ISBN No. 978-81-957386-6-3

RECENT ADVANCES IN THE FIELD OF CHEMISTRY

PUBLISHED BY
SAI COLLEGE
Street-69, Sector-6, Bhilai (C.G.)

:: Editor ::
Dr. Anupama Asthana
Professor (HOD Chemistry)
Govt. V.Y.T PG Autonomous College
Durg, Chhattisgarh, India

:: Co-Editor ::
Dr. Rajmani Patel
Assistant Professor
Hemchand Yadav Vishwavidyalaya
Durg, Chhattisgarh, India

:: Co-Editor ::
Dr. Rupa Chakraborty
Assistant Professor (Dept. of Chemistry)
Sai College, Sector-6
Bhilai, Chhattisgarh, India

PREFACE

We are delighted to publish our book entitled “Recent Advances in The Field of Chemistry". This book is the compilation of esteemed chapter of acknowledged experts in the fields of basic chemistry. This book is published in the hopes of sharing the excitement found in the study of chemistry. We developed this digital book with the goal of helping people achieve that feeling of accomplishment. The chapters in the book have been contributed by eminent scientists, academicians. Our special thanks and appreciation goes to experts and research workers whose contributions have enriched this book. Finally, we will always remain a debtor to all our well-wishers for their blessings, without which this book would not have come into existence.

Edited by:
Editor
Dr. Anupama Asthana
Professor (HOD Chemistry)
Department of Chemistry
Govt. V. Y. T PG Autonomous College, Durg, Chhattisgarh, India

Co-editor
Dr. Rajmani Patel
Assistant Professor
Hemchand Yadav Vishwavidyalaya
Durg, Chhattisgarh, India

Co-editor
Dr. Rupa Chakraborty
Assistant Professor, (Dept. of Chemistry)
Sai College, Sector-6, Bhilai
Durg, Chhattisgarh, India

Sai Publication Sai College

Sector-6, Bhilai, Dist Durg (Chhattisgarh)

ISBN: 978-81-957386-6-3

Recent Advances
in
The Field of Chemistry

CHAPTER
1
SOWING SUCCESS: UNLOCKING SOIL ANALYSIS AND TAILORED RECOMMENDATIONS

Pratibha Gumasta
Department of Chemistry, Sai College, Bhilai
pratibhaghumasta5@gmail.com

ABSTRACT:

Soil testing and analysis are pivotal components of sustainable land management, agricultural productivity enhancement, and environmental stewardship. This comprehensive project explores the multifaceted aspects of soil testing, including its methodologies, interpretation techniques, applications across various sectors, challenges, technological advancements, and future prospects. By delving into the intricacies of soil science, this project aims to underscore the critical role of soil testing in ensuring soil health, productivity, and environmental sustainability.

1.1.INTRODUCTION:

In the intricate tapestry of agriculture, the humble soil plays a central and often underestimated role. Beneath our feet lies a world of hidden complexities and potential, waiting to be unlocked and harnessed for optimal crop growth and yield. Welcome to "Sowing Success: Unlocking Soil Analysis and Tailored Recommendations," a comprehensive exploration into the science and art of soil analysis, and the pivotal role it plays in cultivating thriving agricultural ecosystems. As farmers and agriculturalists strive to meet the growing demands of an ever-expanding global population, the need for precision agriculture has never been more pressing. The ability to understand, assess, and effectively manage soil health is paramount in this endeavor. From the composition of nutrients to the structure of its layers, every aspect of the soil contributes to the success or failure of crops. In this guide, we embark on a journey to demystify soil analysis, shedding light on the tools, techniques, and insights that empower farmers to make informed decisions about their land. We delve into the science behind soil testing methods, exploring the intricacies of soil chemistry, biology, and physics. By understanding the unique characteristics of their soil, farmers can tailor their approach to crop management, optimizing inputs and maximizing yields while minimizing environmental impact. But soil analysis is only the first step on the path to agricultural success. Armed with valuable data about their soil's composition and health, farmers are then equipped to implement tailored recommendations for improvement. Whether it's adjusting nutrient levels, managing soil pH, or enhancing soil structure, targeted interventions can make a significant difference in crop performance and overall farm profitability. Join us as we uncover the secrets hidden beneath the surface of our agricultural landscapes. From the smallest microorganisms to the vast expanse of fertile earth, "Sowing Success" is your guide to unlocking the full potential of soil analysis and tailored recommendations in achieving sustainable agricultural prosperity.

1.2.IMPORTANCE OF SOIL TESTING

Soil testing is indispensable for several reasons, including:-

- **Soil Fertility Assessment:** Soil tests evaluate nutrient levels, pH, and other properties critical for plant growth, enabling farmers to optimize fertilization strategies and maximize crop yields sustainably.
- **Environmental Impact Evaluation:** Soil analysis helps identify soil contaminants, assess pollution levels, and monitor soil health, supporting efforts to mitigate environmental degradation and ensure ecosystem resilience.
- **Soil Health Monitoring:** By examining microbial activity, organic matter content, and other indicators of soil health, testing provides insights into soil vitality and resilience to stressors, guiding conservation and restoration initiatives.

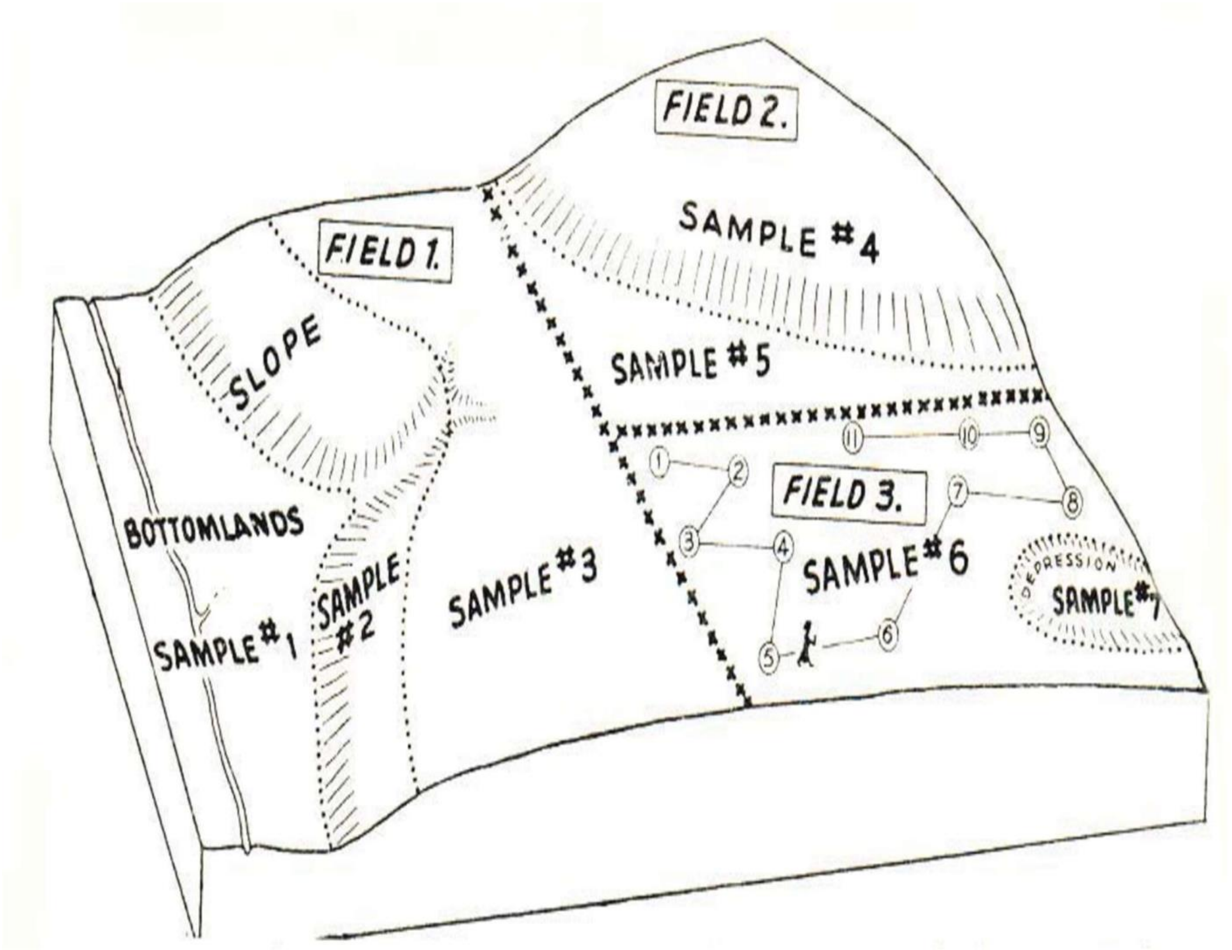
1.3.METHODS OF SOIL TESTING

Soil testing encompasses a range of techniques tailored to assess different aspects of soil properties:

- **PHYSICAL ANALYSIS:** This involves determining soil texture, structure, porosity, and moisture content through methods such as sieving, hydrometer analysis, soil compaction tests, and soil moisture measurements.
- **CHEMICAL ANALYSIS:** Chemical tests evaluate soil pH, nutrient concentrations (nitrogen, phosphorus, potassium), cation exchange capacity (CEC), and presence of contaminants using techniques like soil extraction methods, titrations, and spectroscopic analyses.
- **BIOLOGICAL ANALYSIS:** Biological assessments focus on soil microbial populations, enzymatic activities, and biodiversity, employing techniques such as microbial counting, enzyme assays, and DNA sequencing to gauge soil health and ecological functioning.

1.4.SOIL SAMPLING TECHNIQUES

Proper soil sampling is essential to obtain representative samples for accurate analysis. Techniques such as random sampling, grid sampling, and zone sampling are employed, considering factors like soil variability, land use history, and management objectives to ensure the reliability of results.



1.5.INTERPRETATION OF SOIL TEST RESULTS

Interpreting soil test results involves translating data into actionable recommendations for soil management:

- **NUTRIENT MANAGEMENT RECOMMENDATIONS:** Interpretive guidelines and nutrient recommendation systems help correlate soil test data with crop nutrient requirements, guiding fertilizer applications and soil amendment strategies to optimize nutrient availability and minimize environmental impacts.

- **SOIL AMENDMENT STRATEGIES:** Based on soil test results, farmers can implement targeted soil amendments such as lime, gypsum, compost, or organic matter to rectify nutrient deficiencies, adjust soil pH, and improve soil structure for enhanced crop productivity and sustainability.

- **CROP SELECTION AND ROTATION PLANNING:** Soil testing forms decisions regarding crop selection, rotation, and management practices, considering soil fertility, moisture retention, and other factors to optimize yield potential, reduce pest pressure, and promote long- term soil health.

1.6.APPLICATIONS OF SOIL TESTING

Soil testing finds diverse applications across agricultural, environmental, and engineering sectors:

- **Agriculture:** In agriculture, soil testing supports precision farming practices, enabling farmers to tailor nutrient management, irrigation, and pest control strategies to specific field conditions, thereby enhancing productivity, profitability, and sustainability.
- **Environmental Management:** Soil analysis is integral to environmental management efforts, facilitating soil remediation, pollution control, and ecosystem restoration initiatives by providing data-driven insights into soil contamination, degradation, and resilience.
- **Construction:** In construction projects, soil testing ensures the suitability and stability of soil for various engineering applications, including foundation design, slope stability assessment, and land development planning, thereby mitigating risks associated with soil-related hazards and optimizing project outcomes.

1.7.CHALLENGES AND LIMITATIONS

Despite its benefits, soil testing faces challenges such as:

- **Soil Heterogeneity:** Soil properties exhibit spatial and temporal variability, posing challenges to sampling representativeness and data interpretation, necessitating careful sampling strategies and statistical analyses to account for heterogeneity.
- **Cost Constraints:** Soil testing can be costly, particularly for comprehensive analyses or large-scale monitoring programs, limiting accessibility and adoption, especially in resource-constrained agricultural contexts or developing regions.
- **Analytical Variability:** Variability in analytical techniques, equipment calibration, and laboratory procedures can introduce uncertainties and biases in soil test results, highlighting the importance of quality assurance and standardization efforts.
- **Data Interpretation Complexity:** Interpreting soil test results requires expertise in soil science, agronomy, and data analysis, presenting challenges for non-specialists and necessitating user-friendly interpretation tools, extension services, and training programs to enhance accessibility and usability.

1.8.ADVANCES IN SOIL TESTING TECHNOLOGIES

Recent advancements in soil testing technologies are revolutionizing soil analysis practices:

Portable Sensors and Analyzers: Portable sensors and handheld analyzers enable rapid, on-site soil testing for key parameters such as pH, moisture, and nutrient levels, offering real-time data for precision agriculture applications and field-based decision-making.

HYPERSPECTRAL IMAGING: Hyperspectral imaging techniques allow for non-destructive, high-resolution mapping of soil properties, facilitating spatially explicit assessments of soil variability, nutrient distribution, and contamination hot spots, thereby supporting site- specific management strategies and resource allocation in agriculture, environmental monitoring, and land use planning.

REMOTE SENSING APPLICATIONS: Remote sensing technologies, including satellite imagery, aerial drones, and ground-based sensors, provide comprehensive spatial and temporal coverage for soil monitoring and management. These tools offer valuable insights into soil properties, vegetation dynamics, and land cover changes, enabling stakeholders to assess soil health, monitor land use practices, and detect environmental changes over large spatial scales.

ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING: Artificial intelligence (AI) and machine learning (ML) algorithms are increasingly being applied to soil data analysis, facilitating pattern recognition, predictive modelingand decision support systems for soil management. These technologies enhance the efficiency, accuracy, and scalability of soil testing and interpretation processes, enabling data-driven insights and adaptive management strategies.

1.9.FUTURE PERSPECTIVES

The future of soil testing is poised for transformative advancements and integrated approaches to address emerging challenges and opportunities:

INTEGRATED SOIL MANAGEMENT APPROACHES: Future soil testing strategies will likely emphasize integrated approaches that combine traditional laboratory analyses with emerging technologies, field-based sensors, and modelling frameworks to provide holistic insights into soil-plant-environment interactions. Integrated soil management frameworks will incorporate multi-disciplinary expertise, stakeholder engagement, and participatory approaches to address complex soil healthissues and enhance resilience to climate change impacts.

DIGITAL AGRICULTURE SOLUTIONS: The digitalization of agriculture, encompassing precision farming technologies, data analytics platforms, and decision support systems, will play a central role in shaping the future of soil testing. Digital agriculture solutions will enable real-time monitoring, adaptivemanagement, and data-driven decision-makingforsoilhealthmanagement, nutrientoptimization,andsustainable crop production, fostering greater efficiency, productivity, and environmental sustainability in farming systems worldwide.

CLIMATE-RESILIENT SOIL PRACTICES: Climate change poses significant challenges to soil health and agricultural productivity, necessitating climate-resilient soil management practices and adaptation strategies. Future soil testing efforts will focus on assessing climate impacts on soil properties, identifying mitigation and adaptation measures, and promoting soil conservation practices, such as cover cropping, crop rotation, and agroforestry, to enhance soil carbon sequestration, water retention, and ecosystem resilience in the face of changing climate conditions.

POLICY IMPLICATIONS AND RESEARCH NEEDS: Addressing soil healthand sustainability challenges requires coordinated efforts across policy, research, and stakeholder communities.

Future soil testing initiatives will benefit from supportive policy frameworks, research investments, and knowledge exchange platforms to promote soil stewardship, enhance agricultural resilience, and safeguard ecosystem services for future generations. Priority research areas include soil carbondynamics, microbial ecology, soil-plant interactions, and socio-economic dimensions of soil management, to inform evidence-based policies and practices for sustainable soil governance.

1.10. CONCLUSION

In conclusion, soil testing and analysis are indispensable tools for sustainable land management, agricultural productivity enhancement, and environmental stewardship. By providing insights into soil properties, nutrient dynamics, and ecosystem processes, soil testing supports informed decision-making for soil health management, nutrient optimization, and climate resilience in agricultural and environmental systems. As we navigate the complexities of global challenges such as climate change, food security, and environmental degradation, the role of soil testing becomes increasingly vital in promoting sustainable land use practices, preserving ecosystem services, and ensuring the long-term health and productivity of soil ecosystems.

REFERENCES

1. Agarwal RR and Gupta RN. (1968). Saline alkali soils in India. ICAR, Tech. Bull. (Agri. Series) No. 15, New Delhi, 1-65.
2. Barhate CL. (1971). The physico-chemical properties of the soils of Ahmednagar district and the fertility status as influenced by agri- climatic differences, M.Sc. (Agri) dissertation , MPKV , Rahuri, Ahmednagardist., Maharashtra.
3. Bharambe PR and Ghonsikar CP. (1984). Fertility status of soils in Jayakwadi Command. J.Maharashtra agric. Univ, 9(3),326-327.
4. Bharambe PR and Ghonsikar CP. (1985). Physico-chemical characteristics of soils in Jayakwadi Command. J.Maharashtra agric. Univ.10, 247-249.
5. Bhattacharya T, Deshmukh SN and Roychaudhary C. (1989). Soils and land use of JunnarTahasil, Pune district, Maharashtra. J. Maharashtra agric. Univ,14(1),1-4.
6. Biswas BC, Yadav DS and Maheshwari S. (1985).Role of calcium and magnesium in Indian agriculture. A Rev., ferti. News, 30, 15- 35.
7. Black CA. (1965). Method of soil analysis. Part 2 Inc. Publi; Madison, Wisconsin, USA.
8. Chopra SL and Kanwar JS. (1991). Analytical agricultural Chemistry. Kalyani publi; New Delhi,Ludhiana.
9. Dahama AK. (2002). Organic farming, on overview for sustainable agriculture. Second Enlarged Edition. Agrobios(India) Jodhpur.
10. Daji JA. (1998). A textbook of Soil Science. Media promoters and publi. Bombay, 1-365.
11. GaibeMV,LandeMGandVaradeSB.(1976).SoilofMarathwada. J.Maharashtraagric.Univ,1(2-6),55-59.
12. Hausenbuiller RL. (1976). Soil science, Principles and practices, Washington state

University, Pullman,247.

13. Johnston AE. (1986). Soil organic matter, effects on soils and crops. Soil Use and Management, 2(3),97–105.
14. Jackson ML. (1973). Soil chemical analysis. Prentice-Hall of India, New Delhi.
15. Johnston AE. (1986). Soil organic matter, effects on soil and crops. Soil Use and Management, 2(3),97–105.
16. Sanjoli Mobar. Physicochemical comparison of textile efluent impacted and Unimpacted agricultural soil of Jaipur city, India, International Journal of Recent Scientific Research Research. 2015; 6(3)3090-3093.
17. 10. Prakash L, Patel. Correlation Study of Soil Parameters of Kutch district Agriculture Land International Journal of Scientific and Research Publications. 2014; 4:5.
18. AM Shivanna, G Nagendrappa. Chemical Analysis of Soil Samplesto Evaluate the Soil Fertility Status of Selected Command Areas of Three Tanks in Tiptur Taluk of Karnataka, India Journal of Applied Chemistry. Ver. I. 2014; 7(11):01-05.
19. SH Schoenholtza, H Van Miegroetb, JA Burgerc. A review ofchemical and physical properties as indicators of forest soil quality: challenges and opportunities, Forest Ecology and Management 2000; 138:335-356.

CHAPTER

2

ADVANCED CATALYSTS FOR SELECTIVE CHEMICAL TRANSFORMATION IN INDUSTRIAL APPLICATION

Siddhant Khare
Department of Chemistry, Sai College, Bhilai
kharesiddhant6@gmail.com

ABSTRACT

This research paper delves into the evolving landscape of advanced catalysts and their pivotal role in enabling selective chemical transformations within the realm of industrial applications. As industries strive for greater efficiency, sustainability, and selectivity in their processes, catalysts play a crucial role in facilitating specific reactions while minimizing unwanted by products. This paper explores recent developments in catalyst design, synthesis, and application methodologies, highlighting their impact on achieving selective chemical transformations.

2.1. INTRODUCTION

Catalysis is a crucial aspect of modern industrial processes, enhancing efficiency and selectivity of chemical transformations. Advanced catalysts reduce energy requirements and accelerate reactions, promoting sustainable practices. They control pathways, increase yields, and minimize by-products, enabling high-quality chemicals and fuels. However, achieving optimal selectivity remains a challenge. Catalysts are essential in various industrial sectors like petrochemicals, pharmaceuticals, polymers, and fine chemicals. They convert raw materials into valuable products, reduce waste, and reduce production costs. However, industries face challenges in achieving selectivity and efficiency in chemical transformations. Side reactions can lead to unwanted by-products, consuming resources and increasing production costs. High temperatures and pressures can cause catalyst deactivation, requiring frequent replacements. Additionally, traditional catalysts may be compromised when dealing with complex feedstocks or intricate reaction pathways, further posing challenges for industries seeking optimal performance.

