration of the acid used and leaching time. In general, higher the concentration of the acid and the leaching time, greater is amount of the metal extracted. Simultaneous extraction of copper and electrodeposition from nitric acid / aqua regia leachate of waste printed circuit boards also had been studied by the researchers. Copper recovery was obtained in higher yield from nitric acid than aqua regia however, higher acid concentration in the leachate restricted deposition of the copper. Sulphuric acid combined with hydrogen peroxide (oxidizing agent) is also proved as one of the efficient options for the leaching process of copper. > 95% copper extraction was observed from printed circuit boards (crushed, magnetically separated) leaching with 2M H_2SO_4, 0.2M H_2O_2, at 85ºC, 12 hours leaching time (E Hsu et al (2019). Aqua regia being the universal solvent for the leaching process of Cu. Ag and Au, found very effective however it is highly corrosive in nature. Crushed PCB with particles size < 1mm is invented as optimum size for copper extraction. Highly corrosive nature of the acids enforced to study ammonia based leaching processes which uses ammonium carbonate, NH_3 / NH_4Cl with $CuCl_2$ as oxidant. Copper can form stable complex with ammonia when controlled with proper pH and ammonia concentration, thus it is effective for selective copper extraction (Hsu *et al.,* 2019).

Acid leaching with nitric acid:

$$Cu + 4HNO_3 \rightarrow Cu(NO_3)_2 + 2NO_2 + 2H_2O$$

Acid leaching with sulphuric acid in presence of oxidizing agent:

$$Cu + 2H^+ + H_2O_2 \rightarrow Cu^{+2} + 2H_2O$$

Acid leaching with aqua regia:

$$2Au + 11HCl + 3HNO_3 \rightarrow 2HAuCl_4 + 3NOCl + 6H_2O$$

Cyanidation or Cyanide Leaching:

Cyanide is proved as one of the best and cheaper chemical reagent used as lixiviant (or leach) for selective extraction of gold from alkaline medium. Cyanide leaching is the most effective method for the extraction of silver or gold from the PCB substrate. It involves passing of gold and/ or silver into the alkali metal cyanide solution followed by reduction of these ions with suitable reducing agent. The gold and/or silver entrapped into the PCBs are difficult to dissolve than those present on the surface. Cyanidation is still prominent method in gold mining, but it possesses slow leaching rate and creates the high risk of water body pollution and handling. More attention is needed by the researchers for non-cyanide leaching processes such as halide leaching, thiourea leaching, thiosulphate leaching (Zhang *et al.,* 2012).

$$4Au + 8CN^- \rightarrow 4Au(CN)_2^- + 4e^-$$

Halide Leaching:

It includes three kinds of leaching reagents chloride, bromide and iodide. Gold can exists as Au+ as well as Au+3 in complexation with chloride, bromide and iodide by adjusting the proper chemical conditions. Chloride and chlorine leaching is more preferred industrially but requires specific equipment made up of stainless steel or rubber lining to avoid corrosion. Bromide leaching has safety issues while iodide leaching is expensive (Zhang *et al.,* 2012).

Thiourea Leaching:

Thiourea (sulfurized urea) is an organic complexing agent and reducing agent. It can form strong stable bond with precious metals like gold and base metal like copper. The conditions for extraction of gold and silver from printed circuit boards were investigated using thiourea leaching where 90.87% gold and 59.82% silver were leached in presence of oxidant Fe^{+3}. However, thiourea leaching process has the drawback of poor metal thiourea complex stability and requirement of high reagent concentration (Zhang *et al.,* 2012).

$$Au + 2CS(NH_2)_2 \rightarrow Au(CS(NH_2)_2)^{2+} + e^-$$

Thiosulphate Leaching:

Gold can be leached by sodium thiosulphate as well as ammonium thiosulphate. Gold with thiosulphate gives stable complex in existence of oxygen. Alkaline solution increases the stability of the gold thiosulphate complex. This is because, the tetrathionate, possible oxidation product of thiosulphate can undergo oxidative cleavage under alkaline conditions. At the same time, too much higher pH conditions are also not advisable, as it can lead to disproportionation reaction, allowing the conversion of thiosulphato into sulfidion. Actually, cyanide leaching is more sensitive, for extraction of gold from gold ore or concentrates containing Cu, Mn and or As. However, thiosulphate leaching containing ammoniacal solution is more suitable when more alkaline components are present as the impurities. Greater selectivity, non-toxic and low corrosive properties are the assets of the thiosulphate leaching (Zhang *et al.,* 2012).

Bio Hydrometallurgy:

Bio hydrometallurgy is the novel combination of two different fields where biological redox chemical reactions are used for the metal recovery. Particularly, copper and gold bioleaching from printed circuit boards is very well set procedure due to its low cost, low energy requirement and ecofriendly culture media. Commonly bioleaching, is carried out by using acidithiobacillus ferroxidans and thiooxidans. Particle size of the shredded PCBs, pH of the solution and culture media chemical composition affects the bioleaching process. Suitably prepared culture composition (e.g. $(NH_4)_2SO_4$, KCl, K_2HPO_4, $Ca(NO_3)_2$, and $FeSO_4.\ 7H_2O$) of bacterial species Ferroxidans and thiooxidans can dissolve the metallic part comprising copper, aluminium, zinc and nickel. The chemical reactions involved in copper leaching by microorganism ferroxidan is summarized in equation 1 and equation 2.

$$2Fe^{+2} + (O) + H^+ \rightarrow 2Fe^{+3} + H_2O \qquad \text{equation 1}$$

$$2Fe^{+3} + Cu^0 \rightarrow 2Fe^{+2} + Cu^{+2} \qquad \text{equation 2}$$

Modern bioleaching processes involves bio surfactant producing bacteria for zinc recovery from PCBs. Cyanogenic microorganisms form example chromobacterium violaceum (CV), can bring about the bioleaching of precious metals like Au and Ag.

$$4Au + 8CN^- + O_2 + 2H_2O \rightarrow 4(Au(CN)_2] + 4OH^-$$

Although not found to be as effective as CV, Pseudomonas chlororaphis, is the cyanogenic bacterial strain invented for the gold (8.2%), silver (12.1%), and copper (52.3%) extraction from PCBs (Hsu *et al.,* 2019).

Pyrometallurgy for Metal Recovery:

It is the most common and traditional route used for the separation and recovery the metal. From the technoeconomic point of view, pyrometallurgy, E-waste recycling process, set in copper smelting, is more preferable as the plant can have minimum capacity of 30,000 tons of electronic waste per year. The routes involved in pyrometallurgy process are incineration, smelting in blast furnace or plasma arc, drossing, sintering, high temperature gas phase reactions. Waste electronic and electrical equipment scrap, PCBs etc. are thrown into the blast furnace, then sent to converter and anode furnace then upgraded for electrowining or electrolysis for refining and metal recovery

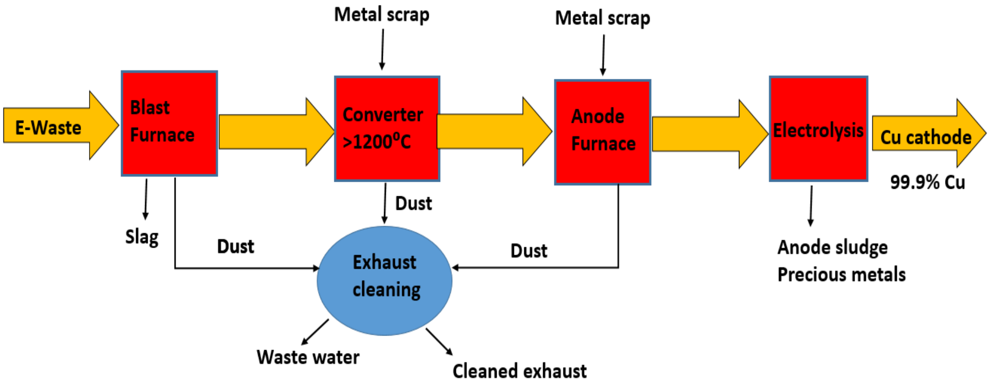


Figure 3: Pyrometallurgy for metal recovery (Source: Hsu *et al.,* 2019)

Solvent Extraction:

Solvent extraction also called liquid-liquid extraction is one alternative option for the metal recovery. It involves distribution of the metal under study between two immiscible phases made of aqueous phase and aliphatic or organic solvent phase. The metal under study can be extracted selectively into the organic phase from the leaching aqueous solvent. The important task in the solvent extraction is to design a special hydrophobic reagent which is capable to have selective interaction with the particular metal in the aqueous phases and pull it from solution containing mixture of various metal ions. The extractants may have acidic, basic or neutral nature. The most widely used acidic extractants include bis-(2-ethyl-hexyl) phosphoric acid (DEHPA), alkyl hydroximes (LIX-84), hydroxyl quinoline (kelex-100), Versatic acid etc., basic extractants include high molecular weight amines such as Primene JMT, tri-n-octylamine (Alamine 335, Adogen 364), triisooctylamine (Alamine 308), tri-n-alkylmethyl ammonium chloride having aliphatic chain of C6 to C8, neutral extractants including tri-n-butyl phosphate (TBP), tri-n-butyl phosphine oxide etc. Great literature is available for the procedures to extract precious and heavy metals from the aqueous chloride, sulphates, nitrates, perchlorate aqueous solutions (Alguacil and Robla, 2022).

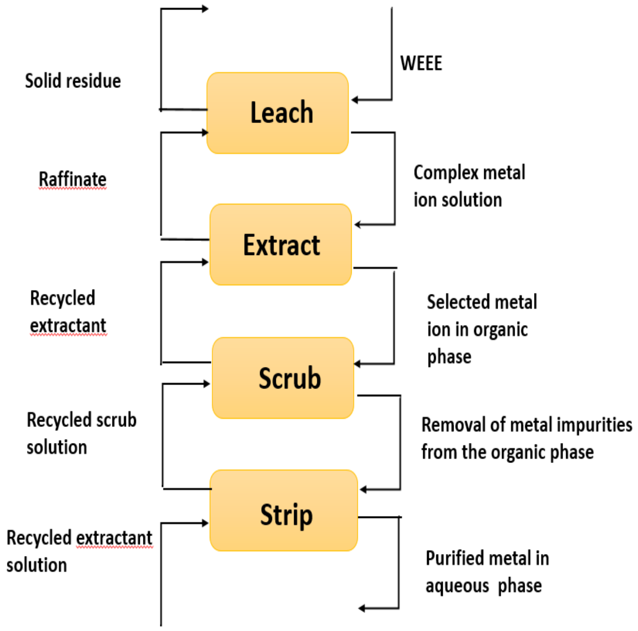


Figure 4: Summary for recovery of metals from leach solution via solvent extraction (Source: Schaeffer *et al.*, 2018)

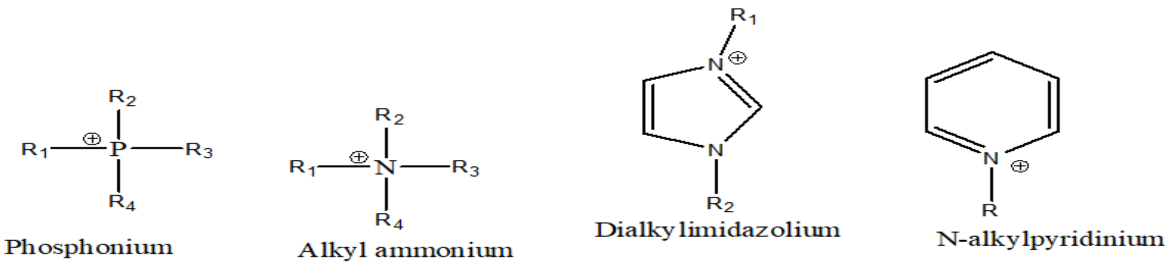
Copper is the major content of all the waste electronic and electrical equipments. Various hydroxyl oximes available with the brand name LIX and ACORGA are commonly used reagents (extractants) in the solvent extraction of copper. Commercial extractants, namely, MIBK (methyl isobutyl ketone), DBC (Diethylene glycol butyl ether, 2-EH (2-Ethyl hexanol) were used for the liquid liquid extraction of gold from halide leach solution, however, they have issues related to safety, selectivity and mass balance. Various monoamide compounds such as N,N-di-n-octylacetamide (DOAA) and N,N-di-n-octyllauramide (DOLA) were studied for liquid-liquid extraction of some precious and base metals commonly found in E-waste. Extraction study was carried out for Au(III), Pt(IV), Pd(II), Rh(III), Fe(III), Zn(II), Cu(II) and Ni(II) in HCl solution using DOAA and DOLA in organic diluent n-dodecane and 2-Ethylhexanol (Narita *et al.,* 2018; Rao, 2021).

High selectivity, excellent extraction efficiency are the pros of liquid-liquid extraction but it has the consequences such as toxic, volatile, inflammable solvent use. To overcome such defects solid phase extraction had pulled the attention. Solid phase extraction uses inert solid support to hold extractant and thus avoids use of organic diluent. Solid support provides adsorption capacity, mechanical strength and chemical stability while the properties of the extractants decides affinity towards specific metal ion (Ding *et al.,* 2019).

Ionic Liquids:

Ionic liquids consist of solvents composed of ions having properties intermediate between organic solvents and molten salt. They are the molten salts composed bulky organic cation and organic or inorganic anion with melting point less than 100^{o}C. Ionic liquids offer environmentally friendly media when compared to the organic volatile solvents used in liquid liquid extraction. They can be tailored to recover metal selectively, decrease waste generation and acid consumption.

Ionic liquids are commonly categorized into following four types based on their cationic part: a) Phosphonium b) Alkylammonium c) Dialkylimidazolium d) N-alkylpyridinium cations



Phosphonium Alkyl ammonium Dialkylimidazolium N-alkylpyridinium

Figure 5: Commonly used Cations in the ionic liquids

Commonly used anions in the ionic liquids are Halides like Chloride (Cl^-), Bromide (Br^-), Iodide (I^-), then Nitrate (NO_3^-), Hydrogen sulfate (HSO_4^-), Sulfate (SO_4^{-2}), trifluoroacetate (CF_3COO^-), trifluorosulfonate ($CF_3SO_3^-$), tetrafluoroborate (BF_4^-), hexafluorophosphate (PF_6^-), bis(trifluoromethanesulfonyl)imide $(CF_3SO_2)_2N^-$

The order in which the anions are showed, represents decrease in coordinating tendency and hydrophilicity. Most frequently mineral acids, alkaline and complexing agents were used for leaching process in hydrometallurgical processes. Ionic liquids replace all these classical leaching reagents providing the higher selectivity for the particular metal under interest against containing the secondary contaminants.

Various alternatives can be adopted to carry out the leaching process with ionic liquids:

- Use of pure ionic liquid as leachant
- Use of ionic liquids mixed with oxidizing agent / reducing agent / complexing ligands
- Use of aqueous solution of ionic liquid or little water with ionic liquid
- Use of ionic liquid in an organic diluent

Copper leaching from waste printed circuit boards was investigated using 1-butyl-3-methyl imidazolium hydrogen sulphate (Ionic liquid (bmim)HSO_4) 80% volume in water with H_2O_2 as oxidant at 70ºC (Huang *et al.,* 2014). Various concentrations of aqueous solutions of imidazolium based ionic liquids along with H_2O_2 as oxidant were studied and reviewed for the recovery of copper and zinc from brass waste. One more precious metal Indium was separated from waste LCD (Liquid Crystal Display) by leaching with the bis (trifluoromethylsulphonyl) imide at 90ºC. In this study, 50% (v/v) of Ionic liquid/ascorbic acid, 24-hour leaching enhanced the separation of indium from iron. Replacing the aqueous solution of Ionic liquid with ascorbic acid promoted the better separation. Combination of imidazolium based ionic liquids with specific complexing agent (e.g. thiourea) and particular oxidant such as ferric sulphate was found suitable for leaching of precious metals like gold and silver from WEEE (Paiva and Nogueira, 2020).

Conclusion:

Development in the technology, short life span and massive sales of electronic and electrical equipment increasing E-waste tonnage worldwide. It seems the earth is revolving with the huge number of electronic gadgets compared to the storage of the elements present in the earth crust. Thus, it will not be the misnomer to call E-waste as the primary source of valuable metals instead of calling it as secondary source for the benefit of mankind. Study and deep investigations of chemical techniques associated with hydrometallurgy, biohydrometallurgy, pyrometalljurgy, solvent extraction, ionic liquids etc. are very important as they make recycling of the metal values feasible. Commercialization of these studied chemical techniques requires low investment cost. Further, it needs proper study of physical and chemical properties of the materials present in the heterogeneous mass of E-waste.

References:

1. Bagwan, W. A. (2024). Electronic waste (E-waste) generation and management scenario of India, and ARIMA forecasting of E-waste processing capacity of Maharashtra state till 2030. *Waste Management Bulletin, 1*, 41–51.
2. Sahdev, S., Induria, T., & Sahu, T. (2024). E-waste management in India. *Sustainability, Agri Food and Environmental Research, 12*(Special Issue).
3. Hsu, E., Barmak, K., West, A. C., & Park, A. A. (2019). Advancements in the treatment and processing of electronic waste with sustainability: A review of metal extraction and recovery technologies. *Green Chemistry, 5*.
4. Obukohwo, A. B. (2023). Review on solvents for extraction of metals from waste electrical and electronic equipment (WEEE). *International Journal of Research in Applied Science and Engineering Technology, 11*(1).
5. Manikandan, S., Inbakandan, D., Nachiyar, C. V., & Namasivayam, S. K. R. (2023). Towards sustainable metal recovery from e-waste: A mini review. *Sustainable Chemistry for the Environment, 2*, 100001.
6. Zhang, Y., Liu, S., Xie, H., Zeng, X., & Li, J. (2012). Current status on leaching precious metals from waste printed circuit boards. *Procedia Environmental Sciences, 16*, 560–568.
7. Alguacil, F. J., & Robla, J. I. (2022). Solvent extraction in the recovery of metals from solutions: Entering the third decade of XXI century. *Desalination and Water Treatment, 265*, 71–93.
8. Schaeffer, N., Passos, H., Billard, I., Papaiconomou, N., & Coutinho, J. A. P. (2018). Recovery of metals from waste electrical and electronic equipment (WEEE) using unconventional solvents based on ionic liquids. *Critical Reviews in Environmental Science and Technology*. https://doi.org/10.1080/10643389.2018.1477417

9. Narita, H., Tanaka, M., Morisaku, K., & Abe, T. (2006). Extraction of gold(III) in hydrochloric acid solution using monoamide compounds. *Hydrometallurgy, 81*, 153–158.
10. Rao, M. D., Singh, K. K., Morrison, C. A., & Love, J. B. (2021). Recycling copper and gold from e-waste by a two-stage leaching and solvent extraction process. *Separation and Purification Technology, 263*, 118400.
11. Ding, Y., Zhang, S., Liu, B., Zheng, H., Chang, C., & Ekberg, C. (2019). Recovery of precious metals from electronic waste and spent catalysts: A review. *Resources, Conservation and Recycling, 141*, 284–298.
12. Huang, J. (2014). Leaching behavior of copper from waste printed circuit boards with Bronsted acidic ionic liquid. *Waste Management, 34*, 483–488.
13. Paiva, A. P., & Nogueira, C. A. (2020). Ionic liquids in the extraction and recycling of critical metals from urban mines. *Waste and Biomass Valorization*.

EVALUATION OF WATER QUALITY CHARACTERISTICS OF KRS BACK WATER

Shreesha Y N*, Divya. J and Vasudha Ranjan
Department of Environmental Science,
JSS Academy of Higher Education and Research, Mysuru 570015, India.
*Corresponding author E-mail: shreesha144@gmail.com

Abstract:

The present study includes the evaluation of physico-chemical properties of KRS backwaters located at Mysuru. The study is conducted from March to May 2025. A total of 15 water samples were collected and analysed for 12 key parameters like pH, temperature, electrical conductivity (EC), total dissolved solids (TDS), total hardness (TH), alkalinity, chloride, dissolved oxygen (DO), turbidity, nitrate, sulphate, and phosphate. The physico chemical characteristics were evaluated. From the results, it was found that, the pH values indicated slightly alkaline conditions throughout the study period, while EC and TDS levels reflected moderate mineral content, indicating suitability for domestic and irrigation use. The DO concentrations remained within limits. The turbidity values showed early signs of elevation during the study, this could be due to seasonal runoff and anthropogenic activity. The nutrient levels such as nitrate and phosphate, though within permissible limits, showed a slight upward trend indicating potential eutrophication risks. These seasonal variations underline the influence of climatic and anthropogenic factors on water quality. The study emphasizes the importance of regular monitoring and sustainable watershed management. Recommendations include eco-sanitation around tourist areas, waste management, and stakeholder engagement to preserve water quality. Overall, this study establishes a scientific baseline for future water quality assessments and informs local authorities and communities on the need for proactive environmental stewardship in ecologically sensitive regions like the KRS backwaters.

Keywords: KRS Backwater, Water Quality, Pre-Monsson Season, Venugopalaswamy Temple, Nutrients.

Introduction:

The freshwater ecosystem including rivers, lakes, reservoirs, and backwaters—are critical for sustaining biodiversity and supporting human needs such as drinking, irrigation, fisheries, and recreation (Sharma & Kansal, 2011). In India, urban expansion, population growth, and agriculture have increased stress on these systems, causing degradation and pollution (Kannel *et al.,* 2007; CPCB, 2019). Among freshwater bodies, backwaters, formed due to river damming or diversion, play a vital yet understudied role in regional water management (Reddy & Chandra, 2013). The Krishna Raja Sagara (KRS) dam was constructed in 1924 across the Cauvery River. The dam serve water for both Karnataka and Tamil Nadu with a storage capacity of 49.45 TMC (Dayal *et al.,* 2024). The area near the Venugopalaswamy Temple, a heritage and pilgrimage site, has witnessed increasing tourist activity. Previous studies, reported that, activities such as religious offerings, domestic waste discharge, and open defecation may degrade water quality. These actions can increase nutrient loads, organic matter, and suspended solids, affecting physico-chemical parameters (Adarsh *et al.,* 2019; Susheela *et al.,* 2014). Despite several studies in the broader Cauvery basin (Mahadev & Gholami, 2010), limited data exist for KRS backwaters, especially around religious zones. Monitoring seasonal variations in water parameters like pH, DO, turbidity, cations and anions are crucial for timely intervention and resource conservation (Mahesh *et al.,* 2013; Gholami & Srikantaswamy, 2009). The evaluation of water quality by considering parameters like pH, EC, TDS, TH, alkalinity, chloride, DO, turbidity, nitrate, phosphate, and sulphate are essential in anthropogenically impacted waters (APHA, 2017; BIS, 2012). The variations in these parameters indicate the pollution from runoff, sewage, and human encroachment.

Materials and Methods:

Collection of Water Samples:

The sample collection is a critical part of any water quality assessment study, as it determines the accuracy and reliability of the subsequent analysis. In the present study, the water samples were collected from the KRS backwaters near Venugopalaswamy Temple for a period of three months—March, April, and May, during the pre-monsoon season of 2025. This period was chosen to study the effects of dry-season water quality changes, when pollution levels can become concentrated due to reduced dilution by rainfall and increased evaporation. The sampling was carried out at regular intervals across the study site to ensure accuracy. A total of 15 water samples were collected, as per APHA guidelines.

Sampling Method:

The water samples were collected in pre-cleaned 1-liter polyethylene bottles to ensure sample integrity. Before sample collection, each bottle was rinsed three times with the water from the respective sampling site to minimize the risk of contamination. To obtain representative samples and avoid interference from the surface debris or atmospheric exchange, the water was collected from a depth of approximately 30 centimeters below the surface.

Experimental Analysis:

Water quality assessment was conducted by analyzing various physico-chemical parameters using standard protocols recommended by the APHA standards. This ensured accuracy, consistency, and comparability of results. The procedures followed for each parameter are listed below. The pH was measured using a digital pH meter, the temperature was recorded using a portable digital thermometer, electrical conductivity was determined by using a conductivity meter calibrated, the total dissolved solid was determined by gravimetric method, Total Hardness by EDTA titrimetric method., the alkalinity was measured by acid titration method, the chloride was determined by argentometric titration, dissolved oxygen was analyzed using the Winkler's method. The nitrate was measured by using UV spectrophotometric method. The phosphate was determined by the UV spectrophotometric method. The sulphate was estimated using the UV spectrophotometric method. The turbidity was measured using a nephelomete

Results and Discussions:

Results For the Month of March-2025

pH: The pH is considered as the basic water quality parameter. In the present study, the pH values in all the water samples showed variations. The higher values were observed in S (11) and lowest values were observed in S (8). In comparison with the WHO standards, the water samples S (11), S (14), S (15) showed within the normal range of the water quality standards. It was also observed that except, S (11), S (14), S(15) the pH values in all the other water samples were found to be below the normal range, indicating mildly acidic conditions across the sampling sites.

Temperature: The water temperature directly influences the biological activity and the chemical solubility. In the present study, the temperature values in all the water samples showed variations. The higher values were observed in S (14) and the lowest values were observed in S(1). All the values are characteristic of pre-monsoon seasonal warming and remained within the WHO standards. The variations could be due to depth, exposure to the sunlight and ambient weather conditions at the time of collection.

Electrical conductivity: The electrical conductivity is a measure of water's ability to conduct electricity, which reflects the concentration of dissolved ions. In the present study, the electrical conductivity values in all the water samples showed variations. The higher values were observed in S (5) and the lowest values were observed in S(15). All the values remained within the WHO standards, indicating the absence of salinity issues. These values indicate the presence of dissolved salts, likely from the weathered rock and runoff.

Total Dissolved Solids: The TDS is a cumulative measure of all the organic and inorganic substances dissolved in water. In the present study, the TDS values in all the water samples showed variations. Higher values were observed in S (8) and lowest values were observed in S(15). All values remained within the WHO standards, indicating relatively clean water with low mineral content.

Dissolved Oxygen: DO is crucial for the survival of aquatic organisms. In the present study, the DO values in all the water samples showed variations. The higher values were observed in S (11) and the lowest values were observed in S (9). In comparison with the WHO standards, the water samples S (3), S (4), S (7), S(8) and S(9), which were marginally below the threshold range of the water quality standards. It was also observed that except, S (3), S (4), S(7), S(8), and S(9) the DO values in all the other water samples were found to be below the normal range. This could be attributed to the microbial decomposition or stagnant conditions reducing the oxygen availability.

Table 1: Physico-Chemical Characteristics of Water Samples Collected in March 2025

Sl.No.	Parameters	WHO Standards	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	Average
1	pH	7.0 – 8.5	6.53	6.27	6.02	6.03	6.04	6.14	6.31	5.98	6.25	6.6	7.32	6.39	6.96	7.04	7.24	6.47
2	Temperature	<35°C	25.4	26.1	27.8	29.3	26.7	28.5	25.9	27.2	29.1	26.4	28.9	27.6	25.8	29.7	26.9	27.36
3	Electrical conductivity	<2500 µS/cm	436	435	447	432	451	446	441	427	440	425	441	439	430	433	424	436.47
4	Total dissolved Solids	≤ 500 mg/L	230	220	230	220	230	230	220	240	230	220	230	230	220	220	210	225.33
5	Dissolved Oxygen	≥ 6 mg/L	6.2	6	5.8	5.7	6	6.1	6.3	5.9	5.6	6	6.4	6	6.2	6.1	6.3	6.06
6	Turbidity	≤ 5 NTU	2.9	3.6	3.5	2.9	3.2	3	3.8	4.4	3.1	2.9	3.6	3	3.3	3.4	3.6	3.32
7	Total Hardness	≤ 500 mg/L	76	89	91	83	82	88	85	87	101	85	100	93	88	92	106	90.07
8	Chloride	≤ 1000 mg/L	23.82	23.32	23.34	23.82	24.3	25.8	26.8	25.31	27.29	25.31	27.79	28.28	31.26	31.76	28.28	26.15
9	Alkalinity	≤200 mg/L	86	98	104	90	108	96	220	104	122	114	108	102	126	122	102	112.13
10	Nitrate	≤ 50 mg/L	0.39	0.28	0.23	0.35	0.18	0.21	0.34	0	0.07	0.64	0	0.1	0	0.19	0.08	0.18
11	Sulphate	≤ 250 mg/L	0.07	0.08	0.05	0	0.04	0.03	0.01	0.07	0.1	0	0.07	0	0.03	0	0	0.03
12	Phosphate	≤ 0.10 mg/L	0.04	0.11	0.03	0.04	0.03	0.03	0.06	0.04	0.02	0.01	0.01	0	0	0.03	0.01	0.03

Turbidity: The turbidity indicates the presence of suspended solids. In the present study, the turbidity values in all the water samples showed variations. The higher values were observed in S (8) and the lowest values were observed in S(1), S(4), and S(10). All the values remained within the WHO standards, indicating that the water was relatively clear and free from the excessive suspended particles.

Total hardness: The total hardness indicates the presence of dissolved calcium and magnesium ions in the water. In the present study, the total hardness values in all the water samples showed variations. The higher values were observed in S (15) and the lowest values were observed in S(1). All the values remained within the WHO standards, indicating that the water is suitable for domestic use without posing scaling or health concerns.

Chloride: The chloride indicates the presence of dissolved salts in the water. In the present study, the chloride values in all the water samples showed variations. The higher values were observed in S (14) and the lowest values were observed in S(2). All the values remained within the WHO standards, indicating minimal intrusion from the sewage or industrial discharges.

Alkalinity: - The alkalinity represents the buffering capacity of water against acidification. In the present study, the alkalinity values in all the water samples showed variations. The higher values were observed in S (7) and the lowest values were observed in S(1). All the values remained within the WHO standards, except S (7) which slightly exceeded it, indicating the adequate buffering capacity to maintain stable pH levels in the water.

Nitrate: The nitrate is an essential nutrient but excessive levels may indicate the pollution from agricultural runoff or sewage. In the present study, the nitrate values in all the water samples showed variations. The higher values were observed in S (10) and the lowest values were observed in S(8), S(11), and S(13). All the values remained within the WHO standards, indicating minimal risk of nitrate contamination or eutrophication.

Sulphate: The Sulphate indicates the presence of dissolved minerals, particularly from the natural rock and the soil sources. In the present study, the sulphate values in all the water samples showed variations. The higher values were observed in S (9) and the lowest values were observed in S(4), S(14), and S(15). All the values remained within the WHO standards, indicating the absence of industrial effluents or Sulphur-bearing minerals in the surrounding geology.

Phosphate: The phosphate indicates the presence of nutrient pollution, often from the agricultural runoff or domestic wastewater. In the present study, the phosphate values in all the water samples showed variations. The higher values were observed in S (2) and the lowest values were observed in S(12), S(13), and S(14). All the values remained within the WHO standards, except for S (2) indicating a increase, potentially due to the presence of organic waste.

Table 2: Physico-Chemical Characteristics of Water Samples Collected in April 2025

Sl.No.	Parameters	WHO Standards	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	Average
1	pH	7.0 – 8.5	8.29	8.49	8.6	8.8	8.84	8.93	8.91	8.86	8.77	8.84	8.96	8.98	9.02	8.79	8.87	8.85
2	Temperature	<35°C	30.1	29.8	30.5	30.9	29.7	31.2	30.6	30.3	29.9	31	30.7	30.2	30.8	31.3	30	30.49
3	Electrical conductivity	< 2500 µS/cm	403	397	407	404	410	393	412	421	396	413	415	406	414	403	405	406.07
4	Total dissolved Solids	≤ 500 mg/L	238	242	236	244	239	247	235	240	245	243	237	241	246	239	234	240.13
5	Dissolved Oxygen	≥ 6 mg/L	7.05	5.85	6.12	5.78	6.3	6	5.95	6.45	5.6	6.15	6.25	5.88	6.05	6.2	5.92	6.11
6	Turbidity	≤ 5 NTU	1.2	1.4	1.3	1.2	1.2	0.7	0.7	1.7	0.6	0.7	1.1	0.7	0.9	1.3	1.2	1.07
7	Total Hardness	≤ 500 mg/L	78	102	85	111	97	75	100	94	88	108	91	82	115	90	96	95.73
8	Chloride	≤ 1000 mg/L	24.7	31.6	28.4	26.9	29.2	25.1	30.6	27.3	23.9	31	24.2	29.9	26.5	28.8	25.8	27.55
9	Alkalinity	≤200 mg/L	89	117	104	92	110	98	115	93	86	101	97	119	90	107	95	101.13
10	Nitrate	≤ 50 mg/L	0.36	0.24	0	0.29	0.08	0.17	0	0.06	0.32	0	0.11	0.63	0.22	0.14	0.03	0.17
11	Sulphate	≤ 250 mg/L	0.06	0	0.04	0.08	0	0.03	0.01	0	0.09	0	0.07	0.02	0	0.05	0	0.03
12	Phosphate	≤ 0.10 mg/L	0.02	0.09	0.01	0.03	0.04	0	0.02	0.06	0	0.03	0.01	0	0.05	0.03	0	0.03

Table 3: - Physico-Chemical Characteristics of Water Samples Collected in May 2025

Sl.No.	Parameters	WHO Standards	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	Average
1	pH	7.0 – 8.5	8.12	9.34	8.75	8.42	9.12	8.68	9.03	8.87	8.2	9.45	8.96	8.59	8.19	9.21	8.31	8.75
2	Temperature	<35°C	29.7	30.4	30.1	29.3	30.6	29.9	30.2	29.1	31	29.5	30	29.6	30.3	30.7	29.2	29.96
3	Electrical conductivity	< 2500 µS/cm	392	428	407	419	395	421	409	430	399	412	390	426	405	417	398	409.87
4	Total dissolved Solids	≤ 500 mg/L	246	268	257	249	264	241	270	252	260	243	265	240	255	266	250	255.07
5	Dissolved Oxygen	≥ 6 mg/L	6.74	7.92	6.18	7.35	6.89	7.11	6.42	7.76	6.7	7.24	6.3	7.59	6.91	6.83	7.07	7
6	Turbidity	≤ 5 NTU	2.1	1.8	2.7	2.3	1.9	2.5	2	2.9	1.7	3	2.6	1.6	2.2	1.5	2.8	2.24
7	Total Hardness	≤ 500 mg/L	118	104	127	93	111	130	97	122	106	90	116	128	103	109	94	109.87
8	Chloride	≤ 1000 mg/L	27.3	39.2	33.2	29.5	36.1	25.8	31.6	38.5	27	34.8	28.4	30.1	32.5	35.7	37.2	32.45
9	Alkalinity	≤200 mg/L	103	137	119	128	112	140	101	134	109	126	117	95	132	122	105	118.67
10	Nitrate	≤ 50 mg/L	0.61	0.53	0.68	0.59	0.66	0.5	0.71	0.54	0.6	0.57	0.65	0.52	0.69	0.55	0.6	0.6
11	Sulphate	≤ 250 mg/L	0.11	0.14	0.12	0.1	0.13	0.09	0.15	0.11	0.1	0.12	0.1	0.13	0.09	0.15	0.11	0.6
12	Phosphate	≤ 0.10 mg/L	0.08	0.07	0.08	0.09	0.06	0.05	0.04	0.09	0.1	0.07	0.06	0.08	0.1	0.05	0.09	0.07

Results For the Month of April 2025

pH: The pH is considered as the basic water quality parameter. In the present study, the pH values in all the water samples showed variations. The higher values were observed in S (13) and the lowest values were observed in S(1). In comparison with the WHO standards, all the samples exceeded the upper WHO limit, indicating strong alkalinity and a potential influence of mineral-rich geological formations or the anthropogenic activities.

Temperature: The water temperature directly influences the biological activity and the chemical solubility. In the present study, the temperature values in all the water samples showed variations. The higher values were observed in S(14) and the lowest values were observed in S(2). All the values are characteristic of pre-monsoon seasonal warming and remained within the WHO standards. The variations could be due to depth, exposure to sunlight and ambient weather conditions at the time of collection.

Electrical conductivity: The electrical conductivity is a measure of water's ability to conduct electricity, which reflects the concentration of dissolved ions. In the present study, the electrical conductivity values in all the water samples showed variations. The higher values were observed in S (8) and the lowest values were observed in S(6). All the values remained within the WHO standards, indicating the absence of salinity issues.

Total Dissolved Solids: The TDS is a cumulative measure of all the organic and inorganic substances dissolved in water. In the present study, the TDS values in all the water samples showed variations. The higher values were observed in S(6) and the lowest values were observed in S(15). All the values remained within the WHO standards, indicating relatively clean water with the low mineral content.

Dissolved Oxygen: The DO is crucial for the survival of aquatic organisms. In the present study, the DO values in all the water samples showed variations. Higher values were observed in S(1) and lowest values were observed in S(9). In comparison with the WHO standards, most of the samples exceeded the minimum WHO requirement, indicating the good oxygen availability to support the aquatic life.

Turbidity: The turbidity indicates the presence of suspended solids. In the present study, the Turbidity values in all the water samples showed variations. The higher values were observed in S(8) and the lowest values were observed in S(11). All values remained within the WHO standards, indicating that the water was relatively clear and free from the excessive suspended particles.

Total hardness: The total hardness indicates the presence of dissolved calcium and magnesium ions in the water. In the present study, the total hardness values in all the water samples showed variations. The higher values were observed in S(13) and the lowest values were observed in S(6). All the values remained within the WHO standards, indicating that the water is suitable for the domestic use without posing scaling or health concerns.

Chloride: - The chloride indicates the presence of dissolved salts in the water. In the present study, the chloride values in all the water samples showed variations. The higher values were observed in S(2) and the lowest values were observed in S(9). All the values remained within the WHO standards.

Alkalinity: The alkalinity represents the buffering capacity of the water against acidification. In the present study, the alkalinity values in all the water samples showed variations. The higher values were observed in S(12) and the lowest values were observed in S(9). All the values remained within the WHO standards, indicating the adequate buffering capacity to maintain stable pH levels in the water.