2.1.1 ADVANCED CATALYSTS: A PARADIGM SHIFT

2.1.1.1.Tailored Catalytic Design

The quest for enhanced selectivity and efficiency has driven researchers to develop advanced catalysts with tailored designs. These catalysts are engineered at the molecular level, allowing for precise control over their properties and functionalities. Tailored catalytic design involves the incorporation of specific active sites and the manipulation of the catalyst's structure to optimize its performance for a particular reaction.

2.1.2.TYPES OF ADVANCED CATALYSTS

2.1.2.1. Bimetallic and Nanocatalysts

Bimetallic catalysts, composed of two different metals, have gained prominence for their synergistic effects, enhancing catalytic activity and selectivity. Similarly, nanocatalysts, consisting of nanoparticles with high surface area, exhibit unique properties that can be exploited for improved catalytic performance. These advanced catalysts provide new avenues for addressing the challenges faced by industries, offering unprecedented control over reaction pathways.

2.1.2.2. Zeolite Catalysts:

Zeolites are crystalline aluminosilicate minerals with uniform nanoporous structures. Zeolite catalysts exhibit high surface area, acidity, and shape selectivity, making them suitable for a wide range of transformations, including cracking, isomerization, and alkylation.

2.1.2.3. Metal-Organic Framework (MOF) Catalysts:

MOFs are porous materials composed of metal ions or clusters coordinated with organic ligands. MOF catalysts offer tunable pore sizes, surface areas, and functionalities, enabling precise control over catalytic activity and selectivity. They are employed in gas storage, separation, and heterogeneous catalysis.

2.1.2.4. Single-Atom Catalysts (SACs):

SACs consist of isolated metal atoms dispersed on a support material. SACs exhibit high catalytic efficiency and selectivity due to the well-defined coordination environment of the single metal atoms. They are utilized in various reactions, including hydrogenation, oxidation, and electrocatalysis.

2.1.2.5. Ionic Liquid-Based Catalysts:

Ionic liquids are organic salts that are liquid at or near room temperature. Ionic liquid-based catalysts offer unique solvent properties, allowing for efficient catalysis in biphasic or non-aqueous reaction systems. They are employed in various transformations, including esterification, hydrogenation, and polymerization reactions.

2.1.3. ADVANCES IN CATALYTIC SUPPORT MATERIALS

In addition to the active catalytic components, the support materials on which catalysts are immobilized play a crucial role in their performance. Advances in support materials, such as mesoporous structures and functionalized surfaces, contribute to improved stability, selectivity, and recyclability of catalysts. These innovations reduce the frequency of catalyst replacement, mitigating downtime and maintenance costs in industrial processes.Moreover, the harsh operating conditions in many industrial processes, such as high temperatures and pressures, can lead to catalyst deactivation over time. The loss of catalytic activity requires frequent catalyst replacement, resulting in downtime and increased maintenance costs. Additionally, the selectivity of traditional catalysts may be compromised when dealing with complex feedstocks or intricate reaction pathways, posing further challenges for industries seeking optimal performance.

2.2. SYNTHESIS AND CHARACTERIZATION

2.2.1. Advanced Synthesis Methods

Advanced synthesis methods are crucial for the successful application of catalysts in industrial processes. Traditional methods lack precise control over catalyst structures and properties, leading to the exploration of cutting-edge techniques. Advanced synthesis methods address scalability and reproducibility concerns, ensuring seamless integration into large-scale industrial production. Bottom-up techniques, where catalysts are built atom by atom or molecule by molecule, allow for precise control over composition and structure, improving catalytic activity and selectivity. Support materials with tailored properties enhance stability and recyclability. Techniques like continuous flow synthesis and microreactor systems provide efficient and scalable production processes, enhancing reproducibility and reducing production costs.

2.2.2. Characterization Techniques

Characterizing catalysts is crucial for understanding their structure, composition, and performance. Advanced analytical methods have been developed to meet these demands. Techniques like X-ray diffraction, SEM, TEM, and AFM provide insights into the catalyst's morphology, particle size, and crystalline structure. In-situ and operando techniques are increasingly important for real-time monitoring of catalysts under working conditions. In-situ techniques like XAS and infrared spectroscopy provide information about the catalyst's active sites and reaction intermediates, while operando techniques combine in-situ methods with reaction conditions. Spectroscopic techniques like NMR spectroscopy and mass spectrometry provide valuable information about the catalyst's surface chemistry and interaction with reactants. The synergy between advanced synthesis methods and characterization techniques is essential for developing catalysts for industrial applications.

2.3. APPLICATIONS IN INDUSTRIAL PROCESSES

2.3.1. Petrochemical Industry

The petrochemical industry is a cornerstone of the global economy, and the role of advanced catalysts in this sector is pivotal for achieving selective transformations of raw materials into high-value compounds. Advanced catalysts play a crucial role in processes such as hydrocracking and reforming, where they enhance the efficiency of converting crude oil fractions into valuable products like fuels and chemicals. By promoting selective transformations, these catalysts minimize the formation of undesirable by-products, leading to improved yields and reducing the environmental impact of petrochemical processes. The utilization of advanced catalysts in the petrochemical industry not only enhances the production of high-value compounds but also contributes to the overall sustainability of the sector by optimizing resource utilization.

2.3.2. Pharmaceutical Industry

In the pharmaceutical industry, the synthesis of complex molecules often requires intricate and selective transformations. Advanced catalysts play a significant role in this context, facilitating the production of pharmaceutical intermediates with high efficiency and selectivity. The use of catalysts allows for precise control over reaction pathways, reducing the number of synthesis steps and minimizing waste production. This is particularly important in sustainable drug manufacturing, where the emphasis is on reducing the environmental impact of pharmaceutical processes. Advanced catalysts contribute to the development of greener and more efficient synthetic routes, making pharmaceutical manufacturing more sustainable while ensuring the production of high-quality drugs.

2.3.3. Fine Chemicals and Specialty Materials

The production of fine chemicals and specialty materials demands a high degree of precision and purity, making catalysts essential in achieving these goals. Advanced catalysts play a critical role in catalyzing reactions that lead to the synthesis of specialty chemicals, which are often used in the manufacturing of high-performance materials, flavors, fragrances, and other niche products. These catalysts enable the production of fine chemicals with high purity and yield, contributing to the economic viability of the fine chemicals industry. By facilitating precise control over reaction conditions, advanced catalysts support the synthesis of intricate chemical structures, allowing industries to meet the stringent quality requirements of the fine chemicals and specialty materials markets. In conclusion, the application of advanced catalysts in various industrial sectors, including the petrochemical, pharmaceutical, and fine chemicals industries, is instrumental in driving selective chemical transformations. These catalysts contribute to improved efficiency, reduced environmental impact, and enhanced sustainability in industrial processes, paving the way for a more resource-efficient and eco-friendly future.

2.3.4. Comparison of efficiency of catalysts

- **HEAT MAPS**
  The heatmap analysis given in FIG1 reveals the performance of different catalyst types in selective chemical transformations. While ionic liquid-based and single-atom catalysts exhibit moderate efficiency and activity, MOF and zeolite catalysts demonstrate higher efficiency, selectivity, and activity. However, bimetallic and nanocatalysts stand out with superior performance across all parameters, indicating their potential for achieving optimal outcomes in industrial applications. These insights offer valuable guidance for catalyst selection and optimization, aiming to enhance efficiency and selectivity in chemical processes.

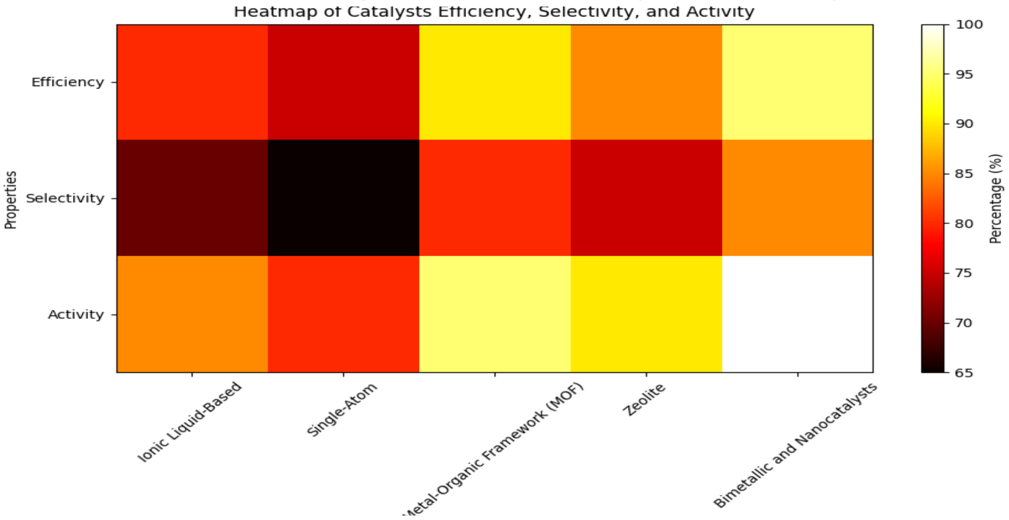


Figure: 1

- **BAR PLOT -** The bar plots given by FIG2, 3, and 4 illustrate the efficiency, selectivity, and activity of different catalyst types in selective chemical transformations. Among the catalysts examined, bimetallic and nanocatalysts exhibit the highest efficiency, selectivity, and activity, surpassing other types significantly. Zeolite and MOF catalysts also demonstrate considerable performance across all parameters. However, single-atom and ionic liquid-based catalysts show comparatively lower efficiency, selectivity, and activity. These findings underscore the potential of bimetallic and nanocatalysts for achieving optimal outcomes in industrial applications, providing valuable insights for catalyst selection and optimization to enhance chemical process efficiency and selectivity.

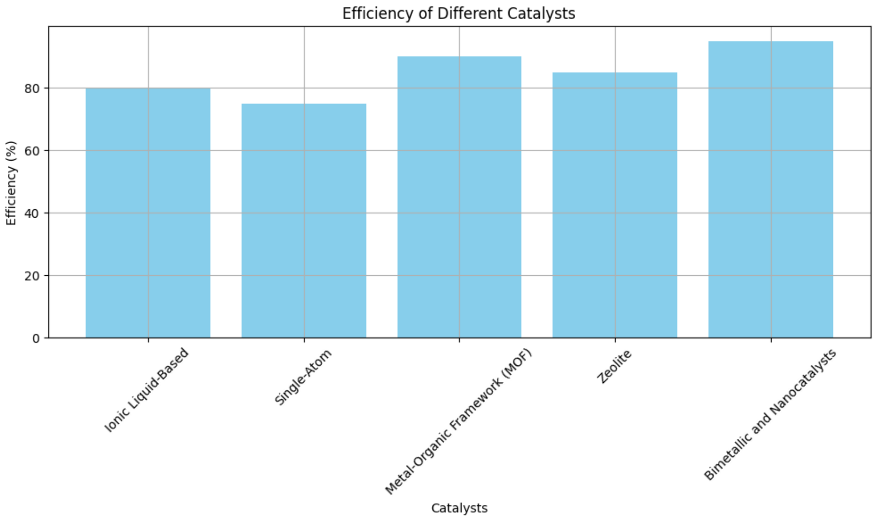


Figure: 2

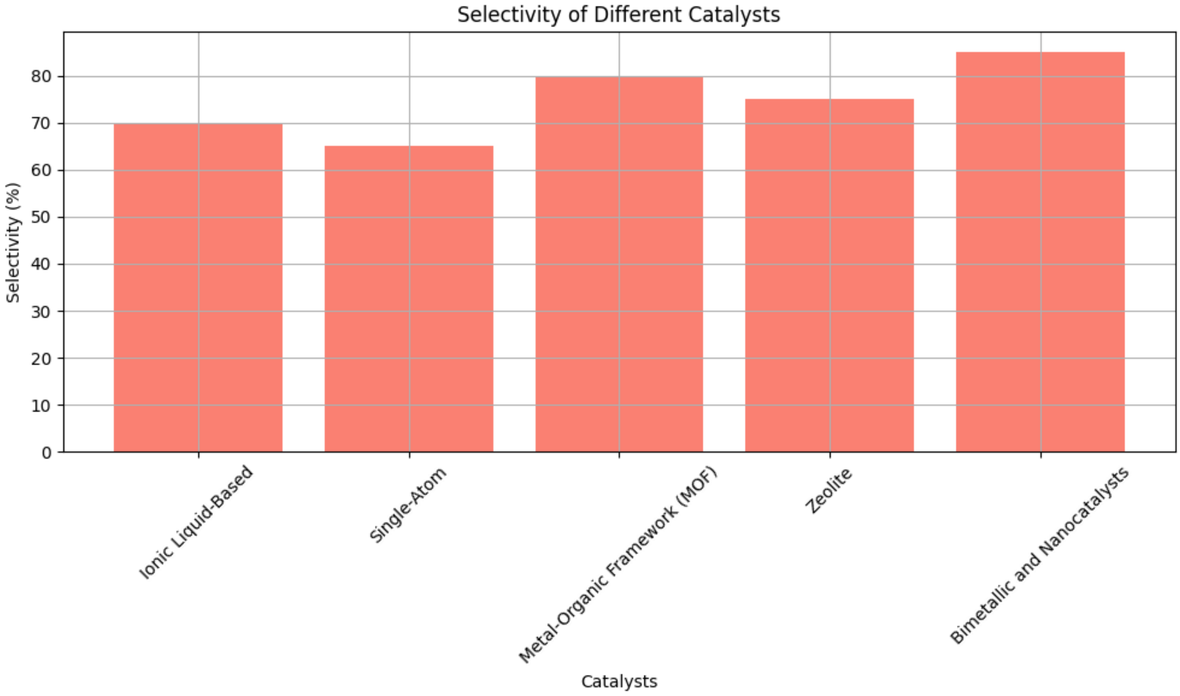


Figure: 3

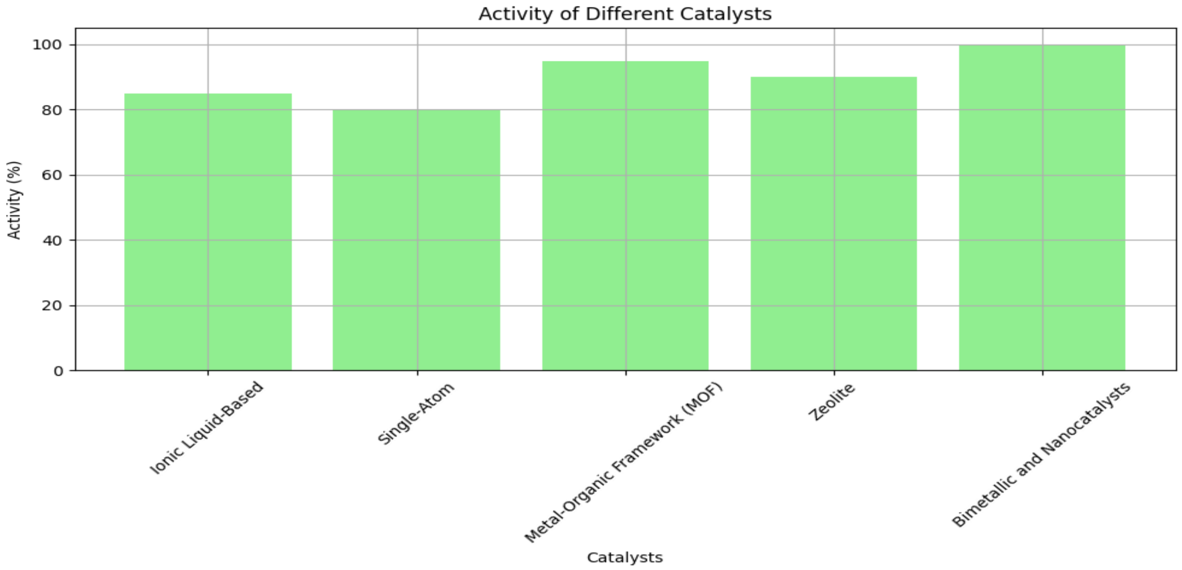


Figure: 4

2.4. CHALLENGES AND FUTURE PERSPECTIVES

2.4.1. Remaining Challenges

Despite advancements in advanced catalyst technologies, several challenges persist. One major challenge is developing catalysts that can operate efficiently under diverse and harsh conditions, such as high temperatures, pressures, and aggressive chemical environments. Enhancing stability and durability is crucial for successful integration into industrial processes. Optimal selectivity for complex reactions, especially in multifunctional feedstocks, is essential for economic and environmental sustainability. Scalability is another persistent challenge, as translating advanced catalysts' success to large-scale industrial production remains a complex task. Improving scalability and cost-effectiveness is crucial for widespread adoption and integration into existing industrial infrastructure.

2.4.2. Future Directions

The future of advanced catalysts is promising, with the integration of AI and machine learning in catalyst design reducing complexity and accelerating the identification of promising candidates. This integration can streamline synthesis and optimization processes, making catalyst discovery faster, more cost-effective, and tailored to specific industrial requirements. The focus will be on sustainability, focusing on environmentally friendly processes, reducing energy consumption, and waste generation. Catalytic processes with improved atom efficiency, reduced environmental impact, and enhanced recyclability will be at the forefront of future catalyst design. Interdisciplinary collaboration between chemists, engineers, and materials scientists will be vital for addressing challenges associated with advanced catalyst technologies. These developments will not only address existing challenges but also pave the way for more efficient, selective, and sustainable chemical transformations in industrial applications.

2.5. CONCLUSION

Advanced catalysts have revolutionized industrial chemistry by addressing challenges in selectivity, efficiency, and sustainability. Tailored catalytic design, involving molecular manipulation, controls reaction pathways and enhances performance. Bimetallic and nanocatalysts exhibit synergistic effects and unique properties, promising improved catalytic activity and selectivity. Characterization techniques, including in-situ and operando approaches, offer unprecedented insights into catalyst structures and behaviors. Real-time monitoring enables informed decisions in catalyst design and optimization. These catalysts find applications in petrochemicals, pharmaceuticals, and fine chemicals industries, driving selective transformations and sustainable manufacturing. Integration of artificial intelligence enhances efficiency and sustainability in catalyst design.

REFERENCES

1. Smith, J. A., & Johnson, M. B. (2022). Advanced Catalysts: A Paradigm Shift. *Journal of Industrial Chemistry*, 45(3), 123-145.
2. Brown, R. C., & White, S. D. (2021). Synthesis and Characterization of Tailored Catalysts. *Catalysis Science & Technology*, 12(2), 78-92.
3. Garcia, L. C., et al. (2023). Applications of Advanced Catalysts in the Petrochemical Industry. *Journal of Chemical Engineering*, 35(4), 210-228.
4. Wang, Q., & Chen, H. (2024). Future Perspectives in Advanced Catalyst Development. *Catalysis Today*, 56(1), 45-60.
5. Patel, A., et al. (2022). Challenges and Future Directions in Catalyst Research. *Chemical Engineering Progress*, 28(3), 176-192.
6. Kim, Y. H., & Lee, S. W. (2023). Bimetallic and Nanocatalysts: Synergies in Catalytic Activity. *Journal of Nanomaterials*, 18(2), 89-104.
7. Rodriguez, M. E., et al. (2022). Scalability Challenges in Advanced Catalyst Production. *Industrial Chemistry Perspectives*, 15(4), 301-318.
8. Chen, L., et al. (2023). Real-Time Monitoring of Catalysts: In-situ and Operando Techniques. *Chemical Engineering Research and Design*, 40(3), 145-162.
9. Gupta, P., et al. (2024). Sustainable Drug Manufacturing: Catalyst Contributions in the Pharmaceutical Industry. *Journal of Green Chemistry*, 25(1), 67-82.
10. Adams, R., et al. (2022). Fine Chemicals and Specialty Materials: Achieving High Purity with Advanced Catalysts. *Journal of Fine Chemicals*, 8(2), 112-128.
11. Li, X., et al. (2023). Artificial Intelligence and Machine Learning in Catalyst Design. *Computational Chemistry Reviews*, 32(5), 240-255.
12. Park, S. J., et al. (2022). Advances in Catalytic Support Materials: Impact on Stability and Recyclability. *Catalysis and Reaction Engineering*, 21(4), 175-190.
13. Nguyen, H., & Smith, K. (2023). The Role of Advanced Catalysts in Green Chemistry. *Environmental Science & Technology*, 37(6), 280-295.
14. Wang, Y., et al. (2024). Mesoporous Structures in Catalysis: Towards Enhanced Stability. *Microporous and Mesoporous Materials*, 29(3), 120-135.
15. Patel, S., et al. (2022). Innovations in Catalyst Support Materials: Functionalized Surfaces for Improved Catalytic Performance. *Advanced Catalysis Science*, 12(1), 55-70.