Nitrate: The nitrate is an essential nutrient but excessive levels may indicate the pollution from the agricultural runoff or sewage. In the present study, the nitrate values in all the water samples showed variations. The higher values were observed in S(12) and the lowest values were observed in S(3), S(7), and S(11). All the values remained within the WHO standards,

Sulphate: The sulphate indicates the presence of dissolved minerals, particularly from the natural rock and the soil sources. In the present study, the sulphate values in all the water samples showed variations. The higher values were observed in S(10) and the lowest values were observed in S(2), S(5), S(7), S(11), S(13), and S(15). All the values remained within the WHO standards, indicating the absence of industrial effluents or sulphur-bearing minerals in the surrounding geology.

Phosphate: The phosphate indicates the presence of nutrient pollution, often from the agricultural runoff or domestic wastewater. In the present study, the phosphate values in all the water samples showed variations. The higher values were observed in S (8) and the lowest values were observed in S(6), S(11), S(12), and S(15). All the values remained within the WHO standards, potentially due to the presence of organic waste or detergent contamination.

Results For the Month of May 2025

pH: The pH is considered as the basic water quality parameter. In the present study, the pH values in all the water samples showed variations. The higher values were observed in S(10) and the lowest values were observed in S(1). In comparison with the WHO standards, all the samples exceeded the upper WHO limit, indicating strong alkalinity and a potential influence of mineral-rich geological formations or the anthropogenic activities.

Temperature: The water temperature directly influences biological activity and chemical solubility. In the present study, the temperature values in all the water samples showed variations. The higher values were observed in S(9) and the lowest values were observed in S(8). All the values are characteristic of pre-monsoon seasonal warming and remained within the WHO standards.

Electrical conductivity: The electrical conductivity is a measure of water's ability to conduct electricity, which reflects the concentration of dissolved ions. In the present study, the electrical conductivity values in all the water samples showed variations. The higher values were observed in S(8) and the lowest values were observed in S(11). All the values remained within the WHO standards.

Total Dissolved Solids: The TDS is a cumulative measure of all the organic and inorganic substances dissolved in water. In the present study, the TDS values in all the water samples showed the variations. The higher values were observed in S(7) and the lowest values were observed in S(12). All the values remained within the WHO standards.

Dissolved Oxygen: The DO is crucial for the survival of aquatic organisms. In the present study, the DO values in all the water samples showed variations. The higher values were observed in S(2) and the lowest values were observed in S(3). In comparison with the WHO standards, most of the samples exceeded the minimum WHO requirement, indicating the good oxygen availability to support the aquatic life.

Turbidity: The turbidity indicates the presence of suspended solids. In the present study, the Turbidity values in all the water samples showed variations. The higher values were observed in S(10) and the lowest values were observed in S(14). All the values remained within the WHO standards, indicating that the water was relatively clear and free from the excessive suspended particles.

Total hardness: The total hardness indicates the presence of dissolved calcium and magnesium ions in water. In the present study, the total hardness values in all the water samples showed variations. The higher values were observed in S (6) and the lowest values were observed in S(10). All the values remained within the WHO standards, indicating that the water is suitable for domestic use without posing scaling or health concerns.

Chloride: The chloride indicates the presence of dissolved salts in the water. In the present study, the chloride values in all the water samples showed variations. The higher values were observed in S(2) and the lowest values were observed in S(6). All the values remained within the WHO standards.

Alkalinity: The alkalinity represents the buffering capacity of water against acidification. In the present study, the alkalinity values in all the water samples showed variations. The higher values were observed in S(6) and the lowest values were observed in S(12). All the values remained within the WHO standards.

Nitrate: The nitrate is an essential nutrient, but excessive levels may indicate the pollution from the agricultural runoff or sewage. In the present study, the nitrate values in all the water samples showed variations. The higher values were observed in S (7) and the lowest values were observed in S(6). All the values remained within the WHO standards.

Sulphate: The sulphate indicates the presence of dissolved minerals, particularly from the natural rock and the soil sources. In the present study, the sulphate values in all the water samples showed variations. The higher values were observed in S (7) and S(14) and the lowest values were observed in S(6) and S(13). All the values remained within the WHO standards.

Phosphate: The phosphate indicates the presence of nutrient pollution, often from agricultural runoff or domestic wastewater. In the present study, the phosphate values in all the water samples showed the variations. The higher values were observed in S (13) and the lowest values were observed in S(7). All the values remained within the WHO standards.

Conclusion:

The present study provides a comprehensive physico-chemical assessment of water quality in the KRS backwaters near Venugopalaswamy Temple, Mysore, during the pre-monsoon months of March, April, and May 2025. Twelve key water quality parameters were analyzed across 15 samples to evaluate the water quality. Results indicate that most parameters, including temperature, turbidity, electrical conductivity, total dissolved solids, total hardness, chloride, nitrate, sulphate, and phosphate remained within the permissible limits prescribed by WHO standards, suggesting that the water is generally free from major chemical contamination and suitable for domestic and irrigation purposes. Alkalinity levels exceeded WHO limits at select locations (notably S7 in March), indicating elevated buffering capacity that may be linked to local lithology or anthropogenic activities. pH levels consistently exceeded the upper WHO limit during April and May, indicating alkaline conditions, possibly due to weathering of carbonate-rich rocks or reduced rainfall dilution. Dissolved Oxygen (DO) values were marginally below the standard in a few samples, especially during March, suggesting localized organic pollution or stagnation. While no immediate health threats were evident, the month-to-month variation highlights the influence of seasonal and site-specific factors such as runoff, temperature, and land use. The findings underscore the importance of routine monitoring to ensure sustained water quality and to detect early signs of nutrient enrichment or anthropogenic contamination. Future studies may include microbial and toxicological assessments for a more holistic evaluation of water suitability.

References:

1. Najar, I. A., & Basheer Khan, A. (2012). Assessment of seasonal variation in water quality of Dal Lake (Kashmir, India) using multivariate statistical techniques. *WIT Transactions on Ecology and the Environment*, *164*, 123–134. https://doi.org/10.2495/WP120111
2. Bhatnagar, A., Hogland, W., Marques, M., & Sillanpää, M. (2013). An overview of the modification methods of activated carbon for its water treatment applications. *Chemical Engineering Journal*, *219*, 499–511. https://doi.org/10.1016/j.cej.2012.12.038
3. Alau, K. K., Gimba, C. E., & Kagbu, J. A. (2015). Preparation and characterization of activated carbon from neem (*Azadirachta indica*) leaf. *International Journal of Environmental Science and Development*, *6*(2), 165–169. https://doi.org/10.7763/IJESD.2015.V6.571

4. Chung, K. T. (2016). Azo dyes and human health: A review. *Journal of Environmental Science and Health, Part C*, *34*(4), 233–261. https://doi.org/10.1080/10590501.2016.1236602
5. Dufatanye Umwali, E., *et al.* (2021). Spatio-seasonal variation of water quality influenced by land use and land cover in Lake Muhazi. *Scientific Reports*, *11*, 17376. https://doi.org/10.1038/s41598-021-96633-9
6. Tiwari, B. K., *et al.* (2021). Evaluation of spatio-temporal changes in surface water quality and their suitability for designated uses: Mettur reservoir, India. *Journal of Water and Climate Change*, *15*(9), 4434–4452. https://doi.org/10.2166/wcc.2024.186
7. Rani, S., & Giri, A. (2023). Impact of seasonal variations on the water quality and zooplankton diversity of pond in Haryana, India (Ph.D. thesis). https://doi.org/10.13140/RG.2.2.32388.03207
8. Toxics, water quality & model correlations. (2023). *Environmental Monitoring and Assessment*, *195*, 529. https://doi.org/10.1007/s10661-023-10529-0
9. Singh, R., *et al.* (2024). Aquatic insects as indicators of water quality: Seasonal distribution patterns in northeast India. *Ecotoxicology and Environmental Safety*, *258*, 114151. https://doi.org/10.1016/j.ecoenv.2023.114151
10. Appraisal of seasonal variations in water quality of Hathaikheda Reservoir, Bhopal. (2024). *World Journal of Applied Research and Review*, *11*(6), 160–170. https://doi.org/10.54061/wjarr.2024.1613
11. Ignatius, G., *et al.* (2024). Multivariate statistical and hydrogeochemical analysis of seasonal groundwater quality in Trivandrum, Kerala, India. *Sustainable Water Resources Management*. https://doi.org/10.1007/s43621-024-00584-w
12. Tiwari, *et al.* (2024). Comparative analysis of water quality index based on seasonal variations in Indian reservoirs. *Water Quality Research Journal*, *60*(1), 19–32. https://doi.org/10.2166/wqrj.2024.106240
13. Sub-seasonal vegetation–water quality relationships. (2024). *Water*, *14*(7), 1058. https://doi.org/10.3390/w14071058
14. Singh, K. P., & Saxena, A. (2025). Seasonal variations and correlation analysis of water quality parameters in the Chambal River, Rajasthan, India. *Water and Environment Research*, *97*, e70035. https://doi.org/10.1002/wer.70035
15. Subramaniyan, A., & Ganesan, S. (2025). Human health risk and water quality assessment due to fluoride and nitrate around Cauvery River basin, southern India. *Environmental Monitoring and Assessment*, *196*(10), 880. https://doi.org/10.1007/s10661-024-12985-5

ONE-POT SYNTHESIS OF HIGHLY FLUORESCENT FURO[2,3-H]QUINOLINE AND FURO[2,3-H]ISOQUINOLINE DERIVATIVES USING FISCHER CARBENE COMPLEX

Priyabrata Roy
Department of Chemistry,
Victoria Institution (College), 78B, A.P.C. Road, Kolkata 700009, India
Corresponding author E-mail: priyo_chem@yahoo.co.in

Abstract:

This chapter presents an efficient synthetic strategy for the construction of furo(2,3-h)quinoline and furo(2,3-h)isoquinoline frameworks via Fischer carbene complex–mediated benzannulation reactions. By employing conjugated dienyne systems with a pyridine-based alkene, the study demonstrates conditions that favor selective annulation, overcoming limitations observed with simple benzene analogues. The work highlights the impact of reaction parameters—including ligand additives, solvent effects, and substrate substituents—on product formation and yield. Notably, the synthesized compounds display strong fluorescence, underscoring their potential utility in both pharmaceutical research and materials science. The chapter further discusses unusual competitive pathways, mechanistic insights, and the optical properties of representative derivatives.

Keywords: Benzannulation, Furo(2,3-h)quinoline, Furo(2,3-h)isoquinoline, Optical Properties, Conjugated Dienyne.

1. Introduction:

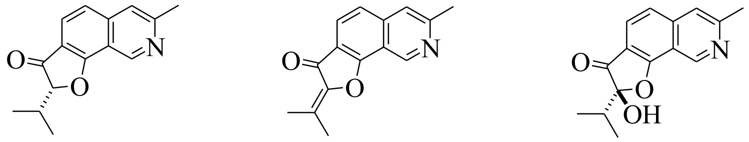
The furoquinoline skeleton is present in many alkaloids like skimmianine and balfouridine.[1] Furo[2,3-*h*]quinoline derivatives are of particular interest as they appear to be very promising photochemotherapeutic agents due to some of its properties, such as high antiproliferative activity, very poor genotoxicity and lack of skin phototoxicity.[2] DNA-intercalators containing a linear or angular planar chromophore with a polyaromatic ring can influence the structures and physiological functions of DNA.[3] Some intercalators such as furocoumarin, acridines, anthraquinones, naphthalimides, and phenanthridine are used in cancer treatment. Angelicin (Fig. 3.1), an angular furocoumarin, has been used to treat pain in the loins and knees,[4] and skin diseases in phototherapy.[5] Guiotto and co-workers have synthesized a series of furoquinolinones,[6] in which the oxygen atom of furocoumarin has been substituted by NH, and some of them showed strong antiproliferative activity against tumor cell lines upon UVA (Ultraviolet Radiation A) irradiation. However, these furoquinolinones also revealed evident skin phototoxicity and marked clastogenic activity due to the formation of covalent monoadducts (MA) with DNA base and covalent DNA–protein cross-links (DPC) upon UVA activation. In the dark, these furoquinolinones exhibit weak antiproliferative activity with a mechanism of action related to topoisomerase II inhibition. In contrast to normal cell, many tumor cells show high expression levels of topoisomerase II, making this enzyme an ideal drug target.[7]

Angelicin: X=O
Furoquinolinone: X=NH

Furo[2,3-*h*]quinoline derivative

Figure 1

Eosinophils are believed to contribute proinflammatory effects in allergic inflammation, including asthma.[8] The cytokines such as hematopoietins, interleukin-5 (IL-5), IL-3 and GM-CSF have been shown to stimulate production of eosinophils in the bone marrow[9] and the same cytokines inhibit eosinophilic apoptosis and prolong survival when eosinophils are cultured.[10] In allergic individuals, large numbers of eosinophils are accumulated and release activated oxygen and toxic granule-derived proteins such as major basic protein and eosinophil cationic protein.[8] Consequently, agents that inhibit the prolongation of eosinophil survival will be another candidate for development of drugs to treat bronchial asthma. Inhibitors of IL-5 mediated prolongation of eosinophil survival, a fungus, *Aspergillus ustus* (Bain.) Thorn & Church TC 1118 was found to produce three novel biologically important isoquinoline alkaloids, e.g., TMC-120A, B and C (Fig. 3.2).[11]

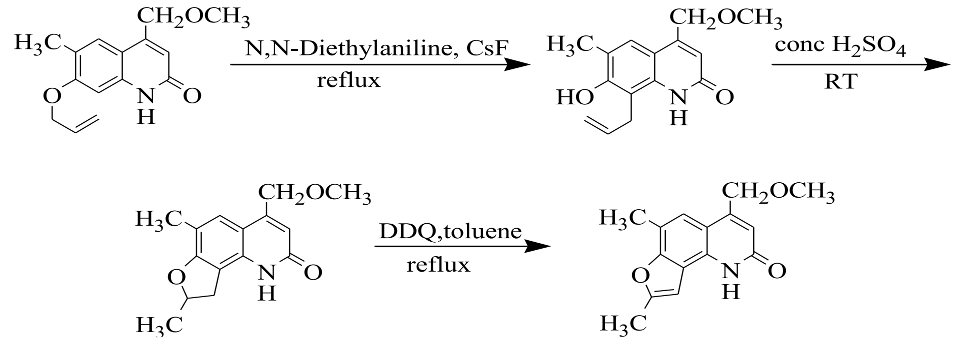


TMC-120 A   TMC-120 B   TMC-120 C

Figure 2

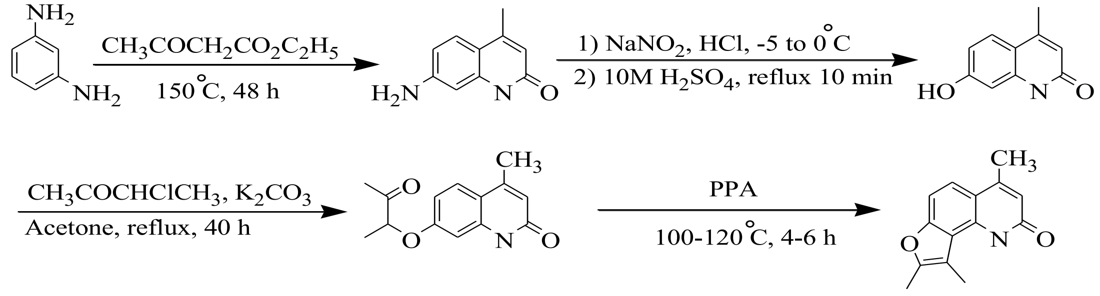
2. Synthesis of Furoquinoline/Furoisoquinoline[3]

Over the last decades, great efforts were made towards the search of their biological significance. In contrast, mild and efficient synthetic strategies of these compounds are less well-known. Chilin and co-workers have synthesized furo[2,3-*h*]quinoline derivative, using the reaction strategy depicted in Scheme 3.1.[12]



Scheme 1

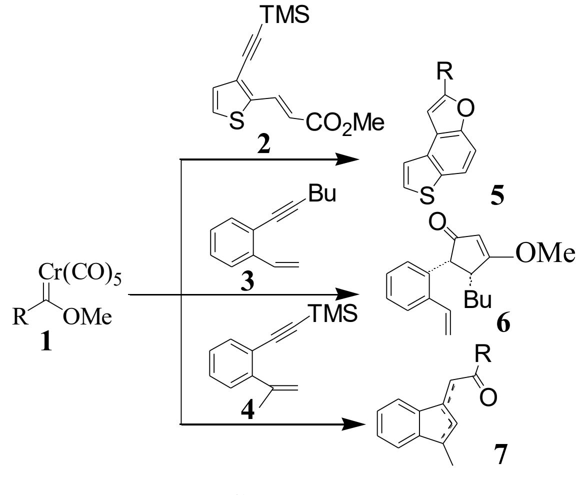
Xie and co-workers established a multistep synthesis of angular furoquinolinones starting from *m*-phenylenediamine and ethyl acetoacetate (Scheme 3.2).[13]



Scheme 2

3. One–Pot Synthesis of Furo[2,3-h]quinoline and furo[2,3-h]isoquinoline Derivatives Using Fischer Carbene Complex

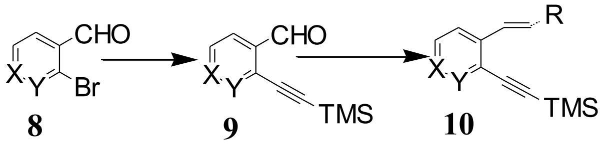
Benzannulation reactions involving the coupling of five-membered 2-alkenyl-3-alkynyl heteroaromatics with Fischer carbene complexes have been successfully reported.[14] However, when the five-membered heteroaromatic core is replaced with a benzene ring, this annulation strategy fails. Specifically, coupling an *o*-alkynylstyrene derivative **3** with carbene complex **1** leads exclusively to products **6**, where annulation occurs within the R substituent and not on the styrene backbone.[15a] Likewise, cyclopentannulation yielding an indane derivative (**7**) was the only outcome when enyne **4** was coupled with carbene complex **1**.[15b]



Scheme 3

This work focuses on exploring the coupling of Fischer carbene complexes with conjugated dienyne systems where the central alkene is embedded within a six-membered aromatic heterocycle, such as pyridine (represented by compound **10**, *Scheme 2*). A major goal of this chapter is to clarify the conditions that favor the formation of furo(2,3-h)quinoline and furo(2,3-h)isoquinoline frameworks — pathways that are often only minor or undesired byproducts in the coupling of *o*-alkynylstyrenes with Fischer carbene complexes.