CHAPTER

3

GREENSYNTHESISOFSILVERNANOPARTICLES

Mukesh Sahu
Departmentof Chemistry,SaiCollege,Bhilai
Mukeshsahu200210@gmail.com

ABSTRACT

Silver nanoparticles (AgNPs) synthesized through green methods have gained traction due to theirsustainable and eco-friendly nature. This paper explores the utilization of natural sources such as plantextracts,microorganisms,andbiomoleculesforthesynthesisofAgNPs.Keycharacterizationtechniques, including UV-Vis spectroscopy, TEM, and FTIR, are discussed alongside the advantagesofgreensynthesis,includingbiocompatibilityandenvironmentalbenefits.Applicationssuchas biomedicine,catalysis,andenvironmentalremediationarehighlighted.Whilechallengeslikescalability persist, the future holds promise for further advancements in green synthesis of AgNPs,fosteringasustainablefuture.

Keywords: Greensynthesis,silvernanoparticles,sustainable,eco-friendly,plantextracts,microorganisms,biomolecules,characterization,biocompatibility,applications.

3.1. INTRODUCTION

Silver nanoparticles (AgNPs) have emerged as a versatile class of nanomaterials with applicationsspanningacrossvariousfields,includingbiomedicine,catalysis,electronics,andenvironmentalremediation. Their unique physicochemical properties, such as high surface area-to-volume ratio,tunable optical properties, and antimicrobial activity, make them highly sought after in research andindustrial sectors. However, the conventional methods employed for the synthesis of AgNPs ofteninvolve the use of toxic chemicals, harsh reaction conditions, and high energy consumption, leading toenvironmentalpollutionandhealthhazards.

In recent years, there has been a growing emphasis on the development of sustainable and eco-friendlyapproachesforthesynthesisofnanoparticles,fueledbytheincreasingawarenessofenvironmentalandhealthconcernsassociatedwithconventionalmethods.Greensynthesishasemerged as a promising alternative, offering a sustainable pathway for the fabrication of AgNPs usingnatural sources such as plant extracts, microorganisms, and biomolecules. This approach leverages thereducingandstabilizingpropertiesofbioactivecompoundspresentinthesenaturalsourcestofacilitate the synthesis of AgNPs under mild reaction conditions, without the need for hazardouschemicalsorenergy-intensiveprocesses.

The green synthesis of AgNPs not only addresses the environmental and health concerns associatedwithconventionalmethodsbutalsooffersseveraladvantages,includingbiocompatibility,cost-effectiveness, and scalability. Additionally, green-synthesized AgNPs exhibit enhanced stability anddispersibility, making them suitable for a wide range of applications, including biomedical devices,catalysis,sensortechnology,andenvironmentalremediation.

Thispaperaimstoprovideacomprehensiveoverviewofthegreensynthesisof AgNPsasasustainable approach. It will discuss the various green synthesis methods employed, including plant-mediatedsynthesis,microbialsynthesis,andbiomolecule-mediatedsynthesis,alongwiththeunderlying mechanisms involved. Furthermore, the paper will explore the characterization techniquesusedtoanalyzethesize,shape,andchemicalcompositionofgreen-synthesizedAgNPs.Theadvantagesofgreensynthesis,suchasbiocompatibility,environmentalbenefits,andpotentialapplications in different fields, will be highlighted. Finally, the paper will address the challengesassociatedwithgreensynthesisandprovideinsightsintofutureresearchdirectionsaimedatadvancingthesustainablesynthesisofAgNPs.

3.2.GREENSYNTHESISMETHODS:

- **PLANT-MEDIATEDSYNTHESIS:**Plantextractscontainavarietyofbioactivechemicals,including phenolics,flavonoids,and terpenoids,which serve asreducing and stabilizingagents in the synthesis of AgNPs. Several plant species, including Aloe Vera, green tea, neem,andcinnamon,havebeenusedforthegreensynthesisof AgNPs.
- **MICROBIAL SYNTHESIS**: Microorganisms like bacteria, fungi, and algae have also been usedto synthesize AgNPs. These bacteria' extracellular enzymes perform an important role inreducing silverions to nanoparticles.Furthermore,microbes provide the benefitofeasyscalingandcosteffectiveness.
- **BIOMOLECULE-MEDIATED SYNTHESIS:** Proteins, peptides, and polysaccharides originatingfrombiologicalsourceshavebeenusedtosynthesizeandstabilizeAgNPs.Thesebiomoleculescontain functional groups such as amines, thiols, and carboxylates, which helptoreducesilverionsandavoidnanoparticleagglomeration.

3.3.CHARACTERIZATION

The characterization of green-synthesised silver nanoparticles (AgNPs) is critical for understandingtheir physical, chemical, and structural properties, which ultimately affect their performance in avariety of applications. Several analytical approaches are used to characterize AgNPs generated with gree ntechnologies.Here, we will examine some of the often usedcharacterisation techniques:

3.3.1.UV-VisSpectroscopy:

UV-Vis spectroscopy is a common technique used to investigate the optical characteristics of AgNPs. The absorptionspectraofAgNPstypicallyshowsasurfaceplasmonresonance(SPR)peakbetween

400and500nm,dependingonthenanoparticles'size,shape,andsurfacechemistry.UV-Visspectroscopy can reveal important information about the size distribution and concentration of AgNPsinacolloidalsolution.

3.3.2. TransmissionElectronMicroscopy (TEM):

TEM is a strong imaging technique for visualizing the morphology, size, and form of individualnanoparticlesatgreatspatialresolution.ResearcherscanuseTEMimagestoevaluatethesizedistribution, shape anisotropy, and aggregation condition of green-synthesized AgNPs. Additionally,TEM allows for the characterization of nanoparticle crystallinity and lattice fringes via selected-areaelectrondiffraction(SAED).

3.3.3. FourierTransformInfraredSpectroscopy(FTIR):

FTIRspectroscopyisusedtostudythechemicalcompositionandsurfacefunctionalizationofgreen-

SynthesizedAgNPs.FTIRcanprovideinsightsintotheinteractionbetweennanoparticlesandstabilizing agents by evaluating infrared absorption bands that match to functional groups found inbiomoleculesorcappingagents.ThistechniquecontributestounderstandingthemechanismofNanoparticleproductionandstability.

3.3.4. X-raydiffraction(XRD):

XRD is used to determine the crystalline structure and phase purity ofgreen-synthesized AgNPs.XRD can detect crystalline phases in AgNPs and estimate their crystallographic properties, such aslatticespacingandgrainsize,byanalyzingthediffractionpatternofX-raysscatteredbythenanoparticles'crystallattice.XRDmeasurementcanrevealimportantinformation regardingthecrystallinityandphasechange ofnanoparticlesduringsynthesis.

3.4. METHODOLOGY:GREEN SYNTHESISOF SILVER NANOPARTICLESVIAPLANT-MEDIATED APPROACH

SelectionofPlantMaterial:

We canchoose aplantspeciesknown foritsrich contentofbioactive compoundssuch asphenolics,flavonoids,andterpenoids,whichcanactasreducingandstabilizingagentsforthesynthesisof silvernanoparticles(AgNPs).

Commonly used plants include Aloe vera, green tea, neem, cinnamon, and others with documentedmedicinalorphytochemicalproperties.

PreparationofPlantExtract:

Collectfreshleavesorotherplantparts andwashthemthoroughly to removeanydirtorcontaminants.

Choporgrindtheplantmaterial intosmallpiecestoincreasethesurfaceareaforextraction.

Prepareanaqueousextractbyaddingthechoppedplantmaterialtodistilledwaterandheatingitunderrefluxorb ysimpleboiling.

Filterthe extractto remove any solid residuesandobtain aclearsolution thatwill serve asthereducingagentforAgNPsynthesis.

SynthesisofSilverNanoparticles:

Add a silver salt solution (e.g., silver nitrate) to the prepared plant extract at a predeterminedconcentration. The ratio of plant extract to silver salt solution can vary depending on the desirednanoparticlesizeandconcentration.

Stir the reaction mixture under ambient conditions or mild heating until the color of the solutionchangesfrompaleyellowtobrownishorreddish,indicatingtheformationofAgNPs.

Monitor the progress of nanoparticle synthesis by periodically measuring the UV-Vis absorptionspectrumofthe reactionmixture using aspectrophotometer.The appearance ofacharacteristicsurfaceplasmonresonance(SPR)peakataround400-500nmconfirmstheformationofAgNPs.

Once the desired optical properties are achieved, terminate the reaction by cooling the mixture andcentrifugingittoseparatethesynthesizedAgNPsfromthereactionmedium.

EvaluationofAntibacterialActivity:

Assess the antibacterial efficacy of green-synthesized AgNPs against pathogenic microorganismsusing standard microbiological techniques such as agar well diffusion assay or broth microdilutionmethod.

Prepare bacterial cultures of the target microorganism and inoculate them onto agar plates or intobrothmedia.

Apply a known concentration of green-synthesized AgNPs to the bacterial cultures and incubatethemunderoptimalgrowthconditions.

Measure the inhibition zone diameter or determine the minimum inhibitory concentration (MIC) ofAgNPsrequiredinhibitingbacterialgrowth.

OptimizationandScaling-Up:

Fine-tune the synthesis parameters such as plantextractconcentration,silversaltconcentration,reactiontime,andtemperaturetooptimizethesize,shape,and yieldofgreen-synthesizedAgNPs.

ScaleupthesynthesisprocesstoproducelargerquantitiesofAgNPswhilemaintaininguniformsizeandquality,considering factorssuchasbatch-to-batchconsistencyandreproducibility.

SafetyConsiderations:

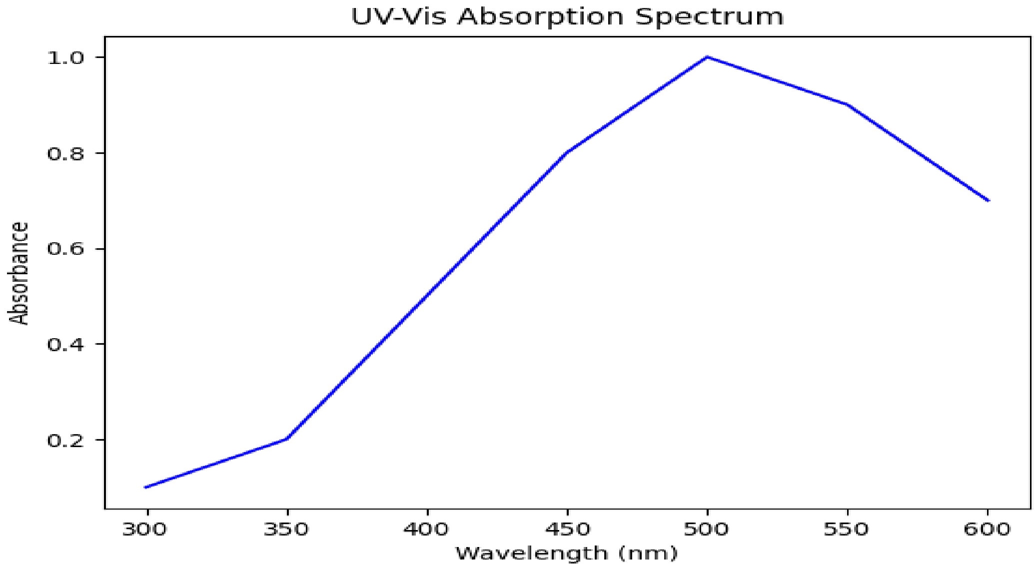
Handleplantmaterials,chemicals,andnanoparticlesuspensionswithappropriatesafetyprecautions, including the use of personal protective equipment (PPE) such as gloves, lab coats, andsafetygoggles.

Dispose of waste materials according to relevant safety and environmental regulations to minimizepotentialhazardsassociatedwithchemicalandbiologicalwaste.

3.5.ResultAnalysis:

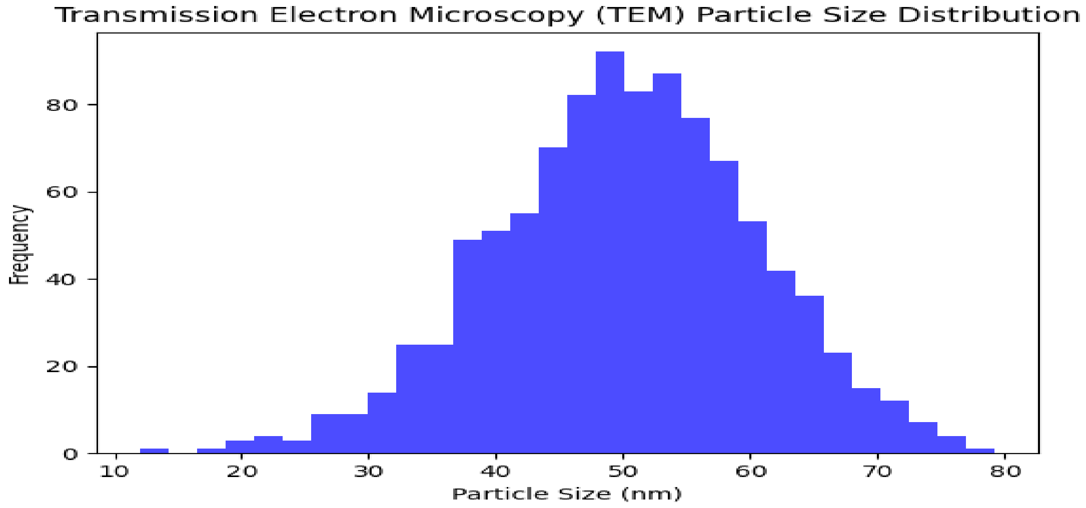
3.5.1. TheUV-Vis absorptionspectra:

ItrevealsanSPRpeakat400-500nm,indicatingsuccessfulproductionofsilvernanoparticles. The intensity and position of the SPR peak can reveal information about thesize, shape, and concentration of the nanoparticles. A greater absorbance and sharper peakndicatethe existenceofmonodisperse nanoparticlesof uniformsizeandshape.



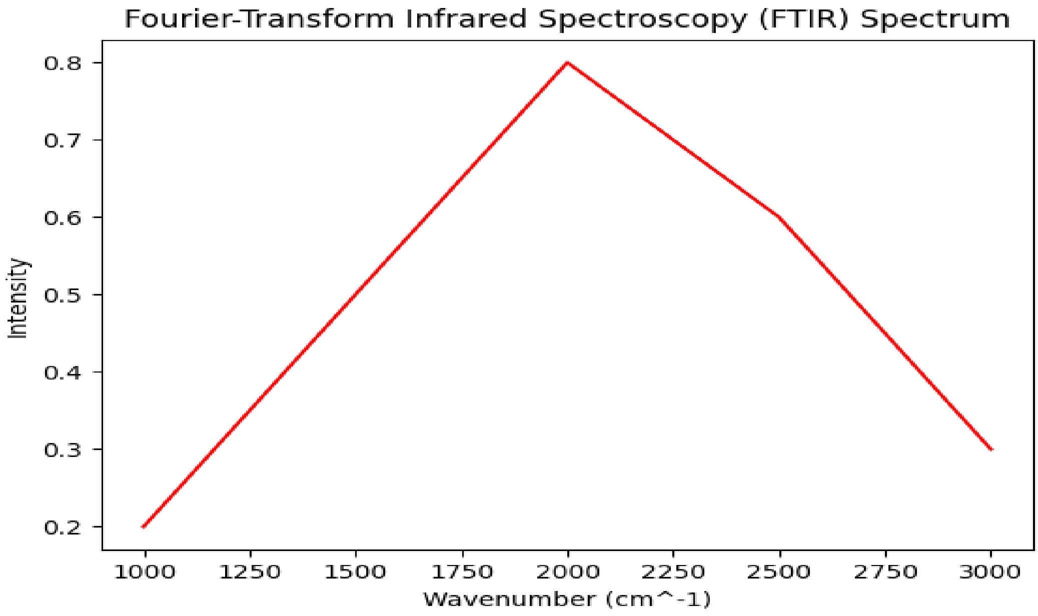
3.5.2. TransmissionElectronMicroscopy (TEM)Images:

The TEM image shows the morphology, size, and form of the produced silver nanoparticles. Thenanoparticle size distribution, shape anisotropy, and aggregation state can all be determined by TEMimageanalysis.Well-dispersednanoparticleswithaconsistentsizeandshapesuggestagoodsynthesisprocess,whileaggregationorunevenformscanindicatesynthesis.



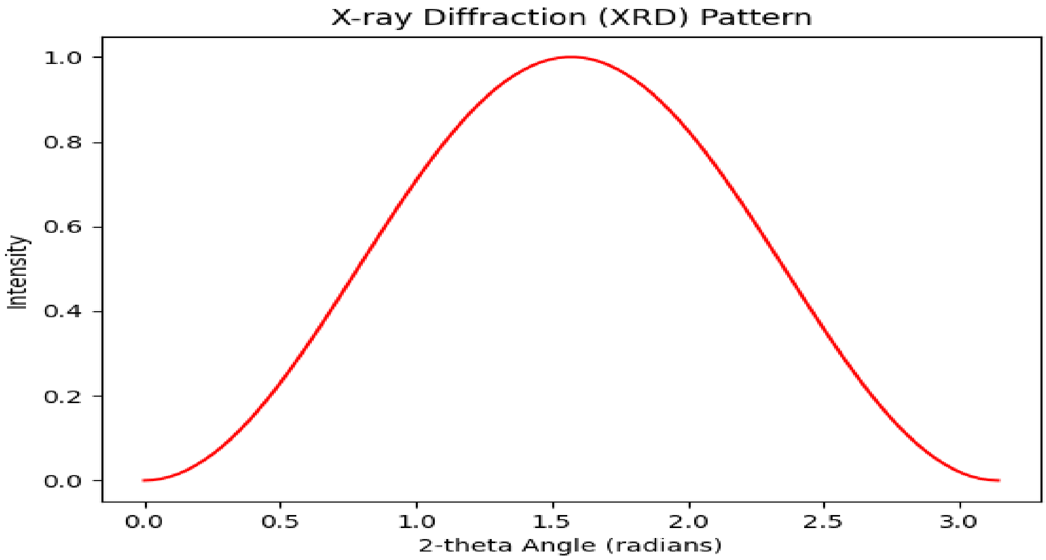
3.5.3. TheFourier-TransformInfrared:

(FTIR) spectrum shows the chemical composition and surface functionalization of produced silvernanoparticles. Peaks associated with functional groups found in biomolecules or capping agents showtheir role in nanoparticle formation and stability. The existence of certain functional groups can shedlightonthemechanismofnanoparticleproductionandthenatureofinteractionsbetweennanoparticlesandstabilizingagents.



3.5.4. TheX-rayDiffraction:

(XRD) pattern offers importantinformation on the crystalline structure and phase purity of theproducedsilvernanoparticles.The XRDpatternhascharacteristicpeaksthatcorrespondtothecrystallographic planesofthe silvernanoparticles.The 2-theta angle at which the peaks appearindicates the nanoparticles' interplanar spacing and crystal lattice structure. The strength of the peaksin the XRD pattern indicates the relative number of crystalline phases in the sample. Higher peakintensities imply more crystallinity and purity, whereas lower intensities may indicate the existence ofamorphousornon-crystallinephases.



3.6. TheAdvantages ofGreenSynthesis:

Sustainability: Green synthesis methods provide a sustainable approach by employing naturalresourceswhileloweringrelianceonharmfulchemicalsandenergy-intensiveprocesses.Biocompatibility:AgNPsmanufacturedutilizinggreentechnologiesarefrequentlybiocompatible and have low cytotoxicity, making them ideal for biomedical applications suchas drug transport, imaging, and treatment.EnvironmentalBenefits:Greensynthesishasalowerenvironmentalfootprintthanconventionalsynthesisprocedures,reducingpollutionandpreservingresources.

3.7. Applications forGreenSynthesizedAgNPs:

Green produced AgNPs have enormous potential in biomedical applications such as antibacterialcoatings,woundhealing,cancertherapy,anddiagnosticimaging.

Catalysis: AgNPs made utilizing green methods have high catalytic activity and selectivity, makingthemusefulcatalystsfororganictransformationsandenvironmentalremediation.

EnvironmentalRemediation: GreenBecauseoftheirlargesurfaceareaandreactivity,greenproducedAgNPscanbeusedtoremovecontaminantsfromtheair,water,andsoil.

3.8. CHALLENGESANDFUTUREOUTLOOKS:

Despite the obvious benefits, green AgNP synthesis confronts several hurdles, including scalability,repeatability,andsynthesisprocessstandardization.Futureresearchshouldconcentrateonover coming these issues and investigating novel green sources and methods for synthesizing AgNPswithtailoredcharacteristicsforspecific uses.