The significance of furo(2,3-h)quinoline derivatives lies in their promise as photochemotherapeutic agents due to properties like potent antiproliferative activity, minimal genotoxicity, and lack of skin phototoxicity.[16] Likewise, the furo(2,3-h)isoquinoline skeleton — found in naturally occurring alkaloids such as TMC-120 A, B, and C — shows moderate inhibition of eosinophil function, indicating possible anti-inflammatory effects.[17]

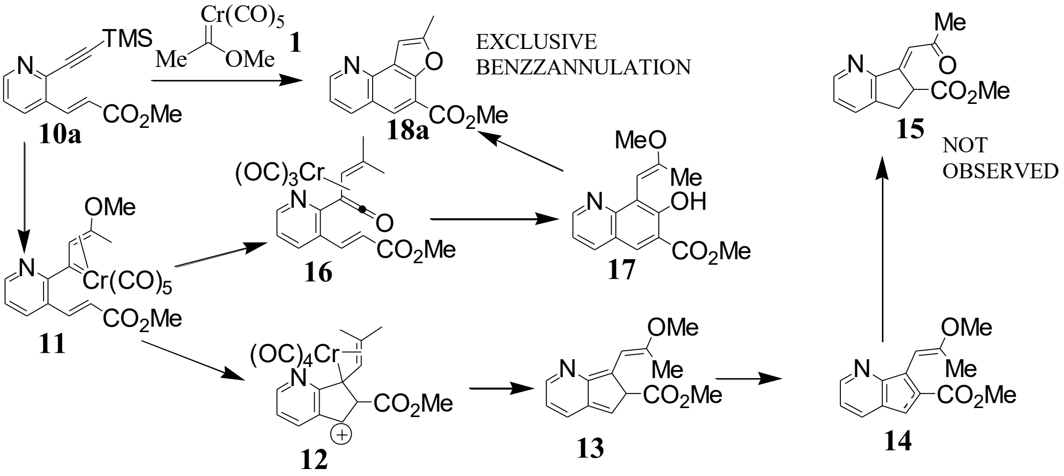


Scheme 4

3.1. Synthesis of Enyne Substrates

The general synthetic route to the key enyne derivatives is shown in *Scheme 2*. A Sonogashira coupling was carried out on a known bromoaldehyde[18] (**8**) using trimethylsilylacetylene,[19] yielding the alkyne aldehyde **9**. A subsequent Wittig reaction on **9** furnished the desired products with good to excellent yields. Notably, with reactive or semi-stabilized ylides, the Wittig reaction exclusively gave the desilylated terminal alkyne **14**, alongside the targeted alkene.

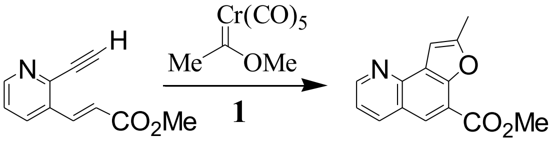
3.2. Initial Coupling Studies: Benzannulation with Pyridine-Based Enyne



Scheme 5

Our study commenced with the reaction of enyne derivative **10a** with Fischer carbene complex **2a**, as summarized in *Table 1*. The initial reaction — the coupling of **10a** and **1** in THF at 80 °C followed by acidic hydrolysis (*Scheme 3*) — proceeded efficiently, providing the benzannulation product **3a** in 49% yield (**Entry a**, *Table 1*).[20] No pentannulation product was observed.[21]

This result suggests that CO insertion takes place at the vinylcarbene stage, balancing C–C bond formation against CO insertion (conversion of **11** to **15** versus **11** to **12**, *Scheme 3*). The successful benzannulation in the pyridine system may arise from the reduced nucleophilicity of the alkene since pyridine is π-deficient.



10a **18a**

Table 1: **Effect of reaction conditions on the coupling of Fischer carbene complex 1 and 2-alkynyl-3-alkenylpyridine 10**[a]

Entry	Solvent	Time	Concn (M)[b]	Yield (%)[c]
A	THF	20	0.4	59
B	THF	10	0.4	31
C	THF-PPh_3	20	0.4	73[d,e]
D	THF-PPh_3	20	0.1	52[d]
E	1,4-Dioxane-PPh_3	20	0.4	64[d]
F	Acetonitrile-PPh_3	20	0.4	58 [d]
G	Acetone-PPh_3	20	0.4	56 [d]

[a] All reaction were conducted at the reflux temperature.

[b] Concentration of carbene and enyne in respective solvent.

[c] Isolated yields.

[d] PPh_3 used: 1.0 equiv.

[e] For experimental details of the optimized condition, see Ref. 7

3.3. Reaction Parameter Effects

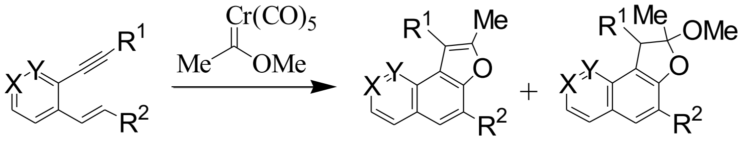
The reaction duration also impacted the yield: reducing reaction time lowered the yield (**Entry b**, *Table 1*). To address possible yield loss due to competing sp^2 nitrogen ligation, the reaction was repeated with a ligand additive (PPh_3), which improved the product formation (**Entry c**).

A notable drop in yield was observed in dilute solution (**Entry d**, *Table 1*). This aligns with Wulff and co-workers' finding[22] that CO insertion is suppressed under dilution, as the coordination of a second alkyne ligand is critical for the CO insertion event. Using other solvents (1,4-dioxane, acetonitrile, acetone) gave inferior yields for **14a**.

4. Scope and Generality

Having synthesized the **furo(2,3-h)quinoline** derivative successfully, we expanded the study to prepare additional analogues, especially varying the substituent at C-6. Various enyne derivatives were reacted with Fischer carbene complex **1** under the optimized conditions (**Entry c**, *Table 1*). In all cases, formation of **furoquinoline** and **furoisoquinoline** products was exclusive.

For substrates where the pure cis-isomer was used (**Entries b and c**), yields were slightly lower. The benzofuran annulation worked equally well for silylated alkynes (**Entries d and g**), which yielded the same products as their terminal analogues following desilylation with catalytic sulfuric acid. Substrates bearing bulky alkyne substituents (e.g., trimethylsilyl groups; **Entries I and J**) showed only a minor yield drop compared to their terminal counterparts (**Entries a and h**).



10 **18** **19**

Table 2: synthesis of furo[2,3-h]quinoline and furo[2,3-h]isoquinoline derivatives through coupling of Fischer carbene complexes with pyridine-bridged enynes[a]

Entry	X	Y	R^1	R^2	Yield 18	Yield 19
a	CH	N	H	CO$_2$Me	73[e]	0
b	CH	N	H	CH$_3$	4[c]	61 (55)[d,e]
c	CH	N	H	Ph	0	67 (62)[d]
d	CH	N	TMS(H)[b]	CO$_2$Et	78	0
e	N	CH	H	H	7[c]	60[e]
f	N	CH	H	CH$_3$	0	58
g	N	CH	TMS(H)[b]	CO$_2$Me	71	0
h	N	CH	H	Ph	0	65[e]
i	CH	N	TMS(H)[b]	CO$_2$Me	64	0
j	N	CH	TMS(H)[b]	Ph	0	55

[a] Puirified *trans* isomer was used as the starting material; [b] In the product, R^1 is H.

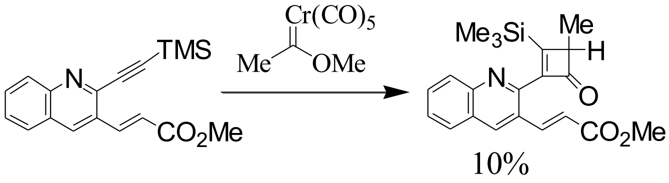
[c] Tentatively identified by ^{1}H NMR, IR, mass spectroscopy and combustion analysis.

[d] The number in parentheses is the yield using the purified *cis* isomer as the starting material.

5. Competitive Pathways

The reaction was also run alongside known chromium-carbene–alkyne coupling processes. Notably, no benzannulation products were isolated when carbene complex **1** was coupled with a 3-alkenyl-2-alkynylquinoline derivative **20** (*Scheme 4*). Instead, a compound tentatively identified as cyclobutenone **21** formed in low yield.[23]

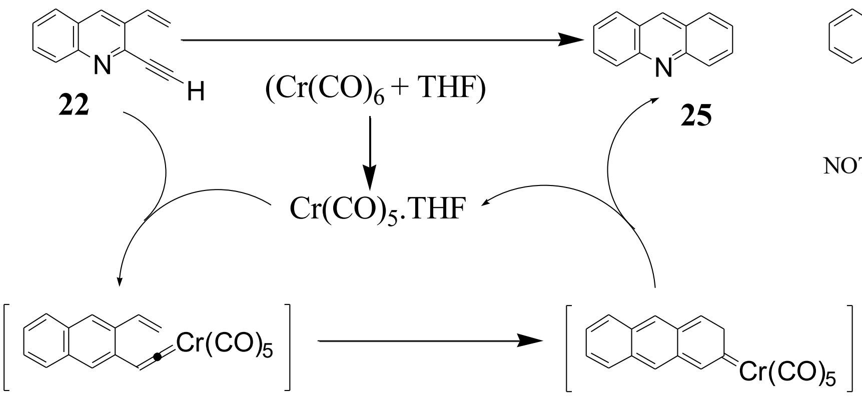
Additionally, an unusual benzannulation product **21** was obtained from the reaction of carbene complex **1** and enyne **20** (*Scheme 5*).



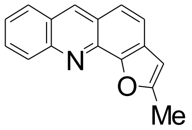
20 **21**

Scheme 4

This product is more plausibly formed by electrocyclization of aromatic enynes rather than via formation of the alternative benzannulation product **26**, given the absence of a fused furan ring. To explain this, *Scheme 2* proposes a mechanism where acridine forms via 6π electrocyclization of vinylidene intermediate **23**, catalyzed in situ by $Cr(CO)_5$.THF generated from residual $Cr(CO)_6$ in the Fischer carbene complex or the reaction medium.[24, 25]



23 **24**



NOT OBSERVED

26

Scheme 5

6. Optical Properties

All synthesized compounds showed strong fluorescence. The optical behaviors of compounds **19e**, **19h**, **19c**, and **18d** were investigated by UV/Vis and photoluminescence spectroscopy in CH_2Cl_2 at room temperature. These results are compiled in *Table 3*.

Table 3: Spectroscopic data of 5-9

Compound	UV/Vis λ_{max} [nm]	Exitation λ_{max} [nm]	Fluorescence λ_{max} [nm]	Φ_{fl} (%)[a]
19e	345, 265	355	427	0.11
19h	355, 251	365	398	0.56
19c	346, 257	356	388	0.21
18d	344, 318, 262	354	403	0.47

[a]Quantum yields were measured by using pyrane in DCM solution as a standard.

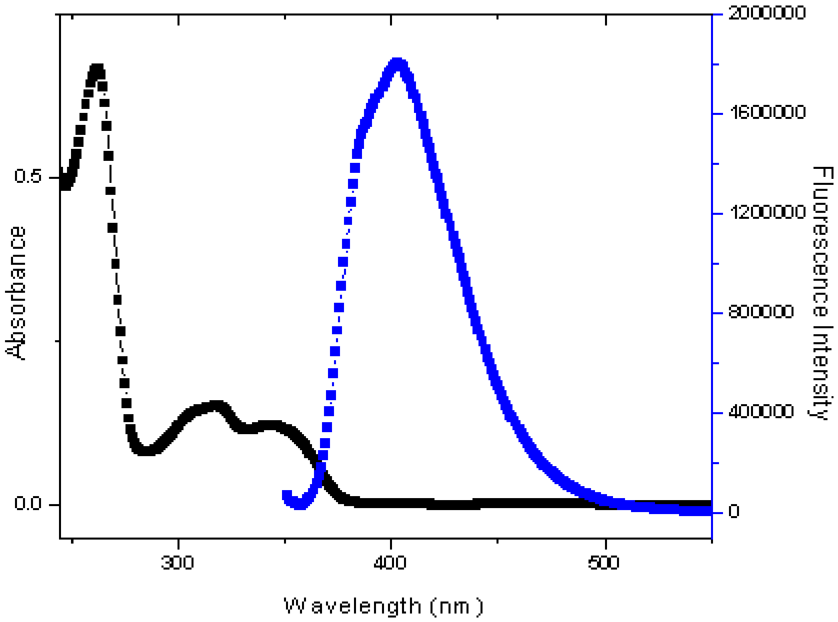


Figure 1: Absorption and emission spectra of 19e (10^{-6}M) in DCM

The absorption spectra feature two electronic transitions: a strong longer-wavelength band at 340–360 nm, likely due to an *n–π* transition involving lone pairs on the oxygen atom, and a shorter wavelength band at 250–265 nm, attributable to *π–π* transitions in the aromatic units. For **18d**, an additional shoulder at 318 nm (*Figure 1*) indicates a transition influenced by its ester functionality. The emission spectra for **5**, **19e**, **19h**, and **19c** consistently appear in the 390–430 nm range (*Figure 1*).

Conclusion:

In summary, we have established a novel route for synthesizing furoquinoline and furoisoquinoline derivatives through benzofuran annulation onto a pyridine core. These frameworks are significant as integral motifs in pharmaceuticals and bioactive compounds and are further notable for their promising fluorescence properties. Detailed optical studies of these systems are currently underway.

References:

1. (a) Jurd, L.; Wong, R. V. *Aust. J. Chem.* 1981, *34*, 1625; (b) Coppola, G. M.; J. *Heterocycl. Chem.* 1983, *20*, 1217.
2. (a) Chilin, A.; Marzano, C.; Baccichetti, F.; Simonato, M.; Guiotto, A. *Bioorg. Med. Chem.* 2003, *11*, 1311; (b) Marzano, C.; Chilin, A.; Baccichetti, F.; Bettio, F.; Guiotto, A.; Miolo, G.; Bordin, F. *Eur. J. Med. Chem.* 2004, *39*, 411.
3. (a) Erkkila, K. E.; Odom, D. T.; Barton, J. K. *Chem. Rev.* 1999, *99*, 2777; (b) Braña, M. F.; Ramos, A. *Curr. Med. Chem.—Anti-Cancer Agents* 2001, *1*, 237; (c) Gibson, D. *Pharmacogenomics* J. 2002, *2*, 275; (d) Ihmels, H.; Otto, D. *Top. Curr. Chem.* 2005, *258*, 161; (e) Martínez, R.; Chacón-García, L. *Curr. Med. Chem.* 2005, *12*, 127; (f) Palchaudhuri,

R.; Hergenrother, P. *J. Curr. Opin. Biotech.* 2007, *18*, 497; (g) Wheate, N. J.; Brodie, C. R.; Collins, J. G.; Kemp, S.; Aldrich-Wright, J. R. *Mini-Rev. Med. Chem.* 2007, *7*, 627.

4. Wang, X.; Wang, Y.; Yuan, J.; Sun, Q.; Liu, J.; Zheng, C. *J. Chromatogr. A* 2004, *1055*, 135.
5. Gambari, R.; Lampronti, I.; Bianchi, N.; Zuccato, C.; Viola, G.; Vedaldi, D.; Dall'Acqua, F. *Top. Heterocycl. Chem.* 2007, *9*, 265.
6. (a) Rodighiero, P.; Guiotto, A.; Chilin, A.; Bordin, F.; Baccichetti, F.; Carlassare, F.; Vedaldi, D.; Caffieri, S.; Pozzan, A.; Dall'Acqua, F. *J. Med. Chem.* 1996, *39*, 1293; (b) Marzano, C.; Chilin, A.; Guiotto, A.; Baccichetti, F.; Carlassare, F.; Bordin, F. *Il Farmaco* 2000, *55*, 650; (c) Chilin, A.; Marzano, C.; Guiotto, A.; Baccichetti, F.; Carlassare, F.; Bordin, F. *J. Med. Chem.* 2002, *45*, 1146; (d) Marzano, C.; Chilin, A.; Bordin, F.; Baccichetti, F.; Guiotto, A. *Bioorg. Med. Chem.* 2002, *10*, 2835; (e) Chilin, A.; Marzano, C.; Baccichetti, F.; Simonato, M.; Guiotto, A. *Bioorg. Med. Chem.* 2003, *11*, 1311; (f) Marzano, C.; Chilin, A.; Baccichetti, F.; Bettio, F.; Guiotto, A.; Miolo, G.; Bordin, F. *Eur. J. Med. Chem.* 2004, *39*, 411.
7. (a) Jahnz, M.; Medina, M. A.; Schwille, P. *ChemBioChem* 2005, *6*, 920; (b) Holden, J. A. *Curr. Med. Chem.—Anti-Cancer Agents* 2001, *1*, 1; (c) Denny, W. A.; Baguley, B. C. *Curr. Top. Med. Chem.* 2003, *3*, 339.
8. Gleich, G. J. *J. Allergy Clin. Immunol.* 1990, *85*, 422.
9. Weller, P. R. *N. Engl. J. Med.* 1991, *324*, 1110.
10. (a) Her, E.; Frazer, J.; Austen K. F.; Owen, W. F. Jr. *J. Clin. Invest.* 1991, *88*, 1982; (b) Rothenberg, M. E.; Owen, W. F. Jr.; Silberstein, D. S.; Woods, J.; Soberman, R. J.; Austen K. F.; Stevens, R. L. *J. Clin. Invest.* 1988, *81*, 1986; (c) Yamaguchi, Y.; Suda, T.; Ohta, S.; Tominaga, K.; Miura, Y.; Kasahara. T. 1991, *78*, 2542.
11. Kohno, J.; Sakurai, M.; Kameda, N.; Nishio, M.; Kawano, K.; Kishi, N.; Okuda T.; Komatsubara S. *J. Antibiot.* 1999, *52*, 913.
12. Chilin, A.; Marzano, C.; Baccichetti, F.; Simonato, M.; Guiotto, A. *Bioorg. Med. Chem.* 2003, *11*, 1311.
13. Xie, L.; Qian, X.; Cui, J.; Xiao, Y.; Wang, K.; Wu, P.; Cong, L. *Bioorg. Med. Chem.* 2008, *16*, 8713.
14. Zhang, Y.; Candelaria, D.; Herndon, J. W. Tetrahedron Lett. 2005, *46(13)*, 2211-2214.
15. (a) Jackson, T. J.; Herndon, J. W. *Tetrahedron* 2001, *57(18)*, 3859-3868. (b) Zhang, L.; Herndon, J. W. *Organometallics* 2004, *23(6)*, 1231-1235.
16. Marzano, C.; Chilin, A.; Baccichetti, F.; Bettio, F.; Guiotto, A.; Miolo, G.; Bordin, F. *European Journal of Medicinal Chemistry* 2004, *39(4)*, 411–419.

17. (a) Kohno, J.; Hiramatsu, H.; Nishio, M.; Sakurai, M.. *Tetrahedron* 1999, *55(37)*, 11247-11252. (b) Slack,G. J.; Puniani, E.; Frisvad, J. C.; Samson, R. A.; MillerJ. D. Mycological Research 2009, *113(5)*, 480–490.
18. bromoaldehyde was prepared by the regioselective ortho-lithiation of 2-bromopyridine and 3-bromopyridine followed by quenching with DMF. Numata, A.; Kondo, Y.; Sakamoto, T. Synthesis 1999, 306-311.
19. (a) Jana, G.P.; Ghorai, B.K. Tetrahedron 2007, 63, 12015-12025. (b) Mukherjee, S.; Jana, G. P.; Ghorai, B. K. J.Organomet. Chem. 2009, *694*, 4100-4106.
20. Roy, P.; Ghorai, B.K. Tetrahedron Lett. 2011, 52, 251-253.
21. Zhang, J.; Zhang, Y.; Schnatter, W. F. K.; Herndon, J. W. *Organometallics* 2006, *25*, 1279-1284.
22. Bos, M.E.; Wulff, W. D.; Miller, R. A.; Chamberlin, S.; Brandvold, T. A. *J. Am. Chem. Soc.* 1991, *113*, 9293-9319.
23. For a related process of cyclobutenone formation, see: Wulff, W. D. In *Comprehensive Organic Synthesis*; Trost, B. M., Fleming, I., Paquette, L. A., Eds.; Pergamon: Oxford,1991; Vol. 5, pp 1065-1113.
24. Li, R.; Zhang, L.; Camacho-Davila, A.; Herndon, J. W. *Tetrahedron Lett.* 2005, *46*, 5117-5120.
25. Maeyama, K.; Iwasawa, N. *J. Org. Chem.* 1999, *64,* 1344-1346.

COSMOLOGICAL MODEL IN $f(Q)$ GRAVITY WITH BIANCHI TYPE III METRIC AND LOG-POLYNOMIAL SCALE FACTOR

Mukunda Dewri
Department of Mathematical Sciences,
Bodoland University, Kokrajhar, BTR, Assam, India
Corresponding author E-mail: dewri11@gmail.com

Abstract:

This chapter studies cosmological dynamics of the model in $f(Q)$ gravity through a Bianchi Type III metric characterized by a log-polynomial scale factor $a(t) = a_1 + a_2 t^n + a_3 lnt$, which signifies an emergent universe model. We formulate field equations, calculate cosmological parameters, and then compare them with observational constraints. The cosmological parameters are presented in figures, and their impact on the universe's evolution, the transition from a phase of slow or no expansion to one of rapid expansion, is discussed within the context of modified gravity theories.

Introduction:

The rapid expansion of the universe, along with the enigmatic characteristics of dark energy, has spurred extensive research into modified gravity theories that build upon Einstein's General Relativity to clarify unresolved cosmological and astrophysical challenges [Ba˜nados & Ferreira (2010); Behera *et al.* (2010); Capozziello *et al.* (2010); Sahoo (2010); Sotiriou & Faraoni (2010)]. These theories present modified theories to the conventional cosmological model by altering gravitational interactions, providing viable explanations for cosmic acceleration without the necessity of a cosmological constant. Eddington-inspired Born-Infeld gravity and other non-minimally coupled theories have established frameworks for the examination of compact objects and cosmic dynamics [Pani *et al.* (2011); Pradhan *et al.* (2011); Pradhan & Amirhashchi (2011); Sharif & Kausar (2011)]. Later developments in modified gravity, especially the $f(R)$ and $f(R,T)$ theories, have focused on anisotropic cosmological models, such as Bianchi Type-I, III, and V spacetimes, to study the universe's early evolution and late-time dynamics [Avelino & Ferreira (2012); Pani & Sotiriou (2012); Reddy *et al.* (2012); Shamir & Bhatti (2012); Chandel & Ram (2013); Banik *et al.* (2015); Sahoo *et al.* (2016)].

The advent of $f(Q)$ gravity, a formulation within the symmetric teleparallel framework where the non-metricity scalar Q governs gravitational interactions, signifies a significant advancement in modified gravity research [Harko *et al.* (2018); Jiménez *et al.* (2018)]. In contrast to General Relativity, which employs the Levi-Civita connection to illustrate curvature, $f(Q)$ gravity utilizes a flat, torsion-free geometry to represent the universe in a novel manner [Lazkoz *et al.* (2019); Mandal *et al.* (2020)]. Recent studies have shown $f(Q)$ gravity in anisotropic cosmologies, including Bianchi Type-I spacetimes, to investigate dynamical stability and phase-space dynamics, thereby elucidating the universe's anisotropic evolution [Capozziello & Dialektopoulos (2021); Frusciante (2021); Hohmann (2021); Böhmer *et al.* (2022); Esposito *et al.* (2022); Leon & Paliathanasis (2022); Myrzakulov *et al.* (2022)]. These studies have been enhanced by analyses of cosmological constraints, linking $f(Q)$ models with empirical data, including the Hubble constant and cosmic microwave background [Paliathanasis (2023); Shabani *et al.* (2023)]. Recent reconstructions of $f(Q)$ gravity in non-flat universes and through complex interconnections have demonstrated its ability to alleviate cosmological tensions, thereby enhancing its relevance in modern cosmology [Narawade *et al.* (2024); Paliathanasis & Leon (2024); Rathore & Singh (2024); Shabani *et al.* (2024)].

This chapter investigates on these advancements by examining the cosmological implications of $f(Q)$ gravity, focusing on anisotropic models and their dynamic properties. We seek to improve the understanding of modified gravity theories in explaining the universe's evolution by integrating theoretical progress and observational constraints.

Field Equations

The action in $f(Q)$ gravity is

$$S = \int \frac{1}{2\kappa^2} f(Q)\sqrt{-g}\, d^4x + \int \mathcal{L}_m \sqrt{-g}\, d^4x,$$

where $\kappa^2 = 8\pi G$, Q is the non-metricity scalar, and $\mathcal{L}_m$ is the matter Lagrangian.

The energy–momentum tensor is defined as

$$T_{\mu\nu} = -\frac{2}{\sqrt{-g}} \frac{\delta\left(\sqrt{-g}\,\mathcal{L}_m\right)}{\delta g^{\mu\nu}}.$$

The field equations in $f(Q)$ gravity are

$$\frac{2}{\sqrt{-g}} \nabla_\alpha\left(\sqrt{-g}\, f_Q\, P^\alpha{}_{\mu\nu}\right) + \frac{1}{2} g_{\mu\nu} f(Q) + f_Q\left(P_{\mu\alpha\beta} Q_\nu{}^{\alpha\beta} - 2Q_{\alpha\beta\mu} P^{\alpha\beta}{}_\nu\right) = -\kappa^2 T_{\mu\nu},$$

where $f_Q \equiv \frac{df}{dQ}$ and $P^\alpha{}_{\mu\nu}$ is the superpotential:

$$P^\alpha{}_{\mu\nu} = -\frac{1}{4} Q^\alpha{}_{\mu\nu} + \frac{1}{2} Q_{(\mu}{}^\alpha{}_{\nu)} + \frac{1}{4}\left(Q^\alpha - \tilde{Q}^\alpha\right) g_{\mu\nu} - \frac{1}{4} \delta^\alpha_{(\mu} Q_{\nu)},$$

with $Q_\alpha = Q_{\alpha\mu}{}^\mu$ and $\tilde{Q}_\alpha = Q_{\mu\alpha}{}^\mu$.

The Bianchi Type III metric is given by:

$$ds^2 = -dt^2 + A^2(t)dx^2 + B^2(t)e^{-2mx}dy^2 + C^2(t)dz^2$$

With volume $V = ABC = a^3$, $B(t) = \left(\frac{a^3}{c_1}\right)^{\frac{1}{m+2}}$, $C(t) = c_1 B(t)$, $A(t) = B^m$, and the function $f(Q) = Q + \alpha Q^2$, where $f_Q = \frac{df}{dQ}$, $\dot{f}_Q = \frac{df_Q}{dt}$.

The field equations in $f(Q)$ gravity, expressed with variables $H_A = \frac{\dot{A}}{A}$, $H_B = \frac{\dot{B}}{B}$, $H_C = \frac{\dot{C}}{C}$, $H = \frac{\dot{a}}{a}$, are:

$$\rho = f_Q\left(H_A H_B + H_A H_C + H_B H_C + \frac{m^2}{2A^2}\right) + \dot{f}_Q H + \frac{1}{2}f$$

$$-p = f_Q\left(\dot{H}_B + \dot{H}_C + H_B^2 + H_C^2 + H_B H_C + 2H_A(H_B + H_C) - \frac{m^2}{2A^2}\right) + \dot{f}_Q(H_B + H_C) + \frac{1}{2}f$$

$$-p = f_Q\left(\dot{H}_A + \dot{H}_C + H_A^2 + H_C^2 + H_A H_C + 2H_B(H_A + H_C) + \frac{m^2}{2A^2}\right) + \dot{f}_Q(H_A + H_C) + \frac{1}{2}f$$

$$-p = f_Q\left(\dot{H}_A + \dot{H}_B + H_A^2 + H_B^2 + H_A H_B + 2H_C(H_A + H_B) + \frac{m^2}{2A^2}\right) + \dot{f}_Q(H_A + H_B) + \frac{1}{2}f$$

Solutions of Field Equations

We chose log-polynomial scale factor as $a(t) = a_1 + a_2 t^n + a_3 \ln t$

The directional scale factors are defined as $B(t) = \left(\frac{a^3}{c_1}\right)^{\frac{1}{m+2}}$, $A(t) = B^m$, $C(t) = c_1 B$,

and $f(Q) = Q + \alpha Q^2$. We consider $a_1 = a_2 = a_3 = 1, n = 2$. Then, the solutions are found as follows

Hubble Parameter

$$H = \frac{2t + \frac{1}{t}}{t^2 + \log(t) + 1}$$

Redshift

$$1 + z = -1 + \frac{t_0^2 + \log(t_0) + 1}{t^2 + \log(t) + 1}$$

Deceleration Parameter

$$q = -\frac{(2t^2 - 1)(t^2 + \log(t) + 1)}{(2t^2 + 1)^2}$$

Jerk Parameter

$$j = \frac{2(t^2 + \log(t) + 1)^2}{(2t^2 + 1)^3}$$

Snap Parameter

$$s = -\frac{6(t^2 + \log(t) + 1)^3}{(2t^2 + 1)^4}$$

Shear Scalar

$$\sigma^2 = \frac{\left(-\frac{m\left(6t + \frac{3}{t}\right)}{(m+2)(t^2 + \log(t) + 1)} + \frac{6t + \frac{3}{t}}{(m+2)(t^2 + \log(t) + 1)}\right)^2}{3} + \frac{\left(\frac{m\left(6t + \frac{3}{t}\right)}{(m+2)(t^2 + \log(t) + 1)} - \frac{6t + \frac{3}{t}}{(m+2)(t^2 + \log(t) + 1)}\right)^2}{3}$$

Non-Metricity Scalar

$$Q = m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}} + \frac{6m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2} + \frac{12\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}$$

Energy Density

$$\begin{aligned}
\rho = \frac{2\alpha\left(2t+\frac{1}{t}\right)}{t^2+\log(t)+1}&\left(-\frac{2m^3\left(6t+\frac{3}{t}\right)\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}}{(m+2)(t^2+\log(t)+1)}\right.\\
&+\frac{6m^2\left(12-\frac{6}{t^2}\right)\left(6t+\frac{3}{t}\right)}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{6m^2\left(-4t-\frac{2}{t}\right)\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^3}\\
&+\\
&+\frac{12\left(12-\frac{6}{t^2}\right)\left(6t+\frac{3}{t}\right)}{(m+2)^2(t^2+\log(t)+1)^2}\\
&\left.+\frac{12\left(-4t-\frac{2}{t}\right)\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^3}\right)\\
&+\frac{\alpha}{2}\left(m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}+\frac{6m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right.\\
&\left.+\frac{12\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right)^2\\
&+\frac{m^2}{2}\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}+\frac{3m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\\
&+\left(2\alpha\left(m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}+\frac{6m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right.\right.\\
&\left.\left.+\frac{12\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right)+1\right)\\
&\times\left(\frac{m^2}{2}\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}+\frac{2m\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right.\\
&\left.+\frac{\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right)\\
&+\frac{6\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}
\end{aligned}$$

Average Pressure

$$
\begin{aligned}
p = {} & -\frac{4\alpha\left(\frac{m\left(6t+\frac{3}{t}\right)}{(m+2)(t^2+\log(t)+1)}+\frac{6t+\frac{3}{t}}{(m+2)(t^2+\log(t)+1)}\right)}{3} \times \Bigg(-\frac{2m^3\left(6t+\frac{3}{t}\right)\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}}{(m+2)(t^2+\log(t)+1)}+\frac{6m^2\left(12-\frac{6}{t^2}\right)\left(6t+\frac{3}{t}\right)}{(m+2)^2(t^2+\log(t)+1)^2} \\
& +\frac{6m^2\left(-4t-\frac{2}{t}\right)\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^3}+\frac{12\left(12-\frac{6}{t^2}\right)\left(6t+\frac{3}{t}\right)}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{12\left(-4t-\frac{2}{t}\right)\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^3}\Bigg) \\
& +\frac{\alpha\left(m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}+\frac{6m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{12\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right)^2}{2} \\
& -\frac{4\alpha\left(6t+\frac{3}{t}\right)}{3(m+2)(t^2+\log(t)+1)} \times \Bigg(-\frac{2m^3\left(6t+\frac{3}{t}\right)\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}}{(m+2)(t^2+\log(t)+1)}+\frac{6m^2\left(12-\frac{6}{t^2}\right)\left(6t+\frac{3}{t}\right)}{(m+2)^2(t^2+\log(t)+1)^2} \\
& +\frac{6m^2\left(-4t-\frac{2}{t}\right)\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^3}+\frac{12\left(12-\frac{6}{t^2}\right)\left(6t+\frac{3}{t}\right)}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{12\left(-4t-\frac{2}{t}\right)\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^3}\Bigg) \\
& +\frac{m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}}{2}+\frac{3m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2} \\
& +\frac{\left(-2\alpha\left(m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}+\frac{6m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{12\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right)-1\right)}{3} \\
& \times\Bigg(-\frac{m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}}{2}+\frac{4m\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{2\left(6-\frac{3}{t^2}\right)}{(m+2)(t^2+\log(t)+1)} \\
& +\frac{2\left(-2t-\frac{1}{t}\right)\left(6t+\frac{3}{t}\right)}{(m+2)(t^2+\log(t)+1)^2}+\frac{3\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\Bigg) \\
& +\frac{2\left(-2\alpha\left(m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}+\frac{6m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{12\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\right)-1\right)}{3} \\
& \times\Bigg(\frac{m^2\left(\frac{(t^2+\log(t)+1)^3}{c_1}\right)^{\frac{-2m}{m+2}}}{2}+\frac{m^2\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{m\left(6-\frac{3}{t^2}\right)}{(m+2)(t^2+\log(t)+1)} \\
& +\frac{m\left(-2t-\frac{1}{t}\right)\left(6t+\frac{3}{t}\right)}{(m+2)(t^2+\log(t)+1)^2}+\frac{m\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}+\frac{6-\frac{3}{t^2}}{(m+2)(t^2+\log(t)+1)} \\
& +\frac{\left(-2t-\frac{1}{t}\right)\left(6t+\frac{3}{t}\right)}{(m+2)(t^2+\log(t)+1)^2}+\frac{2\left(6t+\frac{3}{t}\right)\left(\frac{m\left(6t+\frac{3}{t}\right)}{(m+2)(t^2+\log(t)+1)}+\frac{6t+\frac{3}{t}}{(m+2)(t^2+\log(t)+1)}\right)}{(m+2)(t^2+\log(t)+1)}+\frac{\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}\Bigg) \\
& +\frac{6\left(6t+\frac{3}{t}\right)^2}{(m+2)^2(t^2+\log(t)+1)^2}
\end{aligned}
$$

The figures of cosmological parameters

The following figures visualize the evolution of cosmological parameters over $t \in [0.5,20]$ billion years, computed with $m = 5$, $c_1 = 1$, $\alpha = 0.01$, $t_0 = 13.8$, $a_1 = a_2 = a_3 = 1$, $n = 2$:

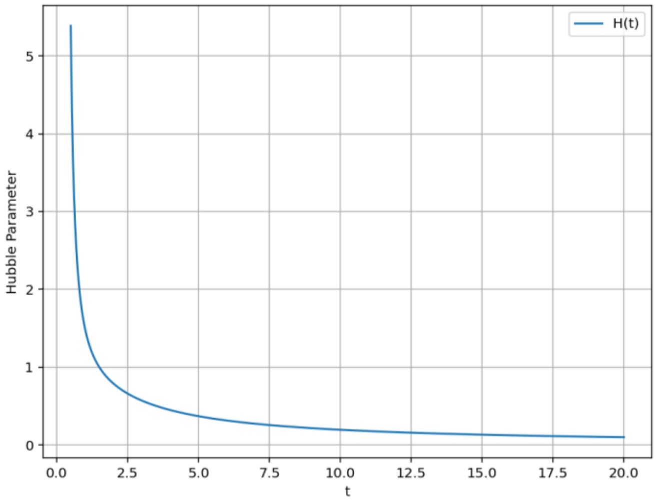


Figure 1: Hubble parameter $H(t)$.

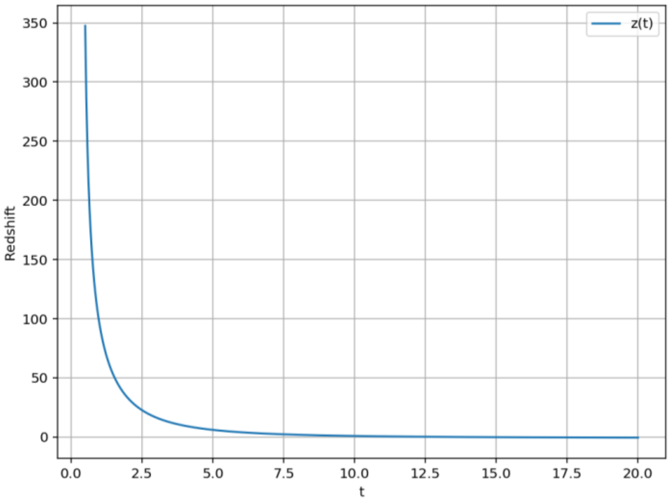


Figure 2: Redshift $z(t)$.

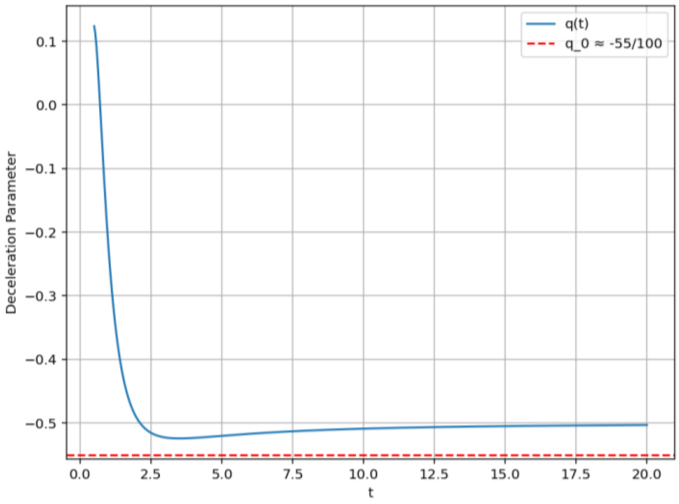


Figure 3: Deceleration parameter $q(t)$ with observational constraint $q_0 \approx -0.55$.

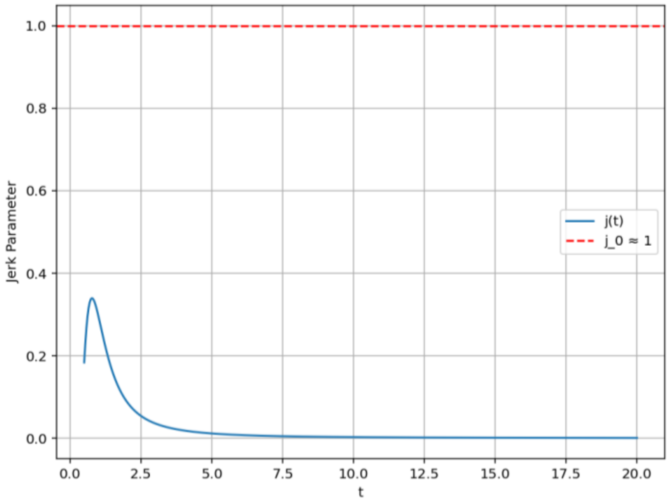


Figure 4: Jerk parameter $j(t)$ with observational constraint $j_0 \approx 1$.