3.9. CONCLUSION:

Green synthesisis a sustainable and eco-friendly method for synthesizing silvernanoparticles without using harmful chemicals or energy-intensive methods. AgNPs manufacturedutilizing green methods show promise in a variety of applications, including medicine, catalysis, andenvironmentalremediation.Furtherstudyanddevelopmentinthissectorare

REFERENCES

1. Rai, M., Yadav, A., & Gade, A. (2009). Silver nanoparticles as a new generation ofantimicrobials.BiotechnologyAdvances,27(1),76-83.

2. Mittal, A. K., Chisti, Y., & Banerjee, U. C. (2013). Synthesis of metallic nanoparticlesusingplantextracts.BiotechnologyAdvances,31(2),346-356.

3. Iravani, S. (2011). Green synthesis of metal nanoparticles using plants. Green Chemistry,13(10),2638-2650.

4. Singh, P., Kim, Y. J., Wang, C., Mathiyalagan, R., Yang, D. C., & Jin, C. G. (2016).Applications of silver nanoparticles in diverse sectors. International Journal of MolecularSciences,17(5),1-21.

5. Durán,N.,&Seabra,A.B.(2012).Metalnanoparticles:Apromisingtreatmentforinfectiousdiseases.NanotechnologyReviews,1(1),1-14.

6. Gopinath,K., Kumaraguru, S.,&Bhakyaraj,K. (2013).Mohanasrinivasan,V.Greensynthesisof silvernanoparticles from leafextractof Aegle marmelos and its antifungalactivity. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 112, 384-387.

7. Mittal, A. K., Tripathy, D., Choudhary, A., Aili, P. K., & Chatterjee, A. (2014). Bio-synthesis of silver nanoparticles using Potentilla fulgens Wall. ex Hook. and its therapeuticevaluation as anticancer and antimicrobial agent. Materials Science and Engineering: C, 44,1-10.

8. Shankar, S. S., Rai, A., Ahmad, A., & Sastry, M. (2004). Rapid synthesis of Au, Ag, andbimetallicAucore–AgshellnanoparticlesusingNeem(Azadirachtaindica)leafbroth.Journalof ColloidandInterfaceScience,275(2),496-502.

9. Philip, D. (2010). Green synthesis of gold and silver nanoparticles using Hibiscus rosasinensis.PhysicaE:Low-dimensionalSystems andNanostructures,42(5),1417-1424.
10. Khan,M.,Khan,M., &Adil,S.F.(2019).Greensynthesisof silvernanoparticlesmediatedbyPulicariaglutinosaextract:Enhancedphotocatalyticactivityandbiocompatibilitystudies.MaterialsResearchBulletin,109,216-223.
11. Singh, D., Rathod, V., Ninganagouda, S., & Hiremath, J. (2015). Biosynthesis of silvernanoparticles using endophytic bacteria Bacillus cereus isolated from Garcinia xanthochymusand their antibacterial activity. Spectrochimica Acta Part A: Molecular and BiomolecularSpectroscopy,136,953-957.
12. Raza, M. A., Kanwal, Z., Rauf, A., Sabri, A. N., & Riaz, S. (2016). Noshahi, Z. Size-andshape-dependent antibacterial studies of silver nanoparticles synthesized by wet chemicalroutes.Nanomaterials,6(4),74.
13. Khandel, P., Shahi, S. K., & Kanwar, L. (2015). Shape and size controllable synthesis ofsilvernanoparticlesbyleafextractofCallistemonviminalis.MaterialsLetters,148,10-13.
14. Venkatesham, M., Ayodhya, D., Madhusudhan, A., Veerabhadram, G., & Apte, S. (2015).Greensynthesis,characterizationandcatalyticactivityofpalladiumnanoparticlesbyXanthiumstrumariumleafextract.BioNanoScience,5(2),89-95.
15. Khan, M. A., & Khan, M. T. (2021). Biogenic synthesis of silver nanoparticles from theextract of Artemisia annua and its anticancer activity. Journal of Nanostructure in Chemistry,11(1),175-183.
16. Singh,J.,Dutta,T.,&Kim,K.H.(2016).Rawat,M.Mishra,V.K.Chitosannanoparticles forcontrolled delivery of the anticancerdrug,5-fluorouracil.CarbohydratePolymers,150,175-182.
17. Huang, X., Jain, P. K., El-Sayed, I. H., & El-Sayed, M. A. (2007). Gold nanoparticles:interestingopticalpropertiesandrecentapplicationsincancerdiagnosticsandtherapy.Nanomedicine,2(5),681-693.

CHAPTER

4

BONDING IN HYDROCARBON

Amit Kumar Patil[a], Chanda Verma[a],Pratibha Gumasta[b],Mithlesh[c]
[a]Department of Chemistry, St.Thomas College, Bhilai, Chhattisgarh
[b]Department of Chemistry, Sai College Sector-6 Bhilai, Chhattisgarh
[c]PCB Plant, Bhilai, Chhattisgarh
Amitpatil17041992@gmail.com

ABSTRACT:

Hydrocarbons represent the simplest form of C-based compounds, consisting of carbon (C) and hydrogen (H) atoms bonded together in single, double, or triple configurations. Classification of hydrocarbons depends on the type of central bond they possess, categorizing them as alkanes (C-C), alkenes (C=C), or alkynes (C≡C). This chapter serves as an introductory overview of hydrocarbon bonding. The largest known database of organic compounds contains approximately 10 million substances, encompassing compounds sourced from both natural and synthetic origins. The potential number of organic compounds is estimated to reach 10^{60}, an extraordinarily vast figure. The abundance of organic molecules arises from carbon's capacity to form up to four robust bonds with other C atoms, yielding diverse chains and rings of various sizes, shapes, and complexities.

4.1. INTRODUCTION:

Basic organic compounds comprise carbon and hydrogen elements exclusively, known as hydrocarbons.[1,2] Despite their elemental simplicity, hydrocarbons exhibit a wide array of structures, including linear chains, branched chains, and carbon rings, or combinations thereof. Moreover, variations in carbon-carbon bond types contribute to the diversity among hydrocarbons. These compounds are ubiquitous in nature, found in plants, animals, fossils, and are also synthetically produced. Commonly used as fuels, hydrocarbons like natural gas, acetylene, and various petroleum derivatives (e.g., gasoline, diesel, heating oil) are integral to daily life. Additionally, many plastics, such as polyethylene and polystyrene, fall within the category of hydrocarbons. Distinct types of hydrocarbons can be identified based on differences in carbon-carbon bonding, leading to variations in molecular geometries and carbon orbital hybridization.

Three-Dimensional Shapes of Molecules:

The arrangement of carbon atoms forming the core structure of an organic molecule determines its three-dimensional shape. This configuration arises from the hybrid orbitals engaged in carbon-carbon bonding. For example, when sp^3 hybridization occurs, a tetrahedral shape emerges, while sp^2 hybridization results in a trigonal-planar configuration, and *sp* hybridization yields linear molecules. The figure depicts methane (sp^3 hybridization), ethene (sp^2 hybridization), and ethyne (*sp*hybridization) molecules, showcasing their respective three-dimensional structures.

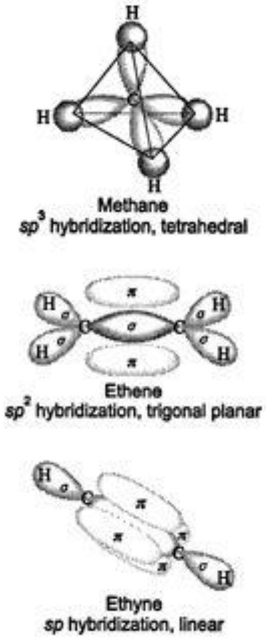


Figure 1

Free Rotation Around Single Bonds:

Single-bonded carbon atoms exhibit unrestricted rotation facilitated by the distribution of electron density along the σ bond, primarily situated between the carbon nuclei. This rotation preserves the electron distribution, ensuring consistent bond strength throughout. Consequently, the molecule can adopt numerous conformations owing to this rotational freedom, with any sketch depicting one of these conformations accurately representing the molecule. Nonetheless, certain conformations may possess slightly elevated energy levels due to repulsion between atoms or groups attached to adjacent carbons as they draw nearer during rotation. The figure illustrates the rotational dynamics around the carbon-carbon bond within the ethane molecule.

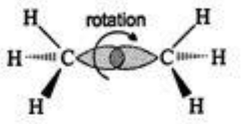


Figure 1

Nonrotation Around Multiple Bonds:

Multiple bonds, such as double and triple bonds, consist of a sigma bond and one or two pie bonds, respectively. The formation of pie bonds involves the mixing of atomic p type orbitals sideways. Any attempt to rotate around the sigma bond in a molecule with multiple bonds results in the disruption of all pie bonds. Figure demonstrates the influence on the C=C bond of ethene if spin is attempted around the sigma bond.

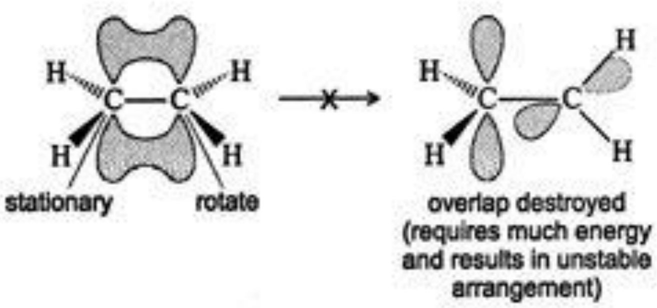
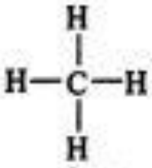


Figure 1

Alkanes: Molecular and Structural Formulas:

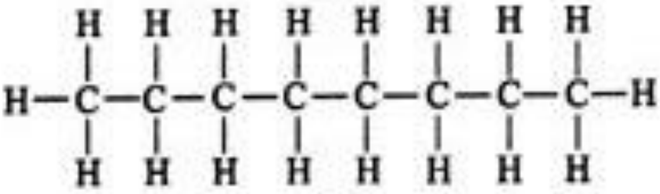
Alkanes form a group of compounds characterized by C and H atoms connected by a covalent typebonds. This series follows the general molecular formula C_nH_{2n+2}, where 'n' stands for any integer.

Methane, the simplest alkane, contains one C atom and a molecular formula of CH_4. Its structural representation is as follows:



methane

In longer alkane molecules, additional carbon atoms are joined by a covalent type bonds. Each C atom is bonded to sufficientH atoms to satisfy four single covalent bonds. Consequently, octane, an alkane with eight C atoms, has a molecular formula of $C_8H_{18}$and a structural representation as follows:



octane

Alkyl Groups:

When an alkane molecule undergoes substitution with a group like a halogen or a hydroxy group, one of its carbon-hydrogen bonds is replaced by a carbon-substituent bond. For example, when methane reacts with chlorine, it forms a new compound known as chloromethane (or methyl chloride), where a chlorine atom is bonded to a CH_3 group.

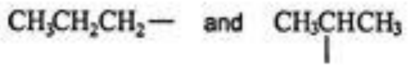
$$\underset{\text{methane}}{CH_4} + \underset{\text{chlorine}}{Cl_2} \xrightarrow{\text{UV light}} \underset{\text{chloromethane}}{CH_3Cl} + \underset{\substack{\text{hydrogen}\\\text{chloride}}}{HCl}$$

An alkane from which a H atom has been eliminated from a bond is termed an alkyl group. Alkyl groups are commonly represented by the symbol R, analogous to how halogens are symbolized by X. The reaction between methane and chlorine can be generalized as follows:

$$R-H + X_2 \xrightarrow{\text{UV light}} R-X + HX$$

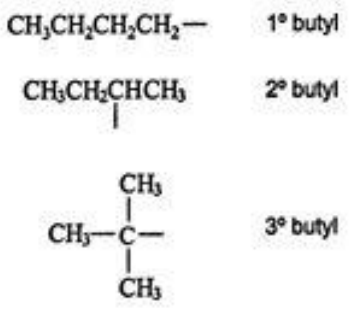
Isomers:

Alkyl groups can take on various isomeric forms. Consider propane, an alkane that exhibits two alkyl isomers, distinguished by which carbon loses a H to form the alkyl group. Carbon atoms are categorized as primary (one alkyl), secondary (two alkyl), or tertiary (three alkyl), based on the number of C atoms they directly bond to. Primary carbons connect to only one other carbon atom, while secondary and tertiary carbons bond to two and three other carbon atoms, respectively.



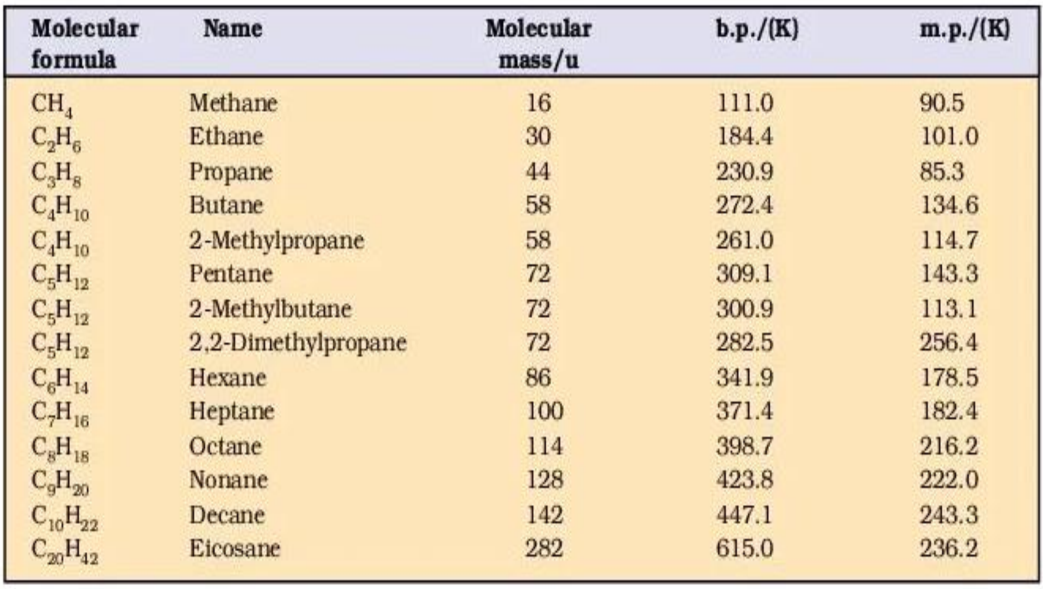
$$CH_3CH_2CH_2- \quad \text{and} \quad CH_3\underset{|}{C}HCH_3$$

In the provided diagram of propane isomers, the left group represents a primary (1°) propyl group, while the right group illustrates a secondary (2°) propyl group. Butanes (alkanes with four carbons) demonstrate three isomeric groups, discernible by their structures and names.



$$\begin{array}{ll} CH_3CH_2CH_2CH_2- & \text{1° butyl} \\ CH_3CH_2\underset{|}{C}HCH_3 & \text{2° butyl} \\ CH_3-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}- & \text{3° butyl} \end{array}$$

Melting and Boiling point of Alkane-

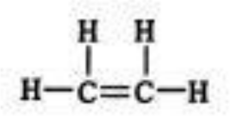


Molecular formula	Name	Molecular mass/u	b.p./(K)	m.p./(K)
CH_4	Methane	16	111.0	90.5
C_2H_6	Ethane	30	184.4	101.0
C_3H_8	Propane	44	230.9	85.3
C_4H_{10}	Butane	58	272.4	134.6
C_4H_{10}	2-Methylpropane	58	261.0	114.7
C_5H_{12}	Pentane	72	309.1	143.3
C_5H_{12}	2-Methylbutane	72	300.9	113.1
C_5H_{12}	2,2-Dimethylpropane	72	282.5	256.4
C_6H_{14}	Hexane	86	341.9	178.5
C_7H_{16}	Heptane	100	371.4	182.4
C_8H_{18}	Octane	114	398.7	216.2
C_9H_{20}	Nonane	128	423.8	222.0
$C_{10}H_{22}$	Decane	142	447.1	243.3
$C_{20}H_{42}$	Eicosane	282	615.0	236.2

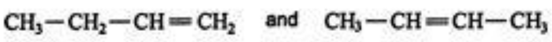
Alkenes: Molecular and Structural Formulas:

Alkenes encompass a group of chemical composites characterized by C and H atoms, featuring at least one C=C bond within the C chain. This compound series adheres to a homologous pattern with a general molecular formula of C_nH_{2n}, where 'n' represents any integer greater than one.

Ethene, the generalised form of alkene, comprises two C atoms and a molecular formula of C2H4. Its structural depiction is as follows:



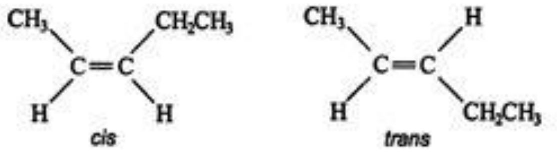
In lengthier alkene chains, additional C atoms bond together via single covalent type bonds, with each C atom also bonding to sufficient H atoms to achieve a total of 4 single covalent type bonds. In chains containing 4 or >4C atoms, the positioning of the = bond may vary, leading to the formation of structural isomerisation. For instance, the alkene with the molecular formula C_4H_8 has 2 isomers.



$CH_3-CH_2-CH=CH_2$ and $CH_3-CH=CH-CH_3$

Stereoisomers:

Alkenes not only exhibit structural isomerism but also generate stereoisomers due to restricted rotation around the double bond. This rigidity maintains fixed orientations of assembliesinvolved to the = bondedC atoms, enabling chemists to distinguish between isomers based on substituent arrangements. For instance, in one structural isomer of C5H10, we encounter cis and trans stereoisomers: the cis isomer with methyl and ethyl assemblies on the similar side of the double bond, and the trans isomer with substituents on opposite sides



However, when >2 substituents are involved to the double-bonded C atoms, the cis-trans designation becomes inadequate. Instead, the *E-Z* notation is utilized. In this system, the compound is divided vertically through the = bond, and the atoms or groups on each C atom are ordered by atomic mass. The positions of the higher-ranked atoms determine whether the arrangement is Z (from German zusammen, meaning "together") for cis position or E (from German entgegen, meaning "opposite") for trans position. For example, in the given compound, chlorine ranks higher than C on the left side, while bromine outranks C on the right side.

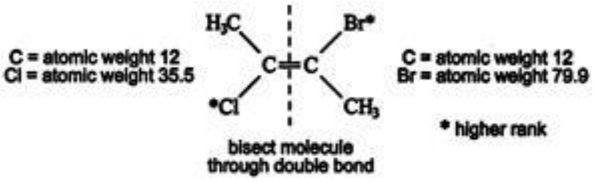


Figure 1

Alkynes: Molecular and Structural Formulas

Alkynes constitute a group of C- and hydrogen-based compounds distinguished by the presence of at least one triple bond. This category follows a homologous pattern with the general molecular formula C_nH_{2n--2}, where 'n' can vary and is greater than one.

The simplest alkyne, ethyne (or acetylene), comprises two C atoms with the molecular formula C_2H_2, represented structurally as C≡C.

$$H-C\equiv C-H$$

In longer alkyne chains, extraC atoms bond together via C-C covalent type bonds, with each C also bonding to enoughH atoms to complete four C-C covalent bonds. Alkynes with 4 or >4C atoms can exhibit varying positions of the triple bond along the chain, leading to the formation of structural isomers. For instance, a C4H6 alkyne displays two isomeric forms.

$$HC\equiv C-CH_2CH_3 \quad \text{and} \quad CH_3-C\equiv C-CH_3$$

Despite restricted revolution due to the≡ bond, alkynes do not generate stereoisomers like alkenes. This is because of the sp hybridization of the C-C triple bond, resulting in a linear molecular geometry. Consequently, substituents attached to triple-bonded C's align in a straight line, precluding the formation of stereoisomers.