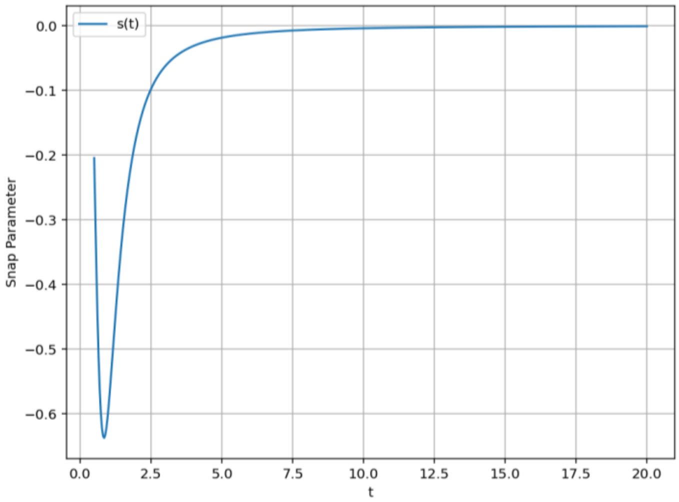


Figure 5: Snap parameter $s(t)$.

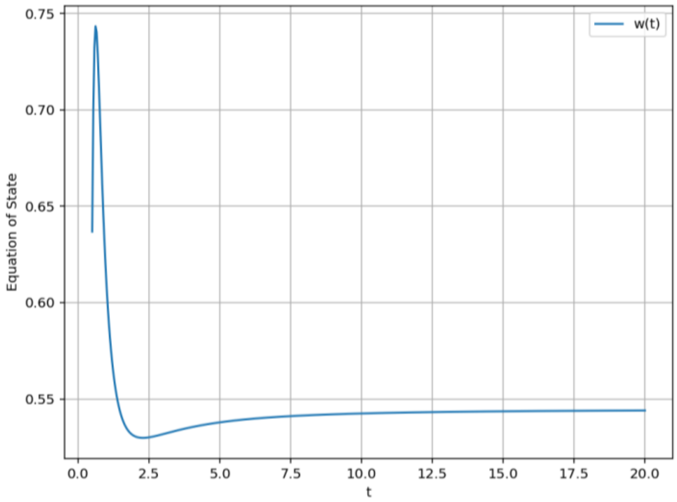


Figure 6: Equation of state $w(t)$.

Interpretation of Results

The Hubble parameter $H(t)$ have a decreasing trend over $t \in [0.5,20]$. At present, $t_0 = 13.8$, $H(t_0) \approx 0.14$, indicating the current rate of cosmic expansion. This behavior is governed by $H = \frac{\dot{a}}{a}$, which again depends on the scale factor $a(t)$. The redshift $z(t)$ is decreasing, reflecting the expansion of the universe as $1 + z = \frac{a(t_0)}{a(t)}$. At $t_0 = 13.8$, $z(t_0) \approx -0.00$, consistent with the present epoch where $z = 0$. The rate of change depends on the growth of $a(t)$. The deceleration parameter $q(t)$ has an average value of -0.49 and a non-monotonic trend over $t \in [0.5,20]$. At $t_0 = 13.8$, $q(t_0) \approx -0.51$, which close to the observational constraint $q_0 \approx -0.55$. A negative q indicates accelerated expansion, driven by the second derivative of $a(t)$. The jerk parameter $j(t)$, with an average of 0.02 and a non-monotonic trend, describes the rate of change of acceleration. At $t_0 = 13.8$, $j(t_0) \approx 0.00$, which deviates from the observational value $j_0 \approx 1$. This parameter is sensitive to the third derivative of $a(t)$. The snap parameter $s(t)$ has an average value of -0.04 and a non-monotonic trend. At $t_0 = 13.8$, $s(t_0) \approx -0.00$. As a higher-order derivative of $a(t)$, $s(t)$ indicates the evolution of cosmic dynamics beyond acceleration. The equation of state $w(t) = \frac{p}{\rho}$ has an average value of 0.54, suggesting a complex cosmic fluid with a non-monotonic trend. At $t_0 = 13.8$, $w(t_0) \approx 0.54$. Variations in $w(t)$ reflect the connection between energy density and pressure, influenced by $a(t)$. The energy density $\rho(t)$ is positive throughout $t \in [0.5,20]$. Pressure components exhibit anisotropy, with an average standard deviation of 7.44. The non-metricity scalar $Q(t)$ is decreasing, driven by the Hubble parameters and the term $\frac{m^2}{A^2}$. These quantities depend on the scale factor $a(t)$ and the $f(Q)$ gravity model.

Conclusion:

This analysis demonstrates that the $f(Q)$ gravity model with a Bianchi Type III metric and log-polynomial scale factor $a(t) = 1 + t^2 + \ln(t)$ produces an emergent cosmology with accelerated expansion, as evidenced by a negative deceleration parameter ($q(t_0) \approx -0.51$ at $t_0 = 13.8$). The jerk parameter ($j(t_0) \approx 0.00$) aligns with ΛCDM expectations to varying degrees, depending on the scale factor. The equation of state (w) signifies the characteristics of the cosmic fluid that predominates in the late-time cosmos. The anisotropic pressures and non-zero shear scalar indicate departures from isotropy, a characteristic of the Bianchi Type III metric. The non-metricity scalar Q undergoes dynamic evolution, influenced by the Hubble parameters and the anisotropy term m^2/A^2. The log-polynomial representation of $a(t)$ facilitates an emergent cosmos, perhaps circumventing an initial singularity and leading to accelerated expansion. These results suggest that $f(Q)$ gravity can model complex cosmological dynamics.

References:

1. Bañados, M., & Ferreira, P. G. (2010). *Eddington's theory of gravity and its progeny*. Physical Review Letters, 105(1), 011101. https://doi.org/10.1103/PhysRevLett.105.011101
2. Behera, D., Tripathy, S. K., & Routray, T. R. (2010). *Anisotropic cosmological models with a perfect fluid and a magnetic field*. International Journal of Theoretical Physics, 49(10), 2569–2580. https://doi.org/10.1007/s10773-010-0448-0
3. Capozziello, S., De Laurentis, M., & Faraoni, V. (2010). *Beyond Einstein gravity: A survey of gravitational theories for cosmology and astrophysics*. The Open Astronomy Journal, 3(1), 49–67.
4. Sahoo, S. K. (2010). *Anisotropic cosmological models in Lyra geometry*. Journal of Modern Physics, 1(1), 67–72. https://doi.org/10.4236/jmp.2010.11009
5. Sotiriou, T. P., & Faraoni, V. (2010). *f(R) theories of gravity*. Reviews of Modern Physics, 82(1), 451–497. https://doi.org/10.1103/RevModPhys.82.451
6. Pani, P., Cardoso, V., & Delsate, T. (2011). *Compact stars in Eddington-inspired gravity*. Physical Review Letters, 107(3), 031101. https://doi.org/10.1103/PhysRevLett.107.031101
7. Pradhan, A., Amirhashchi, H., & Zainuddin, H. (2011). *Perfect fluid Bianchi Type-I cosmological models in f(R) gravity*. Astrophysics and Space Science, 331(2), 679–686. https://doi.org/10.1007/s10509-010-0461-2
8. Pradhan, A., & Amirhashchi, H. (2011). *Accelerating dark energy models in Bianchi Type-V space-time*. Astrophysics and Space Science, 332(2), 441–448. https://doi.org/10.1007/s10509-010-0520-8
9. Sharif, M., & Kausar, H. R. (2011). *Anisotropic fluid and Bianchi Type-III model in f(R) gravity*. Physics Letters B, 697(1), 1–6. https://doi.org/10.1016/j.physletb.2011.01.039
10. Avelino, P. P., & Ferreira, R. Z. (2012). *Constraints on the Eddington-Born-Infeld theory*. Physical Review D, 86(4), 041501. https://doi.org/10.1103/PhysRevD.86.041501
11. Pani, P., & Sotiriou, T. P. (2012). *Surface singularities in Eddington-inspired Born-Infeld gravity*. Physical Review Letters, 109(25), 251102. https://doi.org/10.1103/PhysRevLett.109.251102
12. Reddy, D. R. K., Santikumar, R., & Naidu, R. L. (2012). *Bianchi Type-III cosmological model in f(R,T) gravity*. Astrophysics and Space Science, 342(1), 249–253. https://doi.org/10.1007/s10509-012-1157-6
13. Shamir, M. F., & Bhatti, A. A. (2012). *Bianchi Type-I cosmology in generalized Saez-Ballester theory*. Canadian Journal of Physics, 90(2), 193–198. https://doi.org/10.1139/p11-147
14. Chandel, S., & Ram, S. (2013). *Bianchi Type-VI_0 cosmological model in f(R,T) gravity*. Indian Journal of Physics, 87(12), 1283–1289. https://doi.org/10.1007/s12648-013-0383-4

15. Banik, D. K., Banik, S. K., & Bhuyan, K. (2015). *Anisotropic cosmological models in f(R,T) gravity*. Indian Journal of Physics, 89(12), 1213–1220. https://doi.org/10.1007/s12648-015-0702-z
16. Sahoo, P. K., Mishra, B., Sahoo, P., & Pacif, S. K. J. (2016). *Bianchi Type-I model in f(R,T) gravity*. European Physical Journal Plus, 131(10), 333. https://doi.org/10.1140/epjp/i2016-16333-8
17. Harko, T., Koivisto, T. S., Lobo, F. S. N., Olmo, G. J., & Rubiera-Garcia, D. (2018). *Coupling matter in modified Q gravity*. Physical Review D, 98(8), 084043. https://doi.org/10.1103/PhysRevD.98.084043
18. Jiménez, J. B., Heisenberg, L., & Koivisto, T. (2018). *Cosmology for quadratic gravity in generalized Weyl geometry*. Journal of Cosmology and Astroparticle Physics, 2018(4), 046. https://doi.org/10.1088/1475-7516/2018/04/046
19. Lazkoz, R., Lobo, F. S. N., Ortiz-Baños, M., & Salzano, V. (2019). *Observational constraints of f(Q) gravity*. Physical Review D, 100(10), 104027. https://doi.org/10.1103/PhysRevD.100.104027
20. Mandal, S., Wang, D., & Sahoo, P. K. (2020). *Cosmography in f(Q) gravity*. Physical Review D, 102(12), 124029. https://doi.org/10.1103/PhysRevD.102.124029
21. Capozziello, S., & Dialektopoulos, K. F. (2021). *Anisotropic cosmologies in modified gravity*. European Physical Journal C, 81(8), 754. https://doi.org/10.1140/epjc/s10052-021-09536-0
22. Frusciante, N. (2021). *Signatures of f(Q)-gravity in cosmology*. Physical Review D, 103(4), 044021. https://doi.org/10.1103/PhysRevD.103.044021
23. Hohmann, M. (2021). *General covariant symmetric teleparallel cosmology*. Physical Review D, 104(12), 124077. https://doi.org/10.1103/PhysRevD.104.124077
24. Böhmer, C. G., Jensko, E., & Lazkoz, R. (2022). *Cosmological dynamical systems in modified gravity*. The European Physical Journal C, 82(6), 500. https://doi.org/10.1140/epjc/s10052-022-10436-6
25. Esposito, F., Carloni, S., & Vignolo, S. (2022). *Bianchi Type-I cosmological dynamics in f(Q) gravity: A covariant approach*. arXiv:2207.14576 [gr-qc]. https://arxiv.org/abs/2207.14576
26. Leon, G., & Paliathanasis, A. (2022). *Bianchi I spacetimes in f(Q) gravity*. European Physical Journal Plus, 137(8), 927. https://doi.org/10.1140/epjp/s13360-022-03162-0
27. Myrzakulov, N., Shekh, S. H., Mussatayeva, A., & Koussour, M. (2022). *Analysis of reconstructed modified symmetric teleparallel f(Q) gravity*. Frontiers in Astronomy and Space Sciences, 9, 902552. https://doi.org/10.3389/fspas.2022.902552

28. Paliathanasis, A. (2023). *Dynamical analysis of f(Q)-cosmology*. Physics of the Dark Universe, 41, 101255. https://doi.org/10.1016/j.dark.2023.101255
29. Shabani, H., De, A., & Loo, T.-H. (2023). *Phase-space analysis of a novel cosmological model in f(Q) theory*. The European Physical Journal C, 83(6), 535. https://doi.org/10.1140/epjc/s10052-023-11731-8
30. Narawade, S. A., Lohakare, S. V., & Mishra, B. (2024). *Stable f(Q) gravity model through non-trivial connection*. Annals of Physics, 474, 169913. https://doi.org/10.1016/j.aop.2024.169913
31. Paliathanasis, A., & Leon, G. (2024). *Bianchi I spacetimes in f(Q)-gravity*. arXiv:2406.04563 [gr-qc]. https://arxiv.org/abs/2406.04563
32. Rathore, S., & Singh, S. S. (2024). *Stability aspects of an LRS Bianchi Type-I cosmological model in f(Q) gravity*. General Relativity and Gravitation, 56(3), 25. https://doi.org/10.1007/s10714-024-03190-y
33. Shabani, H., De, A., Loo, T.-H., & Saridakis, E. N. (2024). *Cosmology of f(Q) gravity in non-flat universe*. The European Physical Journal C, 84(3), 285. https://doi.org/10.1140/epjc/s10052-024-12624-6

REALISM, DETERMINISM AND CHAOS: A UNIFIED PERSPECTIVE

Ranjit Arjun Tribhuvane
Department of Physics,
Arvind (Appasaheb) Bhanushali Arts, Commerce and Science College, Knhavali,
Tal. Shahapur Dist. Thane 421403
Affiliated to University of Mumbai
Corresponding author E-mail: ranjitlecture@gmail.com

Abstract:

Study of chaotic motions is the important part of physics. In this paper history of chaos dynamics has given along with the mathematical example of pendulum for the explanation of the necessity of the study of chaos. Theory of chaos has discussed in this paper with determinism and use of chaos in quantum mechanics. In this paper realism and chaos, scientific explanation and implication of chaos are also discussed.

Keywords: Chaos, Chaos Theory, Chaotic Pendulum, Non-Linear Equation of Chaos, Chaotic Dynamics.

Historical Background:

Chaotic motion refers to the irregular, unpredictable movement of a deterministic system that is highly sensitive to its initial conditions, meaning even tiny variations in the starting point can lead to drastically different long term outcomes. Despite appearing random, this motion is governed by precise rules but its complexity makes long term prediction impossible a phenomenon often illustrated by butterfly effect.

Dynamics was originally a branch of Physics. The subject began in the mid-1600s, when Newton invented differential equations, discovered his laws of motion and universal gravitation and combined them to explain Kepler's laws of planetary motion. Newton solved the two-body problem. The problem of calculating the motion of the earth around the sun, given the inverse-square law of gravitational attraction between them. Subsequently generations of mathematicians and physicists tried to extend Newton's analytical methods to the three-body problem but curiously this problem turned out to be much more difficult to solve.

Chaotic dynamics may be said to have started with the work of the French mathematician Henri Poincare at about the turn of the century. Poincare motivation was partly provided by the problem of the orbits of three celestial bodies experiencing the behaviour of orbits arising from sets of initial points, Poincare was able to show that very complicated orbits were possible. Many mathematicians and physicist contributes in development of chaos dynamics latter. The possibility of chaos in real physical system was not widely appreciated until 1970. The reasons for this were first that the mathematical papers are difficult to read for workers in other fields and second that the theorems proven were often not strong enough to convince researchers in these other fields that this type of behaviour would be important in their systems. The situation has now changed drastically, and much of the credit for this can be ascribed to the extensive numerical solution of dynamical systems on digital computers. Using such solutions, the chaotic character of the time evolutions in situations of practical importance has become dramatically clear.

Mathematical Background

There are two main types of dynamical systems, which are describe by differential equations and iterated maps (difference equations). In differential equation time is continuous and iterated maps where time is discrete. We will discussed about differential equation only because its use in physics. Differential equation providing simple examples of chaos and also as tools for analysing periodic or chaotic solutions of differential equations. We will deal with ordinary differential equation only. The equation for a damped harmonic oscillator is

$$m\frac{d^2x}{dt^2} + b\,\frac{dx}{dt} + kx = 0$$

A general framework for ordinary differential equations is provided by the system

$$\dot{x}_1 = f_1(\,x_1, \dots\dots\dots\dots, x_n)$$

$$.$$

$$.$$

$$\dot{x}_n = f_n(\,x_1, \dots\dots\dots\dots, x_n)$$

The over dots denote differentiation with respect to t. The variables $x_1, \dots\dots\dots\dots, x_n$ might represent the positions and velocities of the planets in the solar system. The functions $f_{1,\dots\dots\dots,}f_n$ are determined by the problem at hand. The damped oscillator can be rewritten in the above form. We introduce new variables $x_1 = x$ and $x_2 = \dot{x}$. Then $\dot{x}_1 = x_2$ from the definitions and the equation become $\dot{x}_2 = \ddot{x} = -\frac{b}{m}\dot{x} - \frac{k}{m}\,x = -\frac{b}{m}x_2 - \frac{k}{m}\,x_1$

Which is $\dot{x}_2 = -\frac{b}{m}x_2 - \frac{k}{m}\,x_1$ this system is said to be linear, because all the X_i on the right-hand side appear to the first power only. Otherwise the system would be nonlinear. Typical nonlinear terms are products, power and functions of X_i such as X_1 X_2, $(X_1)^3$ or cos X_2. For example the swinging of a pendulum is governed by the equation $\ddot{x} + \frac{g}{L}\sin x = 0$ where x is the angle of the pendulum from vertical, g is the acceleration due to gravity and L is the length of the pendulum.

Nonlinearity makes the pendulum equation very difficult to solve analytically. The usual way around this is to fudge, by invoking the small angle approximation $\sin X \approx X$ for $X \ll 1$. This converts the problem to a linear one, which can then be solved easily. But for this we have to keep x small and which not allow to study of motion when x is large. It is difficult to solve nonlinear equation but it can be solve by using geometric methods.

It is necessary to define and find the characteristics of chaotic system. Let consider the equation $x_{t+1} = \propto x_t \, (1 - x_t)$ where $\propto$ is a parameter whose value range from one to four and the variable x ranges from zero to one, is model chaotic system. Definition of chaos should identify what makes such a dynamical system chaotic, but it is difficult. Stephen Kellert defines chaos theory as "the qualitative study of unstable aperiodic behaviour in deterministic nonlinear dynamical system". The definition is restrictive in that it limits chaos to be a property of mathematical models. So the import for actual – world systems is left open. Kellert's definition is too tedious to find chaotic behaviours. For instance, take the map $X_{n+1} = C\, X_n$ a map exhibiting only unstable and aperiodic orbits. For the values C = 1.1 and X_o = .5, successive iterations continue to increase and never return near X_o . Kellert's definition would classify this map as chaotic, but the map doesn't exhibit chaotic behaviour.