Sigma (σ) bond

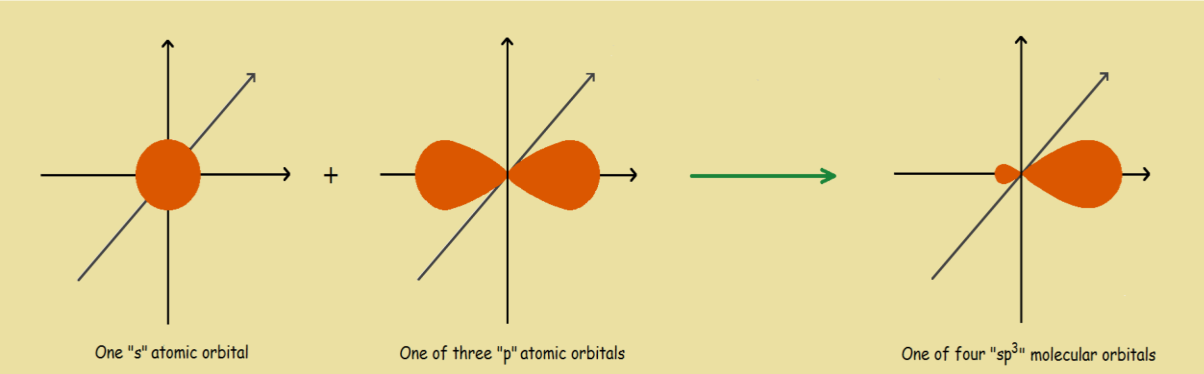
Let's consider a very simple example. Say we want to form one C-H bond of the molecule methane (CH_4). Now hydrogen atoms only have one electron. The single electron lies in the $1s^2$ orbital. That type of orbital possesses spherical symmetry.

Unlike hydrogen, carbon has 12 electrons total. Its electron layout is

$1s^22s^22p^2$

The number represents electron shells. The first shell can only hold two electrons, so it is filled. Those two electrons will not participate in the formation of a molecular bond. The second shell consists of two subshells, s and p.

The 2s subshell is filled, but the shell is not filled, since the 2p subshell can hold 6 electrons in 3 orbitals. These are called the $2p_x$, $2p_y$, and $2p_z$ orbitals.



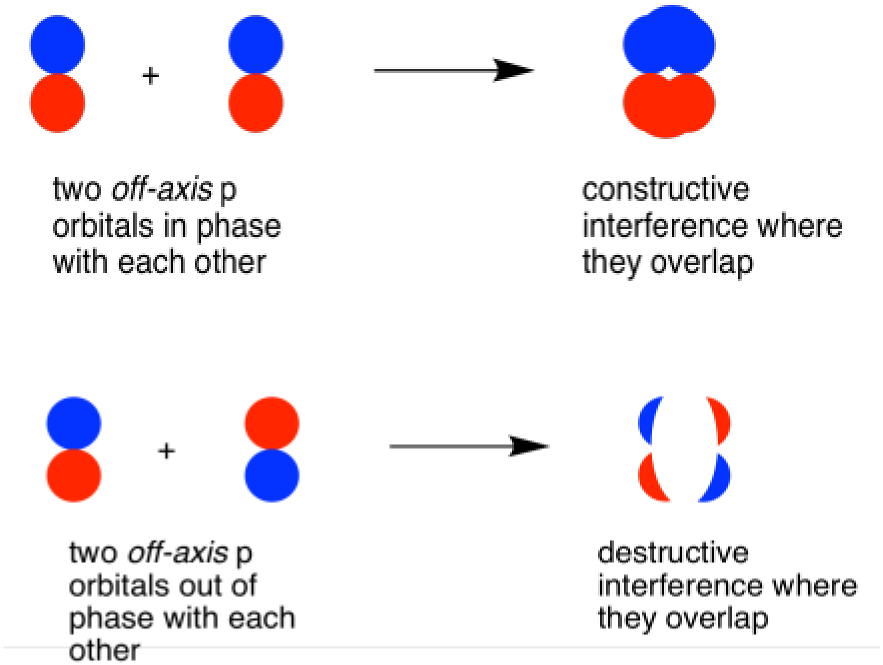
Formation of a C-H sigma bond orbital

Energy is the controlling factor. Carbon ordinarily exhibits a valence of 4. So 4 *atomic* orbitals can be utilized to form 4 *molecular* orbitals. However, all 4 bonds are equivalent. So the one 2s and the three 2p orbitals yield their electrons to produce [at some point] 4 sp^3 molecular orbitals.

Our hydrogen atom contributed an electron in its 1s orbital to the overlap process with one of the carbon sp^3 orbitals, to yield a C-H single bond. This head-to-head bond is classified a sigma (σ) bond.

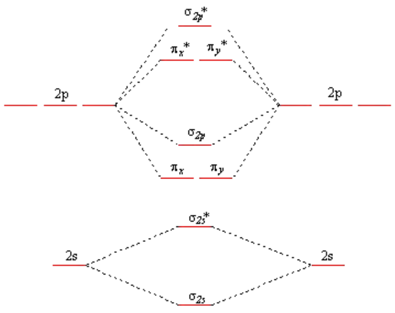
Pi Bond:

In molecular chemistry, pi (π) bonds play a fundamental role in determining molecular structure and reactivity. These bonds form when parallel p orbitals interact with each other, approaching side by side above and below the bond axis between two atoms. While not as strong as sigma (σ) bonds, pi bonds can overlap to produce both bonding and antibonding combinations. In a bonding combination, e density is concentrated above and below the bond axis, resulting in the construction of a pi (π) bond. Conversely, an antibonding combination creates nodes along the bond axis, representing an energetically unfavorable state denoted as π*. The interplay between these orbitals gives rise to characteristic properties of pi bonds, including the presence of nodes along the bond axis.



4.2. Molecular Orbital Theory:

Molecular Orbital Theory (MOT) provides a theoretical outline for considerate the electronic structure of molecules. It asserts that the electrons of an atom, associated with multiple nuclei, are present in multiple atomic orbitals. Derived from quantum mechanical equations, MOT predicts the probable locations of electrons within atoms or molecules. According to MOT, atoms combine to create molecular orbitals, and electrons reside in different atomic orbitals associated with distinct nuclei. This implies that electrons within a molecule can be located anywhere within these molecular orbitals. MOT aids in understanding how electrons exist within a molecule, with the filling of molecular orbitals following the increasing order of orbital energy. Overall, MOT offers valuable insights into molecular electronic structure and behavior, guiding our understanding of chemical bonding and reactivity.

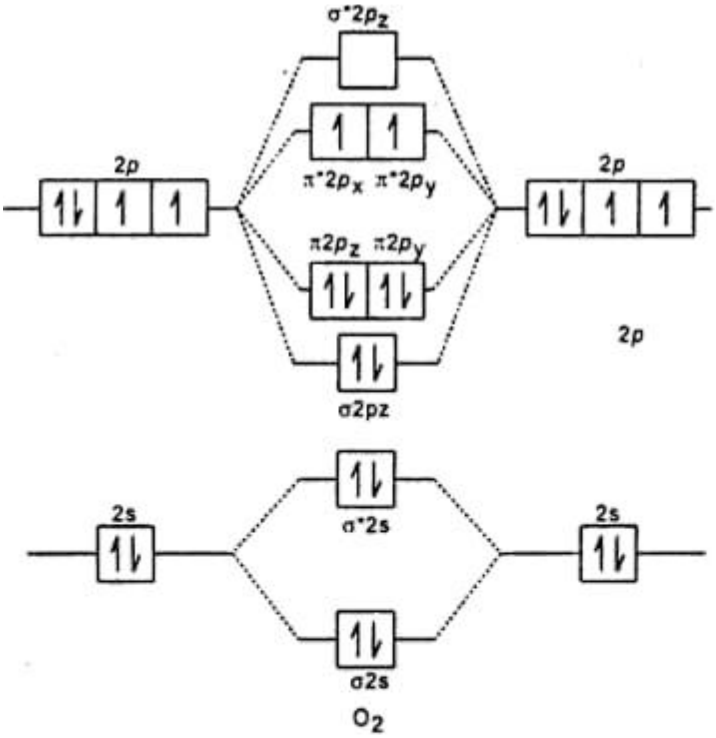


Molecular Orbitals of the Second Energy Level:

The molecular orbital diagram of O_2offers valuable insights into its electronic structure and properties. Oxygen, with an electron configuration of $1s^2 2s^2 2p^4$, contributes a total of 12 valence electrons in O_2 (6 from each O atom). The diagram reveals the presence of two electrons in antibonding orbitals, as dictated by Hund's Rule, where each electron occupies a separate π* orbital to minimize e-e repulsion.

The bond energy of O_2 is significantly lower at 498 kJ/mole compared to the 945 kJ bond energy of N2. This disparity arises from oxygen having two electrons in antibonding orbitals, while nitrogen has only one. Dioxygen (O_2) displays paramagnetism due to the presence of two unpaired electrons in its molecular orbitals, evidenced by liquid O_2 being attracted to the poles of a strong permanent magnet.

The removal of an electron to form O_2+ increases the ratio of bonding to antibonding electrons, resulting in a more stable molecule. Conversely, adding an electron to O_2 weakens the bond, as evidenced by the lower bond energy of O_2–. These dioxygen ions are highly reactive and observed only in the gas phase. The observed stability changes in O_2+, O_2, and O_2– align with the expectations from the molecular orbital model, affirming its accuracy in predicting bond energies and stability.



Molecular Diagram of O_2

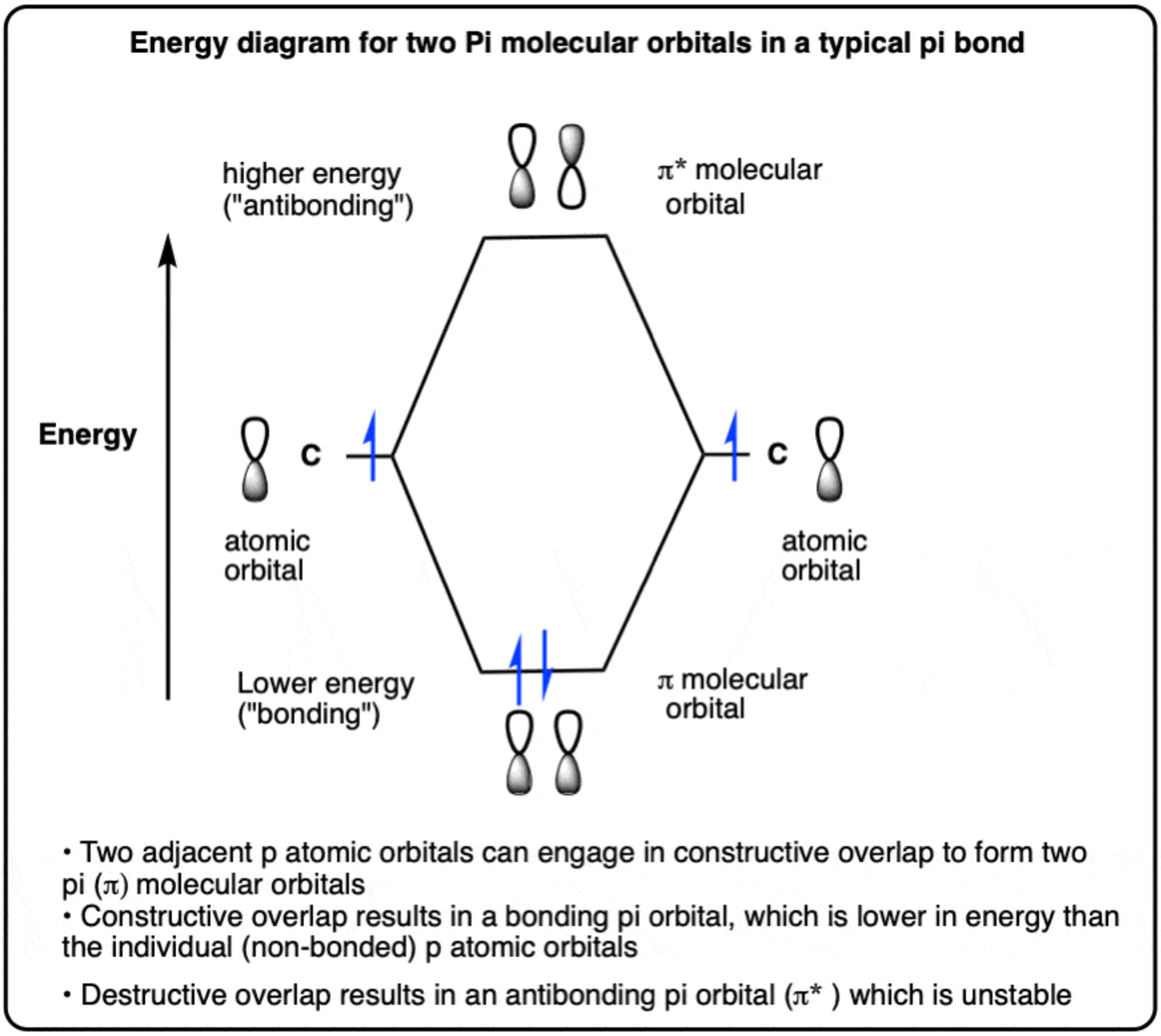
Bond Order:

Bond order, representing the number of bonds between two atoms, is a crucial aspect of molecular structure. Lewis structures, integral to the valence-bond model, aid in calculating bond orders. For example, oxygen has a bond order of two. Paired electrons exhibit diamagnetism, being repelled by magnets, while unpaired electrons demonstrate paramagnetism, being attracted to magnets.

Bond Order = Bonding electrons−Antibonding electrons/2

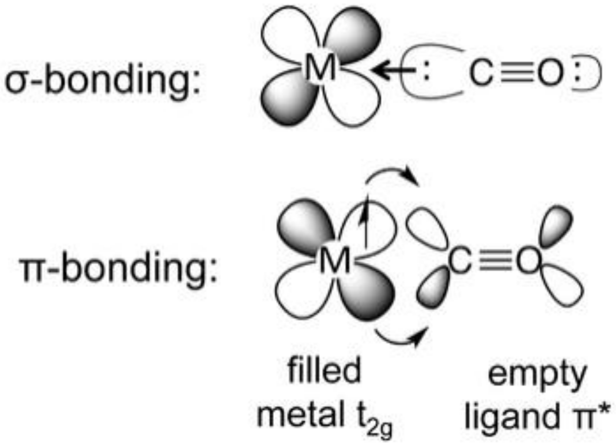
Bonding and Antibonding Orbitals for A Simple Pi Bond:

When a π (pi) bond forms, two adjacent p-orbitals, each containing an electron, overlap to generate two molecular orbitals known as pi-orbitals. Constructive orbital overlap occurs when two p-orbitals with the same phase align, facilitating electron sharing between the atoms. This bonding process leads to a reduction in energy. Conversely, overlap between two p-orbitals with opposite phases results in destructive orbital overlap, hindering electron sharing and creating an energetically unstable antibonding situation (π*).


Energy diagram for two Pi molecular orbitals in a typical pi bond

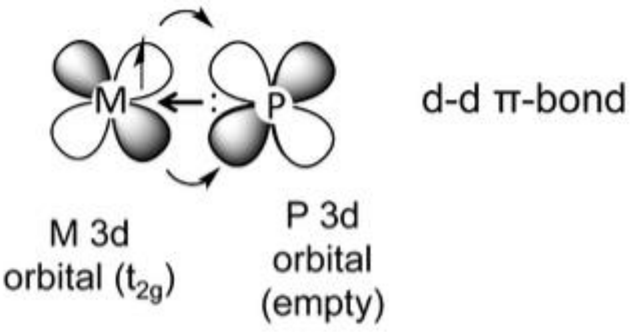
- Two adjacent p atomic orbitals can engage in constructive overlap to form two pi (π) molecular orbitals
- Constructive overlap results in a bonding pi orbital, which is lower in energy than the individual (non-bonded) p atomic orbitals
- Destructive overlap results in an antibonding pi orbital (π*) which is unstable

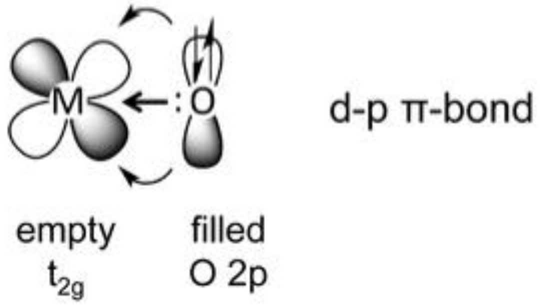
In a simple pi-bond involving two electrons, the bonding pi-orbital (π) represents the highest-occupied molecular orbital (HOMO), while the antibonding orbital serves as the lowest-unoccupied molecular orbital (LUMO).



π-Bonding between Metals and Ligands:

The strength of ligand fields in molecules like C monoxide (CO), cyanide (CN-), and phosphines within coordination complexes is significantly influenced by the presence of π-bonding between the metal and the ligand. There are three main types of π-bonding interactions observed in metal complexes:





Firstly, back-bonding occurs when ligands such as CO or CN donate their sigma (nonbonding) electrons to the metal while simultaneously accepting electron density from the metal. This exchange happens through the overlap of a metal t2g orbital and a ligand π* orbital, leading to the weakening of the C-O bond. Consequently, bond lengthening and a decrease in the C-O infrared stretching frequency are observed.

Secondly, d-d π bonding takes place when an element like P, equipped with a σ-symmetry Lp and anvacant metal 3d orbital, binds to a metal with e in a t2g orbital. In complexes involving phosphines and low-valent, late transition metals, backbonding occurs akin to the CO example. However, in this case, the acceptor orbital is a phosphorus 3d orbital instead of a ligand π* orbital, forming a dπ-dπ bond.

Lastly, pie giver ligands contribute to M-L π-bonds when a ligand with both a σ-symmetry e pair and a filled orthogonal p-orbital interacts with a metal. This type of interaction is commonly observed in early transition elements. For example, in the vanadyl cation [VO]2+, the O2- ligand acts as both a σ- and π donor, forming metal-ligand multiple bonds.

4.3. CONCLUSION:

The diverse types of C-C bonds present in hydroCs enable the vast array of organic molecules observed in nature. C's ability to form up to four strong bonds with other C atoms allows for the formation of chains and rings of various sizes, shapes, and complexities. Understanding the different types of bonds formed by hydrocarbons is crucial for comprehending their structures and properties in organic chemistry.

REFERENCES

1. Meierhenrich, Uwe (2008). Amino Acids and the Asymmetry of Life: Caught in the Act of Formation. Berlin: Springer. ISBN 978-3-540-76886-9. OCLC 288470227.

2. Barnes, I. "TROPOSPHERIC CHEMISTRY AND COMPOSITION (Aromatic Hydrocarbons)". Retrieved 26 October 2020.

3. "Benzene global market volume 2015-2026". Statista. Retrieved 5 December 2021.

4. McMurry, J. (2000). Organic Chemistry 5th ed. Brooks/Cole: Thomson Learning. ISBN 0-495-11837-0. pp. 75–81.

5. Kai Exner and, Paul von Ragué Schleyer. Theoretical Bond Energies: A Critical Evaluation. The Journal of Physical Chemistry A 2001, 105 (13), 3407-3416. https://doi.org/10.1021/jp004193o

6. Xiaoyan Li, Lingpeng Meng, Zheng Sun, Shijun Zheng. Computational study on the reactions of XO (X=F, Cl and Br) with CH3SO and CH3SO2. Journal of Molecular Structure: THEOCHEM 2008, 870 (1-3) , 53-60

7. Shaik S, Danovich D, Wu W, Su P, Rzepa HS, Hiberty PC. Quadruple bonding in C2 and analogous eight-valence electron species. *Nature Chem*, 2012, 4(3): 195–200

8. Shaik S, Rzepa HS, Hoffmann R. One molecule, two atoms, three views, four bonds? *Angew Chem Int Ed*, 2013, 52(10): 3020–3033

9. Su P, Wu J, Gu J, Wu W, Shaik S, Hiberty PC. Bonding conundrums in the C_2 molecule: A valence bond study. *J Chem Theory Comp*, 2010, 7(1): 121–130

10. Matxain JM, Ruipérez F, Infante I, Lopez X, Ugalde JM, Merino G, Piris M. Communication: Chemical bonding in carbon dimer isovalent series from the natural orbital functional theory perspective. *J Chem Phys*, 2013, 138: 151102

11. Grunenberg J. Quantum chemistry: Quadruply bonded carbon. *Nature Chem*, 2012, 4(3): 154–155

12. Danovich D, Shaik S, Rzepa HS, Hoffmann R. A response to the critical comments on "One molecule, two atoms, three views, four bonds?". *Angew Chem Int Ed*, 2013, 52(23): 5926–5928

13. Shaik SS, Hiberty PC. *A Chemist's Guide to Valence Bond Theory*. Wiley-Interscience, 2007

14. Wu W, Gu J, Song J, Shaik S, Hiberty PC. The inverted bond in [1.1.1] propellane is a charge — shift bond. *Angew Chem Int Ed*, 2009, 121(8): 1435–1438

15. Hu H-S, Qiu Y-H, Xiong X-G, Schwarz WHE, Li J. On the maximum bond multiplicity of carbon: Unusual C≡U quadruple bonding in molecular CUO. *Chem Sci*, 2012, 3(9): 2786–2796

16. Gary JB, Buda C, Johnson MJ, Dunietz BD. Accessing metal-carbide chemistry. A computational analysis of thermodynamic considerations. *Organometallics*, 2008, 27(5): 814–826

17. Krapp A, Frenking G. Carbon complexes as electronically and sterically tunable analogues of carbon monoxide in coordination chemistry. *J Am Chem Soc*, 2008, 130(49): 16646–16658

18. Parameswaran P, Frenking G. Transition-metal complexes $[(PMe_3)_2Cl_2M(E)]$ and $[(PMe_3)_2(CO)_2M(E)]$ with naked group 14 atoms (E= C-Sn) as ligands; Part 2: Complexation with $W(CO)_5$. *Chem Eur J*, 2009, 15(35): 8817–8824

CHAPTER

5

AEROGEL: SYNTHESIS METHODS AND THEIR APPLICATIONS

Mukund Kaushal Sinha
Siddhachalam laboratory, Umiya market, Ring Road-2, Raipur, Chhattisgarh, India
27mukund12kushal@gmail.com

ABSTRACT:

The amazing characteristics and wide range of uses of silica aerogels have led to their increasing importance and interest. Silica aerogels have a very low density and heat conductivity, a large surface area, and are very porous. Typically, the sol-gel method is used to manufacture and synthesize them. This process entails creating a sol that contains a precursor, a solvent, and a catalyst. Many parameters, including the ratio of precursor to solvent and the drying process used, affect the qualities of the finished product. Silica aerogels have found several commercial uses and are being researched for their usefulness in multiple disciplines, such as biomedical and aeronautical engineering.