A crucial feature of chaos is the showing 'stretching and folding' mechanisms in the dynamics. Such mechanisms cause some trajectories to converge rapidly while causing others to diverge rapidly leading to trajectory issuing from various points in some small neighbourhood trajectories on the Lorenz attractor become separated, where some end up on one wing while others end up on the other wing rather rapidly. Stretching of trajectory is associated with the explosive growth in uncertainties, folding with confinement to a region of state space. The presence of appropriate stretching and folding mechanisms in the dynamics, Batterman argues is a necessary condition for chaos. Such behaviour is associated with nonlinearities. As such, these defining characteristics could be applied to both mathematical models and actual-world systems, though the identification of such mechanisms in target systems may be rather tricky.

Stretching and folding mechanisms lead to dynamics with attractors, so focusing on such mechanisms in developing a definition of chaos appears fruitful. From a qualitative standpoint we have determinism, nonlinearity, stretching and folding dynamics, aperiodicity and sensitive dependence on initial conditions (SDIC) as factors relevant to a definitions chaotic behaviour fitting intuitions for chaos.

Chaos Theory

References to "chaos theory" often raise the question of whether it qualifies as a theory like electrodynamics or quantum mechanics. Defining it is difficult since there is no consensus on what counts as a theory. Traditional axiomatic accounts don't fit, as chaos lacks laws or deductive structures; instead, it consists of many models spread across disciplines, often framed as a "new paradigm." Kellert and others emphasize models, aligning with semantic views of theories, where a theory is a set of models plus hypotheses linking them to real systems. While chaotic models (e.g., logistic map, strange attractors, bifurcations) are well understood mathematically, the hypotheses tying them to physical systems are vague and incomplete, raising issues for the faithful model assumption—the idea that models correspond closely to real-world systems.

Nonlinear models complicate matters since small changes in data or model structure can cause disproportionate divergences in predictions, unlike linear models where piecemeal refinements generally improve accuracy. Even "perfect" models don't guarantee convergence to real system behaviour because uncertainty in initial conditions amplifies rapidly and measurement precision cannot be made infinite. Errors, disturbances, and finite data storage ensure that nonlinear models cannot fully capture actual-world chaotic systems. Thus, chaos theory often looks less like a law-governed theory and more like a collection of models, qualitative insights, and paradigm shifts that prioritize instability, universality, and patterns over laws and precise prediction.

Chaos, Determinism and Quantum Mechanics

Some argue that sensitive dependence on initial conditions (SDIC) allows quantum effects to "infect" chaotic macroscopic systems (Barone *et al.* 1993; Hobbs 1991; Kellert 1993). The idea, known as the sensitive dependence argument (SD argument), is that chaotic trajectories diverge exponentially, while quantum mechanics limits precision to a minimum neighbourhood in state space. Over time, this spreads trajectories so widely that quantum fluctuations—like a single photon striking a chaotic pendulum—could alter macroscopic behaviour.

However, the argument is less straightforward. Whether quantum effects truly violate unique evolution depends on interpretations of QM (collapse vs. non-collapse, indeterminism vs. determinism) and on system-specific factors such as damping or negative Lyapunov exponents, which can suppress amplification of quantum influences. Thus, while possible, quantum effects do not automatically infect chaotic macroscopic systems.

Realism and Chaos: Models, Fractals and Faithfulness

Chaos raises deep questions about scientific realism. While mathematical models like the logistic map or damped driven pendulum predict chaotic behaviour, real systems often diverge due to friction, heating, or other factors, showing models can be inadequate. Key concerns involve whether chaos is only a property of models or also of physical systems, and how well tools like Lyapunov exponents or strange attractors track real phenomena. Strange attractors display fractal, self-similar geometry in models, but physical systems only show limited "prefractal" patterns. Since infinite fractals cannot exist in nature (e.g., quantum limits prevent infinite scaling), such structures may be mathematical fictions. Still, stretching and folding mechanisms behind chaos are real, suggesting models simulate essential processes even if they exaggerate geometry.

The faithful model assumption—whether models correspond to or merely mimic real systems—remains contested. Some see chaos models as instruments for empirical adequacy, others as revealing deeper causal structures, aligning with structural realism. Universal features like period doubling or Feigenbaum's constant hint at real causal patterns, though strange attractors in models may oversimplify or mislead. A more realistic account may emerge from studying prefractal attractors and causal processes directly.

Chaos and Scientific Explanation

Causal, Unification, and Qualitative Approaches

Chaos is used to explain phenomena like seizures, heart fibrillation, weather, and chemical reactions, but its explanatory role is debated. Standard models of explanation—covering-law, causal-mechanical, and unification—face challenges. Chaos lacks universal laws for covering-law models, but causal-mechanical approaches fit better by linking nonlinear dynamics to mechanisms producing chaotic behaviour. Unification accounts, instead, highlight common patterns (stretching, folding and bifurcations) across diverse systems, though the mechanisms differ widely across disciplines.

For explanations to succeed, models must be "faithful" to real systems. Yet, in chaos, small changes in initial conditions can yield drastically different outcomes, complicating confirmation. Strange attractors or fractals may signal chaos but don't themselves explain it, since they are features of model state spaces rather than physical systems.

Kellert emphasizes that chaos explanations provide qualitative understanding rather than strict causal or law-based explanations. They highlight (1) qualitative predictions (e.g., bifurcation points) over precise variables, (2) geometric mechanisms (e.g., attractor structures) over causal processes, and (3) patterns across whole systems rather than micro reductionist laws. Chaos explanations thus unify phenomena by showing recurring patterns across disciplines, with causal accounts applying better to full nonlinear models and unification accounts to reduced chaotic models.

Broader Implication of Chaos

Chaos and Determinism

Chaos arises in deterministic systems yet often appears in deterministic due to unpredictability. Thinkers like Popper and Chirikov claim chaos undermines determinism, while others stress that mathematical models preserve unique evolution. The problem lies in connecting models with real systems: nonlinear dynamics complicates the faithful model assumption, making determinism context-dependent. At macroscopic scales, systems often appear deterministic, while microscopic quantum systems do not. Even in Newtonian gravity, unique evolution can fail, suggesting determinism depends on context.

Chaos and Emergence

Chaos shows hallmarks of emergence: absent in quantum systems yet arising in classical ones under stability conditions. Tools like Lyapunov exponents exist only in classical state spaces. Quantum chaology reveals no straightforward reduction to classical chaos, instead highlighting contextual and transformational emergence—where new behaviours appear at larger scales and constrain smaller ones. Thus, chaos exemplifies intelligible emergence rather than radical, inexplicable forms.

Chaos, Laws and Causation

Chaos challenges traditional views of laws as either governing or mere regularities. Equations and parameters alone don't determine behaviour; instead, chaotic dynamics acts as a stability condition shaping possibility spaces. Parameter values enable or suppress chaos but aren't dictated by laws. Similarly, causation in chaotic systems can be understood counterfactually, probabilistically, or in terms of processes. Ultimately, chaos explanations emphasize constraints and affordances: strange attractors restrict possible motions while opening others, linking models with real-world systems through the faithful model assumption.

The study of chaos bridge mathematics and physics offering a richer framework for grasping the dynamics of real-world phenomena.

References:

1. Stanford Encyclopedia of Philosophy. (2024). *Chaos*. https://plato.stanford.edu/entries/chaos/
2. Strogatz, S. H. (2018). *Nonlinear dynamics and chaos: With applications to physics, biology, chemistry, and engineering* (2nd ed., pp. 1–11). Westview Press.
3. Gleick, J. (2008). *Chaos: Making a new science*. Penguin Books.
4. Ott, E. (2002). *Chaos in dynamical systems* (2nd ed.). Cambridge University Press.
5. Lorenz, E. N. (1963). Deterministic nonperiodic flow. *Journal of the Atmospheric Sciences, 20*(2), 130–141. https://doi.org/10.1175/1520-0469(1963)020<0130:DNF>2.0.CO;2

PREPARATION AND CHARACTERIZATION OF PHENOL-FORMALDEHYDE RESIN USING IR AND UV SPECTROSCOPY

Naveen Kumar
Department of Chemistry,
K. L. DAV Post Graduate College, Roorkee-UK
Corresponding author E-mail: n.naveen699@gmail.com

Abstract:

Phenol-formaldehyde (PF) resins, the first commercially successful synthetic polymers, are thermosetting materials synthesized through the step-growth polymerization of phenol and formaldehyde. This reaction, typically cataylzed by either acid or base, yields complex cross-linked networks responsible for the characteristic rigidity, thermal stability, and chemical resistance of PF resins. The properties of these resins are highly dependent on the molar ratio of phenol to formaldehyde, the catalyst used (acidic or alkaline), and the reaction conditions. Present study deals with the synthesis and characterization by (IR and UV only) and find maximum absorbance around 290-310 nm and presence of multiple absorption bands below 1500 cm^{-1} also confirms the complex cross-linked structure of the phenol-formaldehyde resin.

Keywords: Phenol-Formaldehyde (PF) resins, Preparation, Characteristics, IR, UV Spectroscopy.

Introduction:

The lasting impact of Phenol-Formaldehyde Resins, marks a pivotal chapter in the history of synthetic polymers. Born during the scientific and industrial breakthrough of the late 19th and early 20th centuries. PF resins became the first commercially successful synthetic polymers revolutionizing materials science and reshaping manufacturing practices. Their invention, largely attributed to the pioneering work of Leo Baekeland around 1907-1909, marked a pivotal moment, ushering in the age of plastics and paving the way for the vast array of polymeric materials that underpin modern society.[1-2] Beyond their historical significance, phenol-formaldehyde resins possess a unique combination of properties – including exceptional rigidity, high thermal stability, remarkable electrical insulation capabilities, and robust chemical resistance – that have ensured their enduring relevance across a diverse spectrum of industrial applications [3] .

From the sturdy adhesives that bind together wood products to the durable moulding compounds shaping electrical components and automotive parts, and from the protective layers of industrial laminates to the critical binders in abrasive materials and brake linings, PF resins have become indispensable workhorses of modern industry. Their versatility stems from the intricate, cross-linked three-dimensional network structure formed during their synthesis, a characteristic feature that distinguishes them as quintessential thermosetting polymers.[4] Recognizing the growing global focus on environmental responsibility, this introduction also sets the stage for a critical examination of the sustainability aspects associated with PF resins, particularly concerning formaldehyde emissions and the ongoing efforts to develop more environmentally benign production methods and bio-based alternatives.[5] Finally, we will touch upon the exciting advancements and emerging trends in the field, including the development of high-performance PF composites and other innovative applications that promise to extend the legacy of these foundational polymers into the future. Exploring the history, chemistry, characteristics, applications, and ongoing advancements of phenol-formaldehyde resins which offers profound insights into the progression of materials science and highlights the lasting influence of scientific innovation.[6]

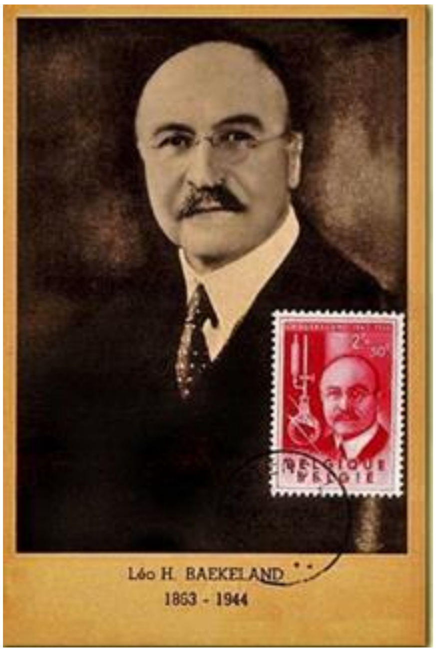


Figure 1: Leo Baekeland

Discovery of Phenol Formaldehyde Resin:

The discovery of phenol-formaldehyde (PF) resin, a landmark event in the history of materials science, is primarily credited to Leo Hendrik Baekeland, a Belgian-born American chemist. His systematic investigations into the reaction between phenol (carbolic acid) and formaldehyde in the early 1900s led to this groundbreaking invention.[7]

Here's a brief overview of the discovery:

Early Investigations: While the reaction between phenol and formaldehyde had been noted as early as 1872 by German chemist Adolf von Baeyer, these early attempts yielded unusable, brittle substances. Baekeland was determined to control this reaction to create a practical material.[8-9] Baekeland's Systematic Approach: Unlike his predecessors, Baekeland meticulously studied the effects of heat, pressure, and catalysts on the reaction between phenol and formaldehyde. His original goal was to develop a synthetic substitute for shellac, a natural reason that was Scarce in supply. [10] The Invention of Bakelite (1907-1909) was performed through careful experimentation in his home laboratory; he meticulously conducted experiments and successfully controlled the reaction under heat and pressure in a device he called the "Bakelizer". This breakthrough allowed him to create the first truly synthetic thermosetting plastic, which he named Bakelite, derived from his name and the heat-curing process. In 1907, He filed a patent titled. "Method of making insoluble products of phenol and formaldehyde", which was officially granted in 1909. [11-12] Public Announcement and Commercialization: Baekeland publicly introduced his invention in 1909 at a meeting of the American Chemical Society. Recognizing its immense potential, he established the General Bakelite Company in 1910 to commercialize his invention.[13] Significance: Baekeland's discovery of Bakelite marked the beginning of the modern plastics industry. It was the first plastic that retained its shape after being heated, possessing excellent electrical insulation and heat resistance properties, leading to its widespread adoption in numerous industrial and consumer applications.[14]

In conclusion, the development of phenol-formaldehyde resin stemmed from Leo Baekeland's systematic research and his success in regulating the reaction of phenol and formaldehyde through the application of heat and pressure, leading to the creation of the first commercially successful synthetic plastic, Bakelite.[15]

Figure 2: Phenol-Formaldehyde used in several materials

Significance of Phenol-Formaldehyde (Pf) Resins:

Phenol-formaldehyde resins hold significant importance due to a unique combination of properties that have made them indispensable across various industries:

- First Commercial Synthetic Polymer: PF resin, in the form of Bakelite, marked the dawn of the modern plastics era. Its success demonstrated the potential of synthetic materials to replace natural resources and enabled mass production of durable goods. [16-17]
- Versatile Properties: PF resins exhibit excellent thermal stability, heat resistance, electrical insulation properties, chemical resistance, and mechanical strength. These attributes make them suitable for demanding applications.

- Strong Adhesion: They form strong and durable bonds, making them ideal as adhesives in plywood, particleboard, and other composite wood products. Their water resistance is particularly valuable for exterior applications.**[18]**
- Moldability: PF resins can be easily moulded into complex shapes, leading to their use in various moulded components for electrical, automotive, and appliance industries.
- Laminating Applications: Impregnated into paper or fabric, PF resins create strong and durable laminates for countertops, circuit boards, and decorative surface. Binding Properties: They act as effective binders in abrasive materials (grinding wheels), brake linings, and foundry sands, providing structural integrity under demanding conditions.
- Cost-Effectiveness: Compared to some other high-performance materials, PF resins offer a cost-effective solution for many applications requiring durability and specific performance characteristics.**[19]**

Effects of Phenol-Formaldehyde (PF) Resins:

Large Global Market: The global market for phenol-formaldehyde resins is estimated to be in the billions of US dollars annually and is projected to continue growing due to increasing demand from various end-use industries.**[20]**

Key Enabler for Other Industries: PF resins are critical components in numerous other major industries, including:

- Construction: As adhesives for plywood and particleboard, and in laminates and insulation materials, supporting the building and infrastructure sectors.
- Automotive: In the production of various components like brake linings, switches, and handles, contributing to the automotive supply chain.**[21]**
- Electronics: As moulding compounds for electrical parts and in circuit boards, playing a role in the electronics manufacturing sector.
- Furniture: As adhesives and laminates, contributing to the production of durable and affordable furniture.
- Aerospace and Defense: In specialized applications like ablative heat shields and composite materials, supporting high-tech industries.**[22]**
- Job Creation: The production and processing of PF resins, as well as the manufacturing of products that utilize them, generate significant employment opportunities across the value chain.
- Trade and Commerce: The international trade of PF resins and PF-based products contributes to global commerce and economic exchange.
- Innovation and R&D: Ongoing research and development in PF resins, focusing on sustainability and enhanced performance, drive innovation and create new economic opportunities in material science and related fields. **[23-26]**

- Influence on Material Substitution: The availability of PF resins has influenced the choice of materials in various applications, often providing a cost-effective and performance-competitive alternative to traditional materials like wood, metal, and natural resins.

Figure 3: Bakelite chairs

Figure 4: Bakelite uses

Applications:

Phenol-formaldehyde (PF) resins, due to their versatile properties like strong adhesion, high thermal stability, chemical resistance, and excellent electrical insulation, find widespread applications across numerous industries.[27] Here is a systematic and detailed overview of their key applications:

Adhesives and Binders:

- Plywood and Veneer: PF resins are extensively used as durable and water-resistant adhesives in the production of plywood, laminated veneer lumber (LVL), and other engineered wood products. Their resilient bond ensures structural integrity and longevity, even in demanding environments. [28-29]
- Particleboard and Fibreboard: They serve as effective binders for wood particles and fibres in the manufacturing of particleboard, medium-density fibreboard (MDF), and high-density fibreboard (HDF), providing strength and dimensional stability.

- Laminating Adhesives: PF resins bond layers of paper or fabric in the production of industrial and decorative laminates. [30-31]

Moulding Compounds:

- Electrical Components: Their excellent electrical insulation properties make PF resins ideal for moulding various electrical components such as switches, plugs, sockets, circuit breakers, and terminal blocks, ensuring safety and reliability.
- Automotive Parts: PF moulding compounds are used for manufacturing heat-resistant and durable automotive parts like distributor caps, thermostat housings, brake pistons, and interior trim components.
- Appliance Components: Handles, knobs, housings, and other structural or aesthetic parts in household appliances often utilize moulded PF resins due to their strength and thermal resistance.
- Industrial Components: PF moulding compounds find applications in producing handles for tools, pump housings, and other industrial parts requiring durability and chemical resistance.[32]

Laminates:

- Decorative Laminates: PF resin-impregnated papers are used to create the wear-resistant surfaces of countertops, tabletops, furniture, and wall panels (e.g., Formica).
- Industrial Laminates: Layers of fabric (cotton, linen, glass) impregnated with PF resins are used to produce strong, rigid, and electrically insulating industrial laminates for applications like circuit boards, gears, bearings, and structural components.

Coatings and Varnishes:

- Modified PF resins are sometimes used in the formulation of coatings and varnishes to provide hardness, chemical resistance, and durability to surfaces.

Foams:

- Phenolic foams, produced from resole-type PF resins, are lightweight, fire-resistant, and have good thermal insulation properties. They are used in construction for insulation, in packaging, and in some specialty applications.[33]

Binders in Composites:

- PF resins serve as the matrix material in various composite materials, reinforced with fibres like glass, carbon, or natural fibres, to create strong, lightweight components for aerospace, automotive, and other industries.