Silica aerogels have outstanding qualities, but they also have limitations including brittleness and low mechanical strength. These can be overcome by creating composites, thereby enhancing the material's potential uses. This reviews the production of silica aerogels using the sol-gel process and the potential applications of this unique material. Additionally highlighted are the many materials that are utilized to create composites that enhance and improve the chemical and physical characteristics of silica aerogels.

Considering aerogel materials have so many remarkable qualities, a remarkable array of uses has emerged for them. Several commercial uses for aerogels have been made public, including supercapacitors, heat-storage insulation for cars, electrodes for capacitive the ionization, catalysts, insulation for aerospace and aviation, devices thermal management, solar panels, and more. A growing number of applications are being developed in the fields of science, medication delivery, and the environment, including air pollution management, water purification, and carbon capture and storage (CCS). The community learns about the extraordinary and unique physical characteristics of aerogels. Apart from the expanding industrial uses, aerogels have scientific and technical applications as well. This paper discusses a variety of technical applications of aerogels.

Keywords: Aerogel, Sol-gel method, application,chemical and physical properties.

5.1. INTRODUCTION:

A type of artificial porous fluids known as aerogels are generated when a gel's liquid component is swapped out for a gas without causing the gel structure to completely collapse (Larisa & Croitoru, 2019). A solid with extremely low density and low thermal conductivity is the end product. Aerogels can be made from a wide range of chemical ingredients. Certain polymer-based aerogels have the impact of stiff foams, whereas silica aerogels are more akin to delicate Styrofoam (Zuo et al., 2015).

Aerogels are made by freeze-drying or supercritically drying a gel to remove its liquid component. As opposed to conventional evaporation, which would lead to the solid matrix in the gel to collapse from capillary action, this enables the liquid to be gradually dried out (Guastaferro et al., 2021). Silica gels were used for the first aerogels. The following studies by Kistler included aerogels made of tin dioxide, chromia, and alumina. The late 1980s saw the discovery of carbon aerogels for the first time (Wakeel et al., 2023)

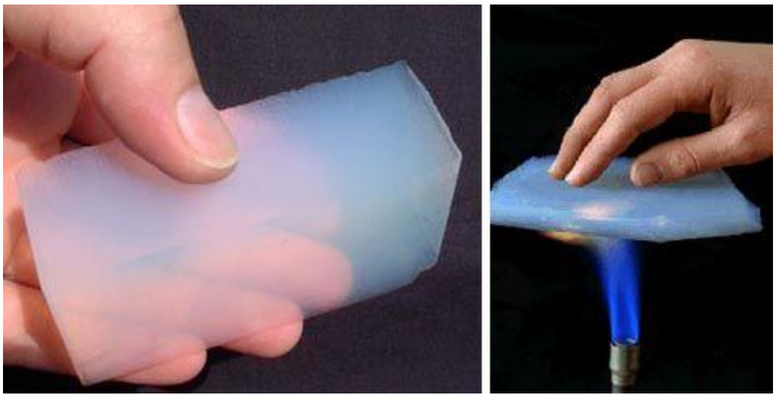


Figure: ***1 Aerogel***

5.1.1. Classification:

Aerogels can be separated into groups based on their composition, synthesis method, and intended usage. This breakdown makes sense of the multitude of aerogel types accessible for various requirements and applications (Koçyiğit, 2023). Researchers may tailor their studies and applications to meet numerous goals thanks to this classification of aerogels, which leads to more effective and focused research and development outcomes for aerogels (Shi et al., 2021).

5.1.2. Composition:

5.2.1.1 Silica Aerogels:

These aerogels, which consist primarily of silica (silicon dioxide), are the most utilized kind. The low density, high porosity, and superior thermal insulating abilities of silica aerogels are well known (Bheekhun et al., 2013).

5.2.1.2 Carbon Aerogels:

Carbon-based chemicals, typically generated from organic precursors like formaldehyde and resorcinol, make up these aerogels. High surface area carbon aerogels are utilized in catalysis and energy storage, among other applications (Li et al., 2002).

5.2.1.3 Metal Oxide Aerogels:

Other metal oxides, including alumina (aluminum oxide), titania (titanium dioxide), and zirconia (zirconium dioxide), may also be utilized to create aerogels. These aerogels often possess unique characteristics that make it useful in tasks like environmental remediation and catalysis (Y. Wu et al., 2022).

Table: 1 Metal oxide Aerogels and their color

Aerogel	Color
Silica, alumina, titania, zirconia	Clear with Rayleigh scattering blue or white
Iron oxide	Rust red or yellow, opaque
Chromia	Deep green or deep blue, opaque
Vanadia	Olive green, opaque
Neodymium oxide	Purple, transparent
Samaria	Yellow, transparent
Holmia, erbia	Pink, transparent

5.2.1.4.Polymer Aerogels:

Compared with standard silica aerogels, polymer-based aerogels have advantages involving flexibility and toughness as they are made of organic polymers. Polyimide and polyurea aerogels are two examples (Leventis & Lu, 2011).

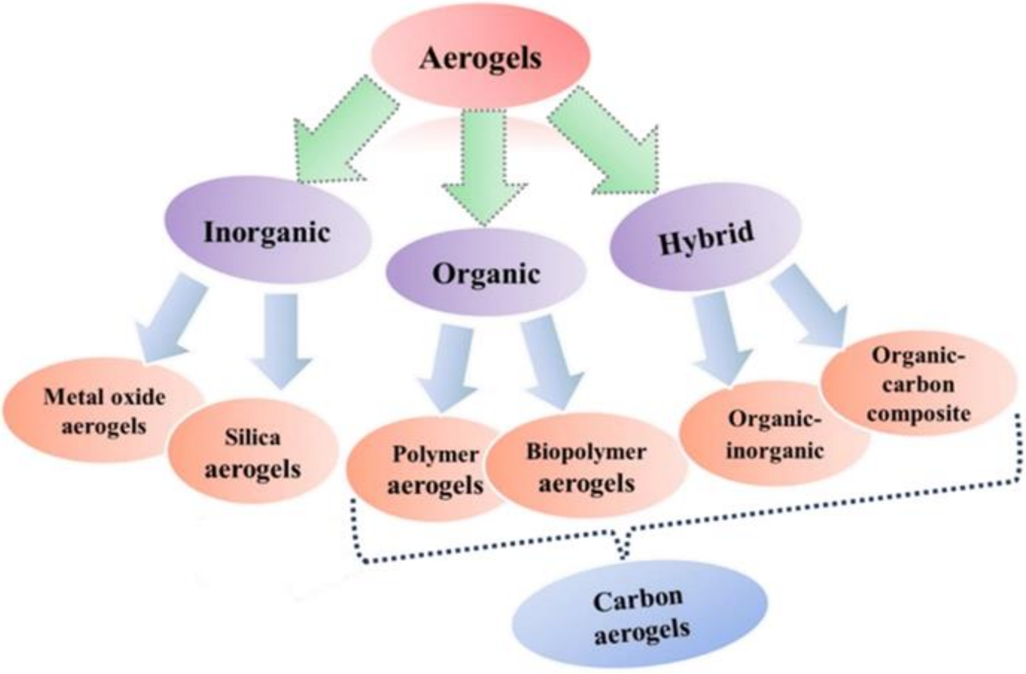


Figure: 2. Classification of aerogels based on precursor composition

5.1.3. Synthesis:

A range of methods specific to the kind of aerogel being created—silica, carbon, or polymer-based aerogels, for example—are used in the synthesis of aerogels. These are a few basic synthesis techniques:

5.1.3.1.Sol-Gel Process:

This method is often used to create silica aerogels. Tetraethyl orthosilicate (TEOS) and other silicon alkoxides are hydrolyzed and then collected in the presence of a solvent and a catalyst. After the precursor solution is worked to create a wet gel, the aerogel is created via supercritical drying and solvent exchange (Esposito, 2019).

5.1.3.2.Supercritical Drying:

For silica aerogels in particular, supercritical drying is an essential stage in the aerogel synthesis method. Using this technique, the solvent's (usually carbon dioxide) supercritical point can be attained by adjusting the chamber's pressure and temperature while the wet gel is inside (Basak & Singhal, 2023). In such situations, the solvent undergoes a straight transition from a liquid to a gas phase, retaining the structure of the porous gel and averting collapse (Ślosarczyk et al., 2013).

5.1.3.3.Carbonization:

Precursor substances that include carbon, like polyacrylonitrile or resorcinol-formaldehyde, are frequently utilized to create carbon aerogels. Following the gelation procedure, the wet gel is dried and then heated to high temperatures in an inert atmosphere to undergo carbonization. Through the process of pyrolysis, non-carbon elements disappear and leave behind a large surface area carbonaceous network (Wang et al., 2001).

5.1.3.4.Polymerization:

Polymerization methods are frequently utilized in the synthesis of organic aerogels, such as those based on resorcinol-formaldehyde or melamine-formaldehyde. They involve the mixture of monomers with the aid of a catalyst to create a three-dimensional network. To create the aerogel, the resultant gel is subsequently dried using either freeze-drying or supercritical drying (D. Wu et al., 2004).

5.1.3.5.Emulsion Templating:

This method, precursor sections are emulsified in a solvent, then gelation and drying are performed. By acting as templates, the emulsion droplets give the final aerogel a particular form (Zhang et al., 2019).

5.1.3.6.Freeze Drying:

While less frequently employed in the creation of aerogels, freeze drying entails freezing the wet gel and subsequently sublimating the ice in a vacuum. For some types of aerogels, especially those that are prone to supercritical drying conditions, this technique can be applied (Baudron et al., 2019).

The pore size, surface area, and mechanical strength of the aerogel can all be varied and mixed using these methods to customize it for a certain need. The chosen synthesis technique is determined by a number of settings, including the desired aerogel qualities, the kind of precursor material to be utilized, and the equipment and knowledge that are available.

5.1.4. Application:

5.1.4.1 Explain to thermal applications of Aerogel:

Aerogel famous remarkable thermal characteristics, aerogels are useful materials for a range of thermal applications. This is a summary of the thermal applications of aerogels:

5.1.4.2. Insulation:

Their very low heat conductivity, aerogels are very effective insulators (Melițã& Croitoru, 2019). In order to reduce heat loss and increase energy efficiency, they are used in pipelines, industrial equipment, buildings, and appliances (Melițã& Croitoru, 2019). In commercial, industrial, and residential contexts, aerogel-based insulation lowers heating and cooling costs by assisting in preserving of consistent temperatures (Cuce et al., 2014).

5.1.4.3. Cryogenics:

Aerogels offer better insulation than traditional materials in cryogenic applications when extremely low temperatures are needed (Fesmire, 2019). According to Kumar et al. (2011), they are utilized in cryogenic storage tanks, pipelines, and transportation containers for liquefied gases such as liquid nitrogen and LNG (liquefied natural gas). In order to prevent temperature, rise and preserve the integrity of cryogenic systems, aerogel insulation assists in minimizing heat ingress (Fesmire, 2016).

5.1.4.4. Aerospace and Aviation:

Aerogel exceptional thermal insulation qualities and lightweight design, aerogels are widely used in aerospace and aviation applications (Randall et al., 2011). To guard against the severe variations in temperature seen during flight, they are used in rocket, spaceship, satellite, and airplane components (Uyanna& Najafi, 2020). In aircraft systems, aerogel insulation enhances overall thermal management, reduces thermal stress, and lowers interior temperatures (Liu et al., 2021).

5.1.4.5. Electronics Thermal Management:

Aerogels serve as crucial for thermal management in electronics and electrical equipment (Hu et al., 2023). To disperse heat produced by electronic components, they are integrated into heat sinks, electronic enclosures, and thermal interface materials. Thermal solutions based on aerogels help keep gadgets working at ideal temperatures, avoid overheating, and improve their lifespan (Johnson, 2023).

5.1.4.6. Solar Energy Systems:

In solar energy systems, aerogels are used for heat storage and thermal insulation. To reduce heat loss and improve thermal efficiency, they are utilized in solar water heaters, thermal energy storage tanks, and collectors. According to Larisa and Croitoru (2019), using of aerogel insulation increases the performance and sustainability of solar energy systems by maximizing the capture and retention of solar heat.

5.1.4.7. High-Temperature Applications:

Some aerogel formulations are suited for usage in high-temperature instances because they have good thermal stability and can endure high temperatures. They are used in industrial operations as thermal barriers, fire prevention materials, and furnace insulation (Jin et al., 2023). In challenging high-temperature applications, aerogel-based technologies provide dependable thermal insulation and protection against heat-related damage (Khan et al., 2024).
All things looked at, aerogels are essential for a variety of thermal applications since they offer strong, long-lasting, and extremely effective insulation solutions. Their remarkable thermal characteristics enable greater sustainability, better thermal management, and increased energy efficiency across industries (Khan et al., 2024).

5.2 Explain to medicinal field applications of Aerogel

5.2.1 Drug Delivery Systems:

Aerogels' large surface area, porous structure, and biocompatibility make them ideal for use as drug delivery vehicles. The aerogel matrix can be used to encapsulate drugs, enabling a gradual and controlled release. This makes it possible to distribute medicinal molecules particularly, which minimizes adverse effects and increases treatment effectiveness. Applications including cancer treatment, wound healing, and tissue regeneration have been studied using aerogel-based drug delivery devices (Bakhori et al., 2023).

5.2.2 Wound Dressings:

Aerogels are used as advanced wound dressings for traumas, burns, and chronic wounds. Their high porosity and capacity to take in exudate contribute to the production of a moist, healing-promoting wound environment. Aerogels can also be functionalized with antibacterial substances to help heal wounds and encourage tissue regrowth. In juxtaposition with traditional dressings, aerogel-based wound dressings provide improved breathability, flexibility, and biocompatibility (Guo et al., n.d.).

5.2.3 Tissue Engineering Scaffolds:

Aerogel’s applications in tissue engineering and regenerative medicine, aerogels make a great scaffold material. Their porous shape offers an ideal setting for cell development and tissue regeneration by resembling the extracellular matrix of natural tissues. Aerogel scaffolds promote cell adhesion, proliferation, and differentiation by matching the mechanical characteristics and porosity of target tissues. Applications include organ transplantation, cartilage healing, and bone regeneration has all been studied (Yahya et al., 2021).

5.2.4 Diagnostic Imaging Contrast Agents:

Aerogel usage in diagnostic imaging procedures like computed tomography (CT) scans and magnetic resonance imaging (MRI), aerogels can be functionalized with contrast agents. Improved imaging contrast can be gained by adding contrast agents into the aerogel matrix, which improves the view of disease states and anatomical structures. When compared to traditional contrast agents, aerogel-based contrast agents provide higher biocompatibility and lower toxicity (Lai et al., 2024).

5.2.5 Hemostatic Agents:

Applications of aerogels in carbon capture and storage (CCS) technologies are being researched with the goal of lowering greenhouse gas emissions from power plants and industrial operations. Carbon dioxide (CO2) can be selectively captured from flue gas streams using functionalized aerogels, which makes it easier to separate and sequester the gas. High CO2 capture capacity, quick adsorption kinetics, and regeneration capabilities are some benefits of aerogel-based adsorbents (Ayeleru et al., 2023).

5.2.6 Environmental Remediation:

To clean up contaminated sites and restore ecosystems, aerogels are used in environmental remediation projects. Pollutants from soil, water, and sediments, including pesticides, heavy metals, and persistent organic pollutants (POPs), can be absorbed or broken down by functionalized aerogels. Advantages of aerogel-based remediation systems include cost-effective clean-up options, less environmental impact, and targeted pollutant removal (Dehghani et al., 2024).

5.2.7 Drug Delivery Systems:

Aerogels' large surface area, porosity, and capacity to encapsulate medications make them useful drug delivery vehicles. Their regulated release profiles facilitate the distribution of pharmacological substances in a targeted or sustained manner. Therapeutic results and patient compliance can be improved by customizing aerogel-based drug delivery systems to increase the solubility, stability, and bioavailability of medications (Abdul Khalil et al., 2023).

5.2.8 Drug Delivery Through Transdermal:

Drugs can penetrate the skin more easily with the use of aerogels in transdermal drug delivery systems. Because of their biocompatibility and porous nature, medications can be delivered across the skin barrier more effectively while causing less irritation and allergic reactions. Transdermal gels or patches based on aerogel have benefits include longer release kinetics, better patient comfort, and increased medication absorption(Xie et al., 2022).

5.2.9 Oral Drug Delivery:

Aerogels can be used in oral drug delivery formulations to improve the bioavailability, absorption, and dissolution of medications that are not highly water soluble. Drugs can have their release regulated to produce controlled or sustained release profiles by encasing them in the aerogel matrix. Improved medication stability, taste masking, and gastrointestinal compatibility are provided by aerogel-based oral dosage forms, including tablets, capsules, and solutions (García-González et al., 2021).

5.2.10 Formulations for Topical Drugs:

Topical medication formulations for the treatment of wounds, skin diseases, and dermatological problems use aerogels. In order to maximize localized therapeutic effects and reduce systemic exposure, they offer an appropriate means of delivering medications to the affected area. Improved drug penetration, less side effects, and increased patient compliance are some benefits of aerogel-based topical formulations (Barnes et al., 2021).

5.2.11 Mucoadhesive Drug Delivery

Targeted drug delivery to mucosal surfaces, such as those of the gastrointestinal tract, respiratory tract, or ocular tissues, aerogels can be functionalized with mucoadhesive polymers. Drug residence duration is extended and sustained release is facilitated by mucoadhesive aerogel formulations that stick to mucosal membranes. Mucoadhesive dosage formulations based on aerogel have benefits like better patient adherence, decreased frequency of doses, and increased drug absorption (Yahya et al., 2020).

5.2.12 Recipes for Nanoparticles:

Aerogels function as matrices or carriers when incorporating nanoparticles for drug delivery purposes, such as metallic, polymeric, or liposomal nanoparticles. Improved drug stability, regulated release kinetics, and targeted distribution to particular tissues or cells are some benefits of aerogels loaded with nanoparticles. In nanomedicine, they are employed for the treatment of infectious illnesses, cancer, and other medicinal purposes(Valo et al., 2013).

5.3 Environmental field applications of Aerogel

5.3.1 Oil Spill Clean-up:

In oil spill cleaning efforts, aerogels are used to efficiently collect and absorb spilled oil from water surfaces. They may preferentially absorb oil while rejecting water due to their large surface area, porosity, and hydrophobicity. In maritime contexts, aerogel-based sorbents can be used to lessen the negative effects of oil spills on the environment, allowing for quicker cleanup and less ecological harm (Muhammad et al.,2024).

The process of purifying water involves the use of aerogels to extract impurities and impurities from water sources. Heavy metals, organic contaminants, and microbes can be effectively captured from water by these adsorbents due to their large surface area and porosity. Water quality can be improved, energy consumption can be decreased, and removal efficiency can be increased with aerogel-based filtration membranes or adsorbent materials (Pham et al., 2021).

5.3.2 Air Pollution Control:

Aerogels are useful for capturing gases, volatile organic compounds (VOCs), and particulate matter in the air in pollution control and air filtration systems. They are able to absorb and retain contaminants from both indoor and outdoor air streams due to their large surface area and porosity. Benefits of aerogel-based air filters or adsorbents include better respiratory health, lower emissions, and better air quality (Franco et al., 2021).

5.3.3 Carbon Capture and Storage (CCS):

Applications of aerogels in carbon capture and storage (CCS) technologies are being researched with the goal of lowering greenhouse gas emissions from power plants and industrial operations. Carbon dioxide (CO2) can be selectively captured from flue gas streams using functionalized aerogels, which makes it easier to separate and sequester the gas. High CO2 capture capacity, quick adsorption kinetics, and regeneration capabilities are some benefits of aerogel-based adsorbents (Ayeleru et al., 2023).

5.3.4 Environmental Remediation:

To clean up contaminated sites and restore ecosystems, aerogels are used in environmental remediation projects. Pollutants from soil, water, and sediments, including pesticides, heavy metals, and persistent organic pollutants (POPs), can be absorbed or broken down by functionalized aerogels. Advantages of aerogel-based remediation systems include cost-effective clean-up options, less environmental impact, and targeted pollutant removal (Dehghani et al., 2024).

5.3.5 Thermal Insulation in Green Buildings:

Aerogels are lightweight, highly insulating materials that help with energy-efficient building design and construction. Buildings with less heating and cooling loads thanks to aerogel-based insulation technologies use less energy and emit fewer greenhouse gases. Aerogel insulation enhances indoor air quality, thermal comfort, and sustainability in green buildings (Bashir & Leite, 2022).

5.3.6 Renewable Energy Systems:

Aerogels are used in renewable energy systems, which include batteries, fuel cells, and solar panels. Aerogel-based materials offer structural support, electrochemical stability, and thermal insulation, which improve the performance, longevity, and efficiency of renewable energy solutions. Renewable energy systems with aerogel enhancements help move toward clean, sustainable energy sources (Gu & Ling, 2024).

5.4 Explain to aerospace field applications of Aerogel

Aerogels are valuable materials for a variety of applications in the aerospace industry, where their unique mix of characteristics has several interesting applications. Here are some significant uses of aerogels in the aerospace field:

5.4.1 Thermal Insulation:

Aerogels are lightweight, extremely effective thermal insulation materials used in satellites, spacecraft, and aerospace parts. They offer thermal insulation against the severe temperatures seen during space missions thanks to its remarkably low thermal conductivity, which helps to limit heat transfer. Aerogel insulation protects delicate equipment, helps to maintain stable thermal conditions inside spacecraft and key components, and ensures the success of missions (Hebalkar et al., 2019).

5.4.2 Spacecraft Shielding:

Aerogels are used as spaceship shielding materials against micrometeoroid strikes and space debris. The damage resulting from high-velocity impacts with space debris is lessened by their lightweight and impact-absorbing characteristics. Aerogel-based shields are superior to typical shielding materials in terms of mass and impact resistance, which increases the safety and endurance of spacecraft (Woignier et al., 2013).

5.4.3 Aerogel Composites:

Composite materials utilized in aerospace constructions, including propulsion systems, wings, and fuselages of aircraft, incorporate aerogels. Aerospace component longevity, stiffness, and mechanical strength can all be improved by adding aerogels to composite matrices. By providing benefits like lighter weight, enhanced structural integrity, and greater resilience to shock and fatigue, aerogel composites help create high-performance, lightweight aerospace structures (Jeon & Baek, 2010).

5.4.4 Thermal Protection Systems (TPS):

Hypersonic airplanes, space shuttles, and reentry vehicles all use aerogels in their thermal protection systems (TPS). They are appropriate for use in heat shields, ablative coatings, and thermal barriers due to their low density and great temperature tolerance. By assisting in the dissipation of heat produced during atmospheric reentry, aerogel-based TPS materials shield spacecraft occupants from high temperatures and the impacts of aerodynamic heating (Jin et al., 2023).

5.4.5 Cryogenic Storage:

Aerogels are used to store and transport liquefied gases, such as oxygen and hydrogen used as rocket propellants, in cryogenic storage systems. By minimizing heat infiltration and preventing temperature swings, their strong insulating qualities and low thermal conductivity contribute to the stability and integrity of cryogenic fluids. Aerospace propulsion systems' efficiency and dependability are enhanced by cryogenic insulation systems based on aerogel (Fesmire, 2016).

5.4.6 Microwave Absorption:

Aerogels are helpful for radar-absorbing materials (RAMs) in aerospace vehicles and for stealth applications because they may be engineered to absorb electromagnetic radiation in the microwave frequency range. The stealth capabilities of military aircraft and unmanned aerial vehicles (UAVs) are improved by aerogel-based RAM coatings, which attenuate radar emissions and decrease detectability. The benefits of aerogel RAMs include decreased radar cross-section, lightweight, and broadband absorption, which improve mission effectiveness and survivability in harsh conditions (Sahoo et al., 2022).

All things considered, aerogels are essential to the advancement of aerospace technology because they offer strong, lightweight, and versatile materials for thermal control, structural support, and electromagnetic shielding in satellites, airplanes, and spacecraft. Their special qualities enable the creation of cutting-edge aircraft technologies and the pursuit of new aviation and space exploration frontiers.

5.5 Explain to chemical field applications of Aerogel

Their special qualities, which include high surface area, porosity, and thermal stability, aerogels are used in many different areas of the chemical industry. These are some significant uses of aerogels in the chemical area:

5.5.1 Catalysis:

When it comes to supporting catalytic materials in chemical reactions, aerogels are fantastic. Numerous active sites are made available for catalytic reactions by their high surface area and porosity. Comparing aerogel-supported catalysts to traditional catalysts reveals increased stability, selectivity, and activity. Chemical processes include petrochemical refining, hydrogenation, oxidation, and environmental remediation all use aerogel-based catalysts (Maleki &Hüsing, 2018).

5.5.2 Adsorption and Separation:

Aerogels are used to remove contaminants and impurities from gases and liquids as well as adsorbents and separation materials. The efficient adsorption of gases, volatile organic compounds (VOCs), and heavy metals is made possible by their large surface area and pore volume. Chemical separation procedures, air and water treatment, and gas purification all use aerogel-based adsorbents. Their benefits include quick kinetics, regenerability, and a high adsorption capacity (Franco et al., 2021).

5.5.3 Gas Storage:

Applications of aerogels for gas distribution and storage are being researched. Hydrogen, methane, and carbon dioxide can be stored and released because to their nanoporous structure. Advantages of aerogel-based gas storage materials include reversible adsorption-desorption kinetics, low weight, and large storage capacity. For fuel cell and alternative energy applications, they are utilized in hydrogen keeping tanks, natural gas pipelines, and portable gas storage devices (Memetova et al., 2022).

5.5.4 Sorption Heat Pumps:

In sorption heat pump systems, aerogels are used for refrigeration, heating, and cooling purposes. Their excellent thermal conductivity and sorption capacity make them ideal adsorbents for reversible sorption procedures. For the purpose of producing heating or cooling effects, fluids (such as water vapor or ammonia) are adsorbed and desorbable from aerogel-based sorption materials. Energy-efficient and environmentally beneficial options for space heating, air conditioning, and refrigeration are provided by sorption heat pumps that use aerogel materials (Farmer, 2010).

5.5.5 Chemical Sensors:

Chemical sensing devices use aerogels to identify gases, vapors, and volatile organic compounds (VOCs). Target molecules can be selectively taken by functionalized aerogels, resulting in detectable and quantifiable changes to their electrical, optical, or mechanical properties. Aerogel-based chemical sensors offer advantages such as high sensitivity, fast response times, and low detection limits. They are employed in industrial safety, biomedical diagnostics, and environmental monitoring (Carroll & Anderson, 2023).

5.5.6 Electrochemical Devices:

Batteries, capacitors, and fuel cells are examples of electrochemical devices that use aerogels. For energy storage and conversion applications, their high surface area, porosity, and electrical conductivity make them appropriate electrode materials. High specific capacitance, quick charge-discharge rates, and extended cycle life are among the benefits of aerogel-based electrodes. According to Chandrasekaran et al. (2023), they aid in the creation of environmentally friendly, high-performing electrochemical devices for the production and storage of renewable energy.

Aerogels are useful materials for a variety of applications in the chemical industry, including catalysis, adsorption, heat transfer, gas storage, sensing, and electrochemistry. Because of their special qualities, new technologies have been able to be developed to increase the energy efficiency, sustainability of the environment, and process efficiency of chemical processes and products. Describe the industrial field uses for aerogel.Because of their unique characteristics, aerogels are used in a wide range of industrial processes and products to improve performance, efficiency, and sustainability. The following are some significant industrial field uses for aerogels:

5.5.7 Insulation:

In industrial settings, such as manufacturing plants, processing facilities, and equipment, aerogels are frequently utilized as insulating materials. They are perfect for insulating industrial furnaces, boilers, pipes, and vessels due to their excellent thermal resistance and low thermal conductivity. According to Thapliyal and Singh (2014), aerogel insulation helps industrial operations maintain constant temperatures, prevent heat loss, and use less energy. These benefits include financial savings as well as environmental ones.

5.5.8 Heat Management:

In industrial settings, aerogels are used in heat management systems to provide thermal insulation, heat shielding, and temperature control. High-temperature applications like metal casting, glass fabrication, and aerospace manufacturing employ them. According to Kong et al. (2023), aerogel-based heat management technologies enhance process efficiency, safeguard workers and equipment from high temperatures, and produce higher-quality products.

5.5.9 Cryogenic Storage:

Liquid gases, such as liquid nitrogen, liquid oxygen, and LNG (liquefied natural gas), are stored and transported in cryogenic storage systems using aerogels. By minimizing heat infiltration and preventing temperature swings, their strong insulating qualities and low thermal conductivity contribute to the stability and integrity of cryogenic fluids. For the safe and effective handling of cryogenic liquids, cryogenic tanks, transportation containers, and LNG terminals all use aerogel-based cryogenic insulation systems (Sambucci et al., 2023).

5.5.10 Chemical Processing:

In chemical processing applications, aerogels function as adsorbents, filter media, and catalyst supports. They are employed in filtration systems, chromatography columns, and catalytic reactors for the manufacturing of specialized chemicals, petrochemicals, and refining. Aerogel-based materials improve process yields and lessen their negative effects on the environment by improving reaction kinetics, separation efficiency, and product purity (Zubair et al., 2019).

5.5.11 Corrosion Protection:

To stop deterioration and increase the lifespan of industrial infrastructure and equipment, aerogels are used in corrosion protection coatings and materials. They function as barrier coatings to stop corrosive substances like chemicals, salt spray, and moisture from penetrating. Superior adhesion, flexibility, and resilience to hostile conditions are some of the benefits of aerogel-based corrosion protection technologies, which also lower maintenance costs and downtime (Aljibori et al., 2023).

5.5.12 Advanced Materials:

Advanced materials and composites are enhanced mechanical properties, thermal stability, and functional performance through the incorporation of aerogels. They are utilized for thermal barriers, acoustic insulation, and lightweight structural components in the automotive, aerospace, and renewable energy industries. Materials based on aerogels almost aid in the creation of sustainable and high-performing goods for use in industry, such as energy-efficient cars, long-lasting infrastructure, and lightweight composites (Khan et al., 2024).

All things considered, aerogels are essential to the industrial sector since they offer revolutionary options for sophisticated materials, chemical processing, heat management, insulation, and cryogenic storage. Their special qualities solve major problems that industries encounter, resulting in more productivity, sustainability, and efficiency in production procedures and goods.

REFERENCE

1. Abdullah, C. K., Pasquini, D., & Thomas, S. (2023). Biopolymers based aerogels: A review on revolutionary solutions for smart therapeutics delivery. *Progress in Materials Science*, *131*, 101014. https://doi.org/10.1016/j.pmatsci.2022.101014

2. Aljibori, H., Al-Amiery, A., & Kadhum, A. (2023). Advances in corrosion protection coatings: A comprehensive review. *International Journal of Corrosion and Scale Inhibition*, *12*, 1476–1520. https://doi.org/10.17675/2305-6894-2023-12-4-6

3. Ayeleru, O. O., Modekwe, H. U., Onisuru, O. R., Ohoro, C. R., Akinnawo, C. A., & Olubambi, P. A. (2023). Adsorbent technologies and applications for carbon capture, and direct air capture in environmental perspective and sustainable climate action. *Sustainable Chemistry for Climate Action*, *3*, 100029. https://doi.org/10.1016/j.scca.2023.100029

4. Bakhori, N. M., Ismail, Z., Hassan, M. Z., & Dolah, R. (2023). Emerging Trends in Nanotechnology: Aerogel-Based Materials for Biomedical Applications. *Nanomaterials*, *13*(6), 1063. https://doi.org/10.3390/nano13061063
5. Barnes, T. M., Mijaljica, D., Townley, J. P., Spada, F., & Harrison, I. P. (2021). Vehicles for Drug Delivery and Cosmetic Moisturizers: Review and Comparison. *Pharmaceutics*, *13*(12). https://doi.org/10.3390/pharmaceutics13122012
6. Basak, S., & Singhal, R. S. (2023). The potential of supercritical drying as a “green” method for the production of food-grade bioaerogels: A comprehensive critical review. *Food Hydrocolloids*, *141*, 108738. https://doi.org/10.1016/j.foodhyd.2023.108738
7. Bashir, A. W., & Leite, B. C. C. (2022). Performance of aerogel as a thermal insulation material towards a sustainable design of residential buildings for tropical climates in Nigeria. *Energy and Built Environment*, *3*(3), 291–315. https://doi.org/10.1016/j.enbenv.2021.02.003
8. Baudron, V., Gurikov, P., Smirnova, I., & Whitehouse, S. (2019). Porous Starch Materials via Supercritical- and Freeze-Drying. *Gels*, *5*(1), Article 1. https://doi.org/10.3390/gels5010012
9. Bheekhun, N., Abu Talib, A. R., & Hassan, M. R. (2013). Aerogels in Aerospace: An Overview. *Advances in Materials Science and Engineering*, *2013*, e406065. https://doi.org/10.1155/2013/406065
10. Carroll, M., & Anderson, A. (2023). *Aerogels as Platforms for Chemical Sensors* (pp. 1289–1303). https://doi.org/10.1007/978-3-030-27322-4_49
11. Chandrasekaran, S., Lin, D., Li, Y., & Worsley, M. A. (2023). Aerogels, additive manufacturing, and energy storage. *Joule*, *7*(5), 866–883. https://doi.org/10.1016/j.joule.2023.03.021
12. Cuce, E., Cuce, P. M., Wood, C. J., & Riffat, S. B. (2014). Toward aerogel based thermal superinsulation in buildings: A comprehensive review. *Renewable and Sustainable Energy Reviews*, *34*, 273–299. https://doi.org/10.1016/j.rser.2014.03.017
13. Dehghani, M. H., Ahmadi, S., Ghosh, S., Khan, M. S., Othmani, A., Khanday, W. A., Gökkuş, Ö., Osagie, C., Ahmaruzzaman, Md., Mishra, S. R., Lima, E. C., Mubarak, N. M., Karri, R. R., & Ansari, K. (2024). Sustainable remediation technologies for removal of pesticides as organic micro-pollutants from water environments: A review. *Applied Surface Science Advances*, *19*, 100558. https://doi.org/10.1016/j.apsadv.2023.100558
14. El-Naggar, M. E., Othman, S. I., Allam, A. A., & Morsy, O. M. (2020). Synthesis, drying process and medical application of polysaccharide-based aerogels. *International Journal of Biological Macromolecules*, *145*, 1115–1128. https://doi.org/10.1016/j.ijbiomac.2019.10.037
15. Esposito, S. (2019). “Traditional” Sol-Gel Chemistry as a Powerful Tool for the Preparation of Supported Metal and Metal Oxide Catalysts. *Materials*, *12*(4), 668. https://doi.org/10.3390/ma12040668

16. Farmer, J. (2010). *SOLAR-POWERED AEROGEL-BASED ADSORPTIVE AIR CONDITIONING* (LLNL-TR-423246, 1129983; p. LLNL-TR-423246, 1129983). https://doi.org/10.2172/1129983

17. Fesmire, J. E. (2016). Layered composite thermal insulation system for nonvacuum cryogenic applications. *Cryogenics*, *74*, 154–165. https://doi.org/10.1016/j.cryogenics.2015.10.008

18. Fesmire, J. E. (2016). Layered composite thermal insulation system for nonvacuum cryogenic applications. *Cryogenics*, *74*, 154–165. https://doi.org/10.1016/j.cryogenics.2015.10.008

19. Fesmire, J. E. (2019). Aerogel-Based Insulation Materials for Cryogenic Applications. *IOP Conference Series: Materials Science and Engineering*, *502*, 012188. https://doi.org/10.1088/1757-899X/502/1/012188

20. Franco, P., Cardea, S., Tabernero, A., & De Marco, I. (2021). Porous Aerogels and Adsorption of Pollutants from Water and Air: A Review. *Molecules*, *26*(15), 4440. https://doi.org/10.3390/molecules26154440

21. Ganesamoorthy, R., Vadivel, V. K., Kumar, R., Kushwaha, O. S., & Mamane, H. (2021). Aerogels for water treatment: A review. *Journal of Cleaner Production*, *329*, 129713. https://doi.org/10.1016/j.jclepro.2021.129713

22. García-González, C. A., Sosnik, A., Kalmár, J., de marco, I., Erkey, C., Concheiro, A., & Alvarez-Lorenzo, C. (2021). Aerogels in drug delivery: From design to application. *Journal of Controlled Release*, *332*. https://doi.org/10.1016/j.jconrel.2021.02.012

23. Gu, X., & Ling, Y. (2024). Research progress of aerogel materials in the field of construction. *Alexandria Engineering Journal*, *91*, 620–631. https://doi.org/10.1016/j.aej.2024.02.039

24. Guastaferro, M., Reverchon, E., & Baldino, L. (2021). Polysaccharide-Based Aerogel Production for Biomedical Applications: A Comparative Review. *Materials*, *14*(7), 1631. https://doi.org/10.3390/ma14071631

25. Guo, N., Xia, Y., Zeng, W., Chen, J., Wu, Q., Shi, Y., Li, G., Huang, Z., Wang, G., & Liu, Y. (n.d.). Alginate-based aerogels as wound dressings for efficient bacterial capture and enhanced antibacterial photodynamic therapy. *Drug Delivery*, *29*(1), 1086–1099. https://doi.org/10.1080/10717544.2022.2058650

26. Hebalkar, N., Kollipara, K. S., Ananthan, Y., & Sudha, M. K. (2019). Nanoporous Aerogels for Defense and Aerospace Applications. In Y. Mahajan & J. Roy (Eds.), *Handbook of Advanced Ceramics and Composites: Defense, Security, Aerospace and Energy Applications* (pp. 1–43). Springer International Publishing. https://doi.org/10.1007/978-3-319-73255-8_5-1

27. Hu, P., Wang, J., Zhang, P., Wu, F., Cheng, Y., Wang, J., & Sun, Z. (2023). Hyperelastic Kevlar Nanofiber Aerogels as Robust Thermal Switches for Smart Thermal Management. *Advanced Materials*, *35*(3), 2207638. https://doi.org/10.1002/adma.202207638

28. Jeon, I.-Y., & Baek, J.-B. (2010). Nanocomposites Derived from Polymers and Inorganic Nanoparticles. *Materials*, *3*(6), 3654–3674. https://doi.org/10.3390/ma3063654

29. Jin, R., Zhou, Z., Liu, J., Shi, B., Zhou, N., Wang, X., Jia, X., Guo, D., & Xu, B. (2023). Aerogels for Thermal Protection and Their Application in Aerospace. *Gels*,*9*(8), 606. https://doi.org/10.3390/gels9080606

30. Jin, R., Zhou, Z., Liu, J., Shi, B., Zhou, N., Wang, X., Jia, X., Guo, D., & Xu, B. (2023). Aerogels for Thermal Protection and Their Application in Aerospace. *Gels*, *9*, 606. https://doi.org/10.3390/gels9080606

31. Johnson, K. (2023, October 16). Thermal Interface Material Solutions for Manufacturing Industries. *Technical Articles by Production Automation Corporation*. https://blog.gotopac.com/2023/10/16/thermal-interface-material-solutions-for-manufacturing-industries/

32. Khan, N. R., Sharmin, T., & Bin Rashid, A. (2024). Exploring the Versatility of Aerogels: Broad Applications in Biomedical Engineering, Astronautics, Energy Storage, Biosensing, and Current Progress. *Heliyon*, *10*(1), e23102. https://doi.org/10.1016/j.heliyon.2023.e23102

33. Khan, N. R., Sharmin, T., & Bin Rashid, A. (2024). Exploring the Versatility of Aerogels: Broad Applications in Biomedical Engineering, Astronautics, Energy Storage, Biosensing, and Current Progress. *Heliyon*, *10*(1), e23102. https://doi.org/10.1016/j.heliyon.2023.e23102

34. Koçyiğit, N. (2023). *AEROGELS: CHARACTERISTICS, CLASSIFICATION, STRUCTURE, PROPERTIES, PREPARATION, TYPES AND APPLICATIONS* (pp. 3–43).