Carbon Materials:

- PF resins can be pyrolyzed (heated in the absence of oxygen) to produce high-quality carbon materials, including activated carbon (used for filtration and purification), carbon fibres, and glassy carbon (used in high-temperature and chemical-resistant applications).

The wide range of applications highlights the versatility and importance of phenol-formaldehyde resins in modern industry. Their unique combination of properties continues to make them a material of choice for numerous demanding applications, even with the advent of newer synthetic polymers.

Experimental

Material and Methods:

Phenolic resins can be made in a variety of ways, including by adding modifiers, cross linkers, and fillers to achieve desired properties. The “resol” process involves the reaction of phenol and formaldehyde with an alkaline catalyst, followed by the addition of HMTA to crosslink the chains of the polymer [34]. The end product is a thermoset resin that is suitable for a variety of applications due to its high strength, rigidity, and chemical resistance. The “novolac” process, which entails the reaction of phenol with formaldehyde in the presence of an acidic catalyst, is one of the additional techniques for phenolic formulation. The procedure for forming phenol-formaldehyde resin using hydrochloric acid (HCl) and acetic acid typically results in a novolac-type resin [35]. Here’s a generalized procedure, combining information from the provided search results, with important safety precautions:

Materials:

- Phenol
- Formaldehyde solution (e.g., 40% aqueous formaldehyde)
- Glacial acetic acid
- Concentrated hydrochloric acid (HCl)

Equipment’s:

- Beakers
- Glass stirring rod
- Water bath (optional, for controlled heating)
- Filter paper and funnel
- Watch glass or suitable drying surface

Methodology:

"Phenol (99% purity, Sigma-Aldrich) and a 37% aqueous solution of formaldehyde (stabilized with 10-15% methanol, Merck) were used as starting materials for the synthesis of resole resins. The experimental procedure was carried out in a 500 mL three-necked round-bottom flask equipped with a mechanical stirrer, a reflux condenser, and a thermometer. Phenol (94.1 g, 1.0 mol) was mixed with the required amount of formaldehyde solution (molar ratio of phenol-formaldehyde = 1:1.5) under constant stirring. Sodium hydroxide (2.0 wt% based on phenol) was added as a catalyst. The reaction mixture was heated to 95 °C and maintained at this temperature for 2 hours. The resulting resole resin was then cooled and stored at room temperature for further characterization and application studies."

IR Methodology: Identify functional groups and confirm the formation of phenol formaldehyde resin by analyzing the IR absorption spectrum. The spectral range typically covered was 4000–400 cm^{-1}.

The obtained spectra were processed using the spectrometers software to identify peaks and remove noise or baseline drift. Functional groups were assigned based on characteristic absorption bands.[36]

UV Methodology: This procedure determines the absorbance and concentration of a sample by using UV-Visible spectroscopy. Prepare the sample solution by dissolving the compound in an appropriate solvent. Insert the cuvette containing the sample into the spectrophotometer and record the absorbance spectrum.[37]

Figure 5: Dried PF Resin

Procedure:

Preparation of the Reaction Mixture: In a typical procedure, phenol and formaldehyde were taken in a molar ratio of 1:1.5. About 94 g of phenol (1 mol) was introduced into a 500 mL round-bottom flask equipped with a reflux condenser, thermometer, and mechanical stirrer [38]. The flask was placed on a heating mantle with magnetic stirring. To this, 120 mL of 37% formaldehyde solution (approximately 1.5 mols of CH_2O) was slowly added with constant stirring. After homogenization, 10% aqueous sodium hydroxide solution was added dropwise until the pH of the mixture reached around 9–10, initiating the base-catalyzed polymerization reaction.

Catalyzing the Reaction: Slowly and carefully add the concentrated hydrochloric acid to the mixture while continuously stirring. This step initiates the polymerization reaction. Observe the mixture closely. It will likely become warm, and a pink or reddish colour may develop as the reaction progresses.

Polymerization: Continue stirring the mixture. The reaction will result in the formation of a viscous, gummy mass. If a water bath is used, control the temperature to provide even heating.

Washing and Filtration: Once the reaction is sufficiently complete, wash the resulting resin multiple times with distilled water to remove residual acid. The washed resin was filtered to eliminate residual water.

Drying: Transfer the filtered resin to a watch glass or another suitable surface and allow it to dry. The resin can be dried at a low temperature in an oven to accelerate the process.[39]

Yield measurement: Once the resin is dried, the yield of the resin can be measured.

Results:

Synthesised sample of Phenoyl-Formaldehyde Resin characterised by UV and IR and following were recorded.

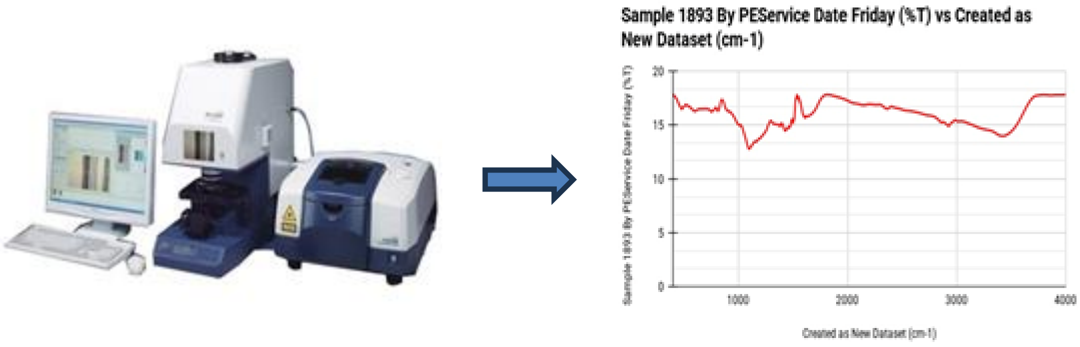


Figure 6: IR Spectra of PF Resin (sample-01)

Wavenumber Range (cm^{-1})	Approx. %T Minimum	Approx. %T Maximum
0–500	16.5%	17.8%
500–1000	13.5%	17.5%
1000–1500	14.0%	18.0%
1500–2000	15.5%	18.5%
2000–2500	15.5%	17.5%
2500–3000	14.5%	16.5%
3000–3500	14.0%	15.5%
3500–4000	16.0%	17.5%

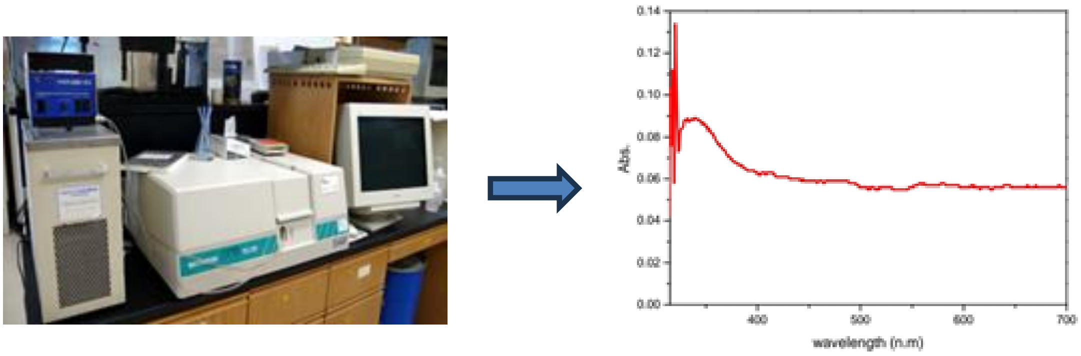


Figure 7: UV Spectra of PF Resin (Sample -01)

Discussion:

The synthesis of the resole resin yielded 85% of a viscous, dark red liquid with a solids content of 70%. FTIR spectra of the cured resole exhibited characteristic peaks at 3300 cm^{-1} (O-H stretching), 2920 cm^{-1} (C-H stretching), 1600 and 1510 cm^{-1} (aromatic C=C stretching), and 1230 cm^{-1} (C-O stretching). The glass transition temperature (Tg) of the cured resole, as determined by DSC, was 115 °C. Tensile testing of the neat cured resole resulted in an average tensile strength of 35 ± 2 MPa and a Young's modulus of 2.5 ± 0.1 GPa."The infrared (IR) spectrum of the phenol-formaldehyde resin displays characteristic absorption bands that confirm the presence of key functional groups associated with this type of polymer. The presence of multiple absorption bands below 1500 cm^{-1} also confirms the complex cross-linked structure of the phenol-formaldehyde resin, which includes aromatic rings and methylene (-CH2-) linkages.[39] The UV-Vis spectrum of the phenol-formaldehyde resin shows a broad absorption band in the ultraviolet region, with a maximum absorbance around 290–310 nm. This is characteristic of the π–π^* transitions associated with the aromatic rings present in the phenol moiety. Overall, the UV-Vis spectrum supports the structure of the phenol-formaldehyde resin, indicating the presence of aromatic rings [40].

Conclusion:

Phenol-formaldehyde (PF) resin stands as a significant synthetic polymer with a rich history, being the first commercially successful synthetic resin (Bakelite). Its formation through the reaction of phenol and formaldehyde, catalyzed by either acids (producing novolacs) or bases (producing resoles), yields materials with a unique combination of properties. PF resins exhibit excellent thermal stability, heat resistance, electrical insulation, chemical resistance, dimensional stability, hardness, and good adhesion, making them suitable for a wide array of demanding applications. While offering many benefits, the use of formaldehyde in PF resin production raises environmental and health concerns due to its toxicity and potential carcinogenicity. Responsible handling, proper curing, and ongoing research into safer alternatives are crucial. Furthermore, PF resins are thermosetting plastics that are non-degradable, posing challenges for recycling and contributing to environmental pollution.

References:

1. Kopf, P. W. (2002). *Encyclopaedia of Polymer Science and Technology* (Vol. 7, p. 322).
2. Poljansek, I., & Krajnc, M. (2005). *Acta Chimica Slovenica, 52*, 238.
3. Cardona, F., & Moscou, C. (2009). In *Proceedings of the 20th Australasian Conference on the Mechanics of Structures and Materials* (p. 317). Taylor & Francis.
4. Gardziella, A., Pilato, L. A., & Knop, A. (2013). *Phenolic resins: Chemistry, applications, standardization, safety and ecology* (Chapter 3, p. 83). Springer.
5. Cardona, F., & Sultan, M. T. H. (2016). *BioResources, 11*, 965.

6. Asim, M., Saba, N., Jawaid, M., Nasir, M., Pervaiz, M., & Alothman, O. Y. (2018). *Current Analytical Chemistry, 14*, 185.
7. Younesi-Kordkheili, H., & Pizzi, A. (2018). *European Journal of Wood and Wood Products, 76*, 871.
8. Sarika, P. R., Nancarrow, P., Khansaheb, A., & Ibrahim, T. (2020). Bio-based alternatives to phenol and formaldehyde for the production of resins. *Polymers, 12*, 2237.
9. Xu, Y. R., Guo, L. F., Zhang, H. N., Zhai, H. M., & Ren, H. (2019). Research status, industrial application demand and prospects of phenolic resin. *RSC Advances, 9*, 28924–28935.
10. Vitkalova, I. A., Torlova, A. S., & Pikalov, E. S. (2017). *Nauchnyi Obzor. Tekhnicheskiye Nauki*, (2), 15–28.
11. Kochnova, Z. A., Zhavoronok, E. S., & Chalykh, A. E. (2006). *Epoksidnye smoly i otverditeli: promyshlennye produkty (Epoxy resins and curing agents: Industrial products)*. Moscow: Peint-Media.
12. Nikiforov, V. M. (2009). *Tekhnologiya metallov i drugikh konstruktsionnykh materialov (Technology of metals and other structural materials)*. St. Petersburg: Politekhnika.
13. Ashpina, O. (2016). *Chem. J.*, 24–30.
14. Strelkov, V. P., Ivanov, B. K., & Tsvetkov, V. E. (2011). *Vestnik Moskovskogo Gosudarstvennogo Universiteta Lesa – Lesnoi Vestnik*, (5), 141–147.
15. Ashpina, O. (2016). *Chem. J.*, 24–30.
16. BiznesStat. (n.d.). *Analiz rynka fenoloformal'degidnykh smol v Rossii v 2011–2015 gg, prognoz na 2016–2020 gg (Analysis of the market of phenol-formaldehyde resins in Russia for 2011–2015 and forecast for 2016–2020)*. https://businesstat.ru/images/demo/phenol-formal-dehyde_resin_russia_2016.pdf
17. Vorob'ev, V. A., & Andrianov, R. A. (1980). *Tekhnologiya polymerov (Technology of polymers)*. Moscow: Vysshaya Shkola.
18. Kopf, P. W. (2006). In *Kirk-Othmer Encyclopedia of Chemical Technology* (Vol. 18, pp. 756–802).
19. Kadykova, Yu. A., & Levkina, N. L. (2017). *Russian Journal of Applied Chemistry, 90*(2), 244–251.
20. Knop, A., & Scheib, W. (1979). *Chemistry and application of phenolic resins* (pp. 5–8). New York: Springer-Verlag.
21. *Bakelite materials in industry*. (1935). *Bakelite Review, 7*(3), 30–36.
22. Baekeland, L. H. (1909). Method of making insoluble products of phenol and formaldehyde. U.S. Patent No. 942,699.

23. He, G., & Riedl, B. (2003). Phenol-urea-formaldehyde cocondensed resol resins: Their synthesis, curing kinetics, and network properties. *Journal of Polymer Science Part B: Polymer Physics, 41*, 1929–1938.
24. Ozaki, J., Ohizumi, W., & Oya, A. (2000). A TG-MS study of poly(vinyl butyral)/phenol-formaldehyde resin blend fiber. *Carbon, 38*, 1515–1519.
25. Jiang, H., Wang, J., Wu, S., Yuan, Z., Hu, Z., Wu, R., & Liu, Q. (2012). The pyrolysis mechanism of phenol-formaldehyde resin. *Polymer Degradation and Stability, 97*, 1527–1533.
26. Liu, J. N., Hou, Q. F., Hu, R. F., & Wang, W. Q. (2011). Modification and application of phenolic resin. *Pioneering with Science and Technology Monthly, 29*, 134–136.
27. Xue, B., & Zhang, X. L. (2007). Application and development trend of phenolic resin. *Thermosetting Resin, 4*, 47–50.
28. Liu, S. Q., Ning, P. C., & Ding, Z. M. (2016). Research progress of modified phenolic resin. *Thermosetting Resin, 31*, 64–70.
29. Wang, D. X., Chen, Z. M., Zhang, G. X., Liang, X. C., Li, B. H., Cao, X. Q., & Wang, C. (2016). Study on fast-curing phenol-formaldehyde resin adhesive. *Chemical Adhesion, 38*, 447–449.
30. Fenichell, S. (1996). *Plastic: The making of an artificial world*. HarperCollins.
31. Trimborn, C. (2004). Galalith – Jewelry milk stone. *Ganoskin Jewelry Making Resources*.
32. Meikle, J. L. (1995). *American plastic: A cultural history* (p. 53). Rutgers University Press.
33. Ibrahim, J. (2015, May 27). Faturan oxidization. *Amber Island Islamic Antiques & Arts*. Retrieved February 4, 2018.
34. Hirano, K., et al. (2013). Phenolic resins—100 years of progress and their future. *Reactive & Functional Polymers*.
35. Baekeland, L. H. (1909). Method of making insoluble products of phenol and formaldehyde. U.S. Patent No. 942,699.
36. Mauzy, B. E. (2001). *Bakelite in the kitchen* (2nd ed.). Atglen, PA: Schiffer Publishing.
37. Brandt, A. (2007). Bakelite: The beautiful plastic. *Antique Shoppe Newspaper*.
38. Davidov, C., & Dawes, G. R. (1988). *The Bakelite jewelry book* (1st ed.). New York: Abbeville Press.
39. *Bakelite materials in industry*. (1935). *Bakelite Review, 7*(3), 30–36.
40. The Old Timer. (1935). I remember when. *Bakelite Review, 7*(3), 24–28.

Matter & Motion: Explorations in Physical and Chemical Science Volume I

(ISBN: 978-81-992068-8-5)

About Editors

Dr. Shakuntala Avdhutrao Shinde serves as the Associate Professor and Head of the Department of Physics at SharadChandra Arts, Commerce and Science College, Naigaon, Dist-Nanded, where she has been a dedicated faculty member for the past fourteen years. A distinguished academician and researcher, Dr. Shinde holds a Ph.D. in Astrophysics from Swami Ramanand Teerth Marathwada University, Nanded. Her scholarly contributions include the publication of over 25 research papers in reputed national and international journals. In addition to her academic pursuits, she has successfully completed a Minor Research Project (MRP) and holds one Indian patent to her credit. Dr. Shinde's consistent engagement in teaching, research, and innovation reflects her commitment to academic excellence and scientific advancement in the field of physics.

Dr. Kushal Radheshyam Lanjewar, M.Sc. (Chemistry), Ph.D., is currently serving as Assistant Professor and Head of the Department of Chemistry at Mohsinbhai Zaweri Mahavidyalaya, Desaiganj (Wadsa), Dist. Gadchiroli, affiliated with Gondwana University, Gadchiroli. With 12 years of teaching experience and 4 years in the chemical industry, Dr. Lanjewar has a strong foundation in both academic and applied chemistry. He has published over 25 research articles in reputed national and international journals and authored three practical handbooks. As a recognized Ph.D. Supervisor under Gondwana University, he has also contributed as a reviewer for numerous research articles and book chapters. His research interests span organic synthesis, medicinal chemistry, catalysis, green chemistry, phytochemistry, and nanomaterials, reflecting his versatile engagement with contemporary scientific advancements.

Dr. Rajanish Saikia serves as Assistant Professor in the Department of Physics and holds the position of Academic Vice Principal at Nanda Nath Saikia College, Titabar. He earned his Ph.D. in Condensed Matter Physics from Gauhati University in 2004 and holds a Master's degree in Physics with specialization in Electronics and Radio Physics. Dr. Saikia is a dedicated researcher with over 10 publications in reputed national and international journals, particularly in the areas of clay minerals and plant fibers. His current research interests include Condensed Matter Physics, Materials Science, and Electronics. Passionate about science outreach, he actively promotes scientific awareness through student-centered and rural community initiatives. As the Secretary of the Assam Science Society, Titabar Branch, Dr. Saikia continues to inspire and contribute significantly to the advancement of science education and public engagement.

Mr. Swagatam Deva Nath, M.Sc. in Physics, is an Assistant Professor in the Department of Physics at Nanda Nath Saikia College, Titabar, Assam, with over ten years of teaching and academic experience. His primary areas of expertise include Space and Atmospheric Physics, with growing interest in Semiconductor Physics and Electronics. Known for his interactive and inclusive teaching approach, Mr. Nath is dedicated to making physics both accessible and engaging for undergraduate students. He plays an active role in student assessment, mentoring, and career counseling, guiding students toward higher education and careers in science and technology. Beyond the classroom, he is deeply involved in science outreach programs aimed at promoting scientific awareness and critical thinking in local schools and rural communities. His work reflects a strong commitment to academic excellence and community engagement.

Bhumi Publishing

ISBN 978-81-992068-8-5
9 788199 206885