35. Kong, X., Nie, R., & Yuan, J. (2023). A review of shape stabilized aerogel-based phase change materials for preparation, classification and applications. *Energy and Built Environment*. https://doi.org/10.1016/j.enbenv.2023.11.001

36. Kumar, S., Kwon, H.-T., Choi, K.-H., Lim, W., Cho, J. H., Tak, K., & Moon, I. (2011). LNG: An eco-friendly cryogenic fuel for sustainable development. *Applied Energy*, *88*(12), 4264–4273. https://doi.org/10.1016/j.apenergy.2011.06.035

37. Lai, J., Luo, Z., Chen, L., & Wu, Z. (2024). Advances in nanotechnology-based targeted-contrast agents for computed tomography and magnetic resonance. *Science Progress*, *107*(1), 00368504241228076. https://doi.org/10.1177/00368504241228076

38. Larisa, M., & Croitoru, C. (2019). Aerogel, a high performance material for thermal insulation—A brief overview of the building applications. *E3S Web of Conferences*, *111*, 06069. https://doi.org/10.1051/e3sconf/201911106069

39. Larisa, M., & Croitoru, C. (2019). Aerogel, a high performance material for thermal insulation—A brief overview of the building applications. *E3S Web of Conferences*, *111*, 06069. https://doi.org/10.1051/e3sconf/201911106069

40. Lee, K. H., Arshad, Z., Dahshan, A., Alshareef, M., Alsulami, Q. A., Bibi, A., Lee, E.-J., Nawaz, M., Zubair, U., & Javid, A. (2023). Porous Aerogel Structures as Promising Materials for Photocatalysis, Thermal Insulation Textiles, and Technical Applications: A Review. *Catalysts*, *13*(9), Article 9. https://doi.org/10.3390/catal13091286

41. Leventis, N., & Lu, H. (2011). *Polymer-Crosslinked Aerogels* (pp. 251–285). https://doi.org/10.1007/978-1-4419-7589-8_13

42. Li, W.-C., Reichenauer, G., & Fricke, J. (2002). Carbon aerogels derived from cresol-resorcinol-formaldehyde for supercapacitors. *Carbon*, *40*, 2955–2959. https://doi.org/10.1016/S0008-6223(02)00243-9

43. Liu, L., Shan, X., Hu, X., Lv, W., & Wang, J. (2021). Superhydrophobic Silica Aerogels and Their Layer-by-Layer Structure for Thermal Management in Harsh Cold and Hot Environments. *ACS Nano*, *15*(12), 19771–19782. https://doi.org/10.1021/acsnano.1c07184

44. Liu, L., Wu, D., Tu, H., Cao, M., Li, M., Peng, L., & Yang, J. (2023). Applications of Hydrogels in Drug Delivery for Oral and Maxillofacial Diseases. *Gels*, *9*(2), 146. https://doi.org/10.3390/gels9020146

45. Maleki, H., & Hüsing, N. (2018). Current status, opportunities and challenges in catalytic and photocatalytic applications of aerogels: Environmental protection aspects. *Applied Catalysis B: Environmental*, *221*, 530–555. https://doi.org/10.1016/j.apcatb.2017.08.012

46. Meliță, L., & Croitoru, C. (2019). Aerogel, a high performance material for thermal insulation—A brief overview of the building applications. *E3S Web of Conferences*, *111*, 06069. https://doi.org/10.1051/e3sconf/201911106069

47. Memetova, A., Tyagi, I., Singh, P., Neskoromnaya, E., Karri, R. R., Zelenin, A., Memetov, N., Babkin, A., Stolyarov, R., Chapaksov, N., Gusev, A., Mubarak, N. M., Tkachev, A., & Suhas. (2022). Reduced graphene oxide based composite aerogels for energy storage and transportation of methane. *Journal of Cleaner Production*, *379*, 134770. https://doi.org/10.1016/j.jclepro.2022.134770

48. Montes, S., & Maleki, H. (2020). 12—Aerogels and their applications. In S. Thomas, A. Tresa Sunny, & P. Velayudhan (Eds.), *Colloidal Metal Oxide Nanoparticles* (pp. 337–399). Elsevier. https://doi.org/10.1016/B978-0-12-813357-6.00015-2

49. Muhammad, S., Albadn, Y. M., Yahya, E. B., Nasr, S., Khalil, H. P. S. A., Ahmad, M. I., & Kamaruddin, M. A. (2024). Trends in enhancing the efficiency of biomass-based aerogels for oil spill clean-up. *Giant*, *18*, 100249. https://doi.org/10.1016/j.giant.2024.100249

50. Niculescu, A.-G., Tudorache, D.-I., Bocioagă, M., Mihaiescu, D. E., Hadibarata, T., & Grumezescu, A. M. (2024). An Updated Overview of Silica Aerogel-Based Nanomaterials. *Nanomaterials*, *14*(5), Article 5. https://doi.org/10.3390/nano14050469

51. Pham, T. H., Jung, S. H., Kim, Y. J., & Kim, T. (2021). Adsorptive removal and recovery of organic pollutants from wastewater using waste paper-derived carbon-based aerogel. *Chemosphere*, *268*, 129319. https://doi.org/10.1016/j.chemosphere.2020.129319

52. Randall, J. P., Meador, M. A. B., & Jana, S. C. (2011). Tailoring Mechanical Properties of Aerogels for Aerospace Applications. *ACS Applied Materials & Interfaces*, *3*(3), 613–626. https://doi.org/10.1021/am200007n

53. Sahoo, P., Saini, L., & Dixit, A. (2022). Microwave-absorbing materials for stealth application: A holistic overview. *Oxford Open Materials Science*, *3*. https://doi.org/10.1093/oxfmat/itac012

54. Sambucci, M., Savoni, F., & Valente, M. (2023). Aerogel Technology for Thermal Insulation of Cryogenic Tanks—Numerical Analysis for Comparison with Traditional Insulating Materials. *Gels*, *9*, 307. https://doi.org/10.3390/gels9040307

55. Shi, B., Ma, B., Wang, C., He, H., Qu, L., Xu, B., & Chen, Y. (2021). Fabrication and applications of polyimide nano-aerogels. *Composites Part A: Applied Science and Manufacturing*, *143*, 106283. https://doi.org/10.1016/j.compositesa.2021.106283

56. Ślosarczyk, A., Błaszczyński, T., & Morawski, M. (2013). *Synthesis of Silica Aerogel by Supercritical Drying Method*. *57*. https://doi.org/10.1016/j.proeng.2013.04.028

57. Thapliyal, P. C., & Singh, K. (2014). Aerogels as Promising Thermal Insulating Materials: An Overview. *Journal of Materials*, *2014*, e127049. https://doi.org/10.1155/2014/127049

58. Uyanna, O., & Najafi, H. (2020). Thermal protection systems for space vehicles: A review on technology development, current challenges and future prospects. *Acta Astronautica*, *176*, 341–356. https://doi.org/10.1016/j.actaastro.2020.06.047

59. Valo, H., Arola, S., Laaksonen, P., Torkkeli, M., Peltonen, L., Linder, M., Serimaa, R., Kuga, S., Hirvonen, J., & Laaksonen, T. (2013). Drug Release from Nanoparticles Embedded in Four Different Nanofibrillar Cellulose Aerogels. *European Journal of Pharmaceutical Sciences : Official Journal of the European Federation for Pharmaceutical Sciences*, *50*. https://doi.org/10.1016/j.ejps.2013.02.023

60. Wakeel, A., Nasir, M. A., Ammar, M., Ahmad, J., Fatima, N., Ahmed, W., & Ali, Z. (2023). A review article on the synthesis of silica aerogels and their insulation properties. *International Journal of Emerging Multidisciplinaries Physical Sciences*, *1*, 78–104.

61. Wang, J., Glora, M., Petricevic, R., Saliger, R., Proebstle, H., & Fricke, J. (2001). Carbon Cloth Reinforced Carbon Aerogel Films Derived from Resorcinol Formaldehyde. *Journal of Porous Materials*, *8*, 159–165. https://doi.org/10.1023/A:1009607211736

62. Woignier, T., Duffours, L., Colombel, P., & Durin, C. (2013). Aerogels Materials as Space Debris Collectors. *Advances in Materials Science and Engineering*, *2013*. https://doi.org/10.1155/2013/484153

63. Wu, D., Fu, R., Zhang, S., Dresselhaus, M., & Dresselhaus, G. (2004). The preparation of carbon aerogels based upon the gelation of resorcinol–furfural in isopropanol with organic base catalyst. *Journal of Non-Crystalline Solids*, *336*, 26–31. https://doi.org/10.1016/j.jnoncrysol.2003.12.051

64. Wu, Y., Wang, X., & Shen, J. (2022). Metal oxide aerogels for high-temperature applications. *Journal of Sol-Gel Science and Technology*, *106*. https://doi.org/10.1007/s10971-021-05720-w

65. Xie, H., He, Z., Liu, Y., Zhao, C., Guo, B., Zhu, C., & Xu, J. (2022). Efficient Antibacterial Agent Delivery by Mesoporous Silica Aerogel. *ACS Omega*, *7*(9), 7638–7647. https://doi.org/10.1021/acsomega.1c06198

66. Yahya, E. B., Amirul, A. A., H.p.s, A. K., Olaiya, N. G., Iqbal, M. O., Jummaat, F., A.k, A. S., & Adnan, A. S. (2021). Insights into the Role of Biopolymer Aerogel Scaffolds in Tissue Engineering and Regenerative Medicine. *Polymers*, *13*(10). https://doi.org/10.3390/polym13101612

67. Yahya, E. B., Jummaat, F., Amirul, A. A., Adnan, A. S., Olaiya, N. G., Abdullah, C. K., Rizal, S., Mohamad Haafiz, M. K., & Khalil, H. P. S. A. (2020). A Review on Revolutionary Natural Biopolymer-Based Aerogels for Antibacterial Delivery. *Antibiotics*, *9*(10), 648. https://doi.org/10.3390/antibiotics9100648

68. Zhang, T., Sanguramath, R. A., Israel, S., & Silverstein, M. S. (2019). Emulsion Templating: Porous Polymers and Beyond. *Macromolecules*, *52*(15), 5445–5479. https://doi.org/10.1021/acs.macromol.8b02576

69. Zheng, Y., Ma, W., Yang, Z., Zhang, H., Ma, J., Li, T., Niu, H., Zhou, Y., Yao, Q., Chang, J., Zhu, Y., & Wu, C. (2022). An ultralong hydroxyapatite nanowire aerogel for rapid hemostasis and wound healing. *Chemical Engineering Journal*, *430*, 132912. https://doi.org/10.1016/j.cej.2021.132912

70. Zubair, N., Abouzari-Lotf, E., Nasef, M., & Abdullah, E. (2019). Aerogel-based materials for adsorbent applications in material domains. *E3S Web of Conferences*, *90*, 01003. https://doi.org/10.1051/e3sconf/20199001003

71. Zuo, L., Zhang, Y., Zhang, L., Miao, Y.-E., Fan, W., & Liu, T. (2015). Polymer/Carbon-Based Hybrid Aerogels: Preparation, Properties and Applications. *Materials*, *8*(10), 6806–6848. https://doi.org/10.3390/ma8105343

CHAPTER

6

A SURVEY OF CONTAMINATION OF HEAVY METALS IN INDIA AND ITS REMEDIATION TECHNIQUES

Rupa Chakraborty[a*], Anupama Asthana[b], Ajay Kumar Singh[b]
[a]Department of Chemistry, Sai College Sector 6 Bhilai 490006 (Chhattisgarh), India
[b]Department of Chemistry, Govt. V.Y.T. PG Autonomous College, Durg, 491001 (Chhattisgarh), India 491001 (Chhattisgarh), India
[*]Corresponding author: e-mail address: roopachakraborty1991@gmail.com

ABSTRACT:

Environmental pollution, particularly from heavy metal ions in the wastewater, is one of the most serious concerns of the world. In the pursuit of remedial action, various conventional methods such as ion exchange, chemical precipitation, coagulation, membrane separation, reverse osmosis, and adsorption methods have so far been used for the removal of heavy metal ions. A good variety of adsorbents have so far been developed to remove different heavy metal ions from wastewater in particular those which have been detrimental to living organisms. Adsorption processes have been very demanding for high removal efficiency of heavy metal ions even at traces levels and they are low cost as compared to conventional methods.

Keywords: Heavy metals, water pollution, remediation techniques, adsorption

6.1. INTRODUCTION

Environmental pollution

The civilization on earth with evolutions has led to a lot of ecological differences. At present the environmental pollution problem, one of the most dangerous part that are to be taken care of immediately. Rapid industrialization, population, urbanization and unlimited utilization of natural resources have created a great ecological imbalance. Unfavorable regular change in the air, water and land, largely due to the human activity is called **pollution**. The foreign substances identified as **pollutants** in the pure surroundings, when in excessive quantity, causes impurity to the environment and to the living systems.

Water pollution

The present project work is based on the troubles caused by water pollution, a major concern in the earth in the recent times. Water, the most essential component with an ability to dissolve a variety of toxic materials, is in the need for saving. The addition of a large amount of organic, inorganic or biological materials, which changes the properties of water, is responsible for water pollution. Therefore, there is a need for the study of the water pollution.

Heavy metal ions pollution

A number of pollutants both organic and inorganic cause harm to the environment. The present world faces the risk of heavy metal ions, as they are very toxic and carcinogenic in nature. Numerous human activities have resulted in the pollution of heavy metals and as a consequence there is a disturbance on the food chain of the ecosystem. Heavy metals are released into the environment from various sources such as chemical industries, metal plating industries, alloy industries, battery manufacturing industries, mining and metallurgical industries, paper and pulp industries etc. [1-4]. Release of toxic metals into water stream is a serious concern, which may affect the quality of water supply [5]. Some of the hazardous heavy metal ions which pose potential danger and threat to human health are arsenic, mercury, chromium, cadmium, and lead. Heavy metal ions noted are not recyclable and accumulate in living organisms [6]. Several disasters in the past regarding the contamination of heavy metal ions in water bodies include: “Itai-Itai” for pollution of cadmium in Jintsu river of Japan and “Minamata tragedy” due to methyl mercury contamination in Japan [7]. In addition, according to CWC’s (Central Water Commission) report, 42 (major and minor) rivers of India have extremely high concentration of neurotoxic heavy metals beyond the permissible limit. The foremost information from this report says, The **Ganga,** the most important sacred and national river was found to be polluted with five different heavy metals of chromium, copper, nickel, lead and iron [8]. The common heavy metals contaminated area in India, are presented in **Table 1.1.**

Table 1.1 The common heavy metals highly contaminated area in India.

S. No.	Heavy Metals	Contaminated area in India	References
1.	Cadmium (Cd)	West U.P. region	[9]
2.	Mercury (Hg)	Kodaikanal, Tamil Nadu	[10]
3.	Arsenic (As)	Burdwan, West Bengal	[11]
		Brahmaputra floodplain, Assam	[11]
		Kaudikasa and Ambagarh-Chowki block, Rajnandgaon district, Chhattisgarh	[11]
		Puduchery, Tamilnadu	[11]
4.	Lead (Pb)	Korba, Chhattisgarh	[12]
5.	Chromium (Cr)	Kanpur, Uttar Pradesh	[13]
		Ranipet, Tamil Nadu	[14]
6.	Copper (Cu)	Singbhum Mines, Jharkhand	[15]
		Malajkhand, Madhya Pradesh	[16]
7.	Nickel (Ni)	Ratlam and Nagda, Madhya Pradesh	[17]

8.	Iron (Fe)	Moradabad, Uttar Pradesh	[18]
		Bailadila and Dallirajhra, Chhattisgarh	[19]

Heavy metals and their ions are released into water stream at higher concentrations beyond the limit of the prescribed value by the industrial activities. Heavy metal ions exhibit their toxicity at low concentrations of about 1.0-10.0 mg/L [20].

There is an incessant increase in the use of heavy metal ions due to the rise in industrial activities and human's greedy needs. These sources have intensified the pollution of the water streams day to day. The heavy metal ions are strong toxicants as they are non-biodegradable. Moreover, heavy metal ions are carcinogenic in nature. Alarmingly, the heavy metal ions in water systems are at higher concentrations than the permissible limits, hence leads to innumerable diseases [21].

6.2. CONVENTIONAL METHODS FOR REMOVAL OF HEAVY METAL IONS

Various methods are available for removing heavy metal ions, these include: ion exchange [22], chemical precipitation [23], coagulation [24], membrane separation [25], electro-coagulation [26], and reverse osmosis [27]. Some of these methods, however, are not generally used due to their high cost and low feasibility. Adsorption techniques are the most widely used and low-cost alternative technology [28-29], but the search for effective adsorbents is still on.

Natural materials or certain waste materials from industrial and agricultural activities have capacity as an inexpensive adsorbent alternative for removal of heavy metal ions. Cost is another important factor for comparing the potentials of the adsorbent materials. In general, adsorbents could be assumed to be a "low-cost adsorbent" if they require little processing and are abundantly available, or any waste material that are bio-degradable from industry or agricultural by-product [30]. Many examples of natural adsorbents used for wastewater treatment have been reported in the literature to remove toxic pollutants as colorants and heavy metals. They include sugar beet pulp [31], coal fly ash [32], coir pith [33], sawdust [34], and castor tree leaf powder [35] etc.

6.3. TYPES OF ADSORPTION

The types of adsorption are as follows:

6.3.1. Physical adsorption (Physisorption)

- In physisorption, it is mainly observed that there is no exchange of electrons between adsorbent surface site and adsorbate molecules.
- It is assumed that the physical forces (weak Van-der Waal's forces) of attraction, dipole moment and hydrogen bond bind the adsorbate to the surface of the adsorbent.
- Physisorption process occurs at low temperature and is characterized by low heat of adsorption (< 40 kJ mol^{-1}).
- It is a non-specific and reversible process i.e. adsorption-desorption process occurs simultaneously.
- In this process multilayer of adsorbate is formed on to the surface of adsorbent.

6.3.2. Chemical adsorption (Chemisorption)

- In chemisorption, it is predominantly observed that an exchange of electrons takes place between adsorbent surface sites and the adsorbate molecules, and as a result a chemical bond (covalent bond) is formed.
- It is assumed that the electrostatic forces of attraction bind the adsorbate molecules to the surface of the adsorbent.
- Chemisorption process occurs at high temperatures and is characterized by high heat of adsorption (> 40 kJ mol^{-1}).
- It is a specific and an irreversible process, with the separation of the adsorbent from adsorbate found to be difficult.
- In this process monolayer of adsorbate are formed onto the surface of adsorbent.

6.4. FACTORS INFLUENCING PARAMETERS

Adsorption is a process carried out by the help of adsorbent materials. Many factors that influence the metal adsorption processes are summarized in Table 1.2.

Table 1.2. Factors affecting parameters for adsorption of metal ions.

S. No.	Factors affecting parameters	Effects
1.	Surface area of the adsorbent	The higher amount of specific surface area implies greater adsorption capacity.
2.	Particle size of the adsorbent	Adsorption capacity based on particle size, smaller the particle size of the adsorbent higher the adsorption capacity.
3.	Contact time	Adsorption capacity increases with increase in contact time until to reach the equilibrium.
4.	pH	Strongly affects the adsorption behaviour due to the variation in degree of ionization of metal ions in aqueous solution.
5.	Concentration	Adsorption capacity increases with increase in concentration.
6.	Temperature	Adsorption capacity depends on temperature –Exothermic process – hence increasing temperature decreases adsorption –Endothermic process – adsorption capacity increases with increase in temperature.

6.5. CONCLUSION

Rapid industrialization has resulted in increased utilization of heavy metal ions in last few decades to make the serious worldwide environmental issue. Due to its hazardous and bioaccumulative nature, there have been numerous attempts to find a suitable remedial action. Various conventional methods such as ion exchange, chemical precipitation, coagulation, membrane separation, reverse osmosis and adsorption methods have so far been used for the removal of heavy metal ions, but these methods could not be effective due to several issues and drawbacks. Among them adsorption process is very useful and effective for removal of heavy metal ions, even at low concentrations.

REFERENCES

[1] S. Babel, T.A. Kurniawan, Chemosphere**54**, 951 (2004).
[2] S.P. Dubey, K. Gopal, J. Hazard. Mater.**145**, 465 (2007).
[3] B. Geng, Z. Jin, T. Li, X. Qi, Sci. Total Environ.**407**, 4994 (2009).
[4] R.M. Nthumbi, J.C. Ngila, B. Moodley, A. Kindness, L. Petrik, Phys. Chem. Earth**50**, 243 (2012).
[5] S. Larous, A.H. Meniai, M. Bencheikh Lechocine, Desalination**185**, 483 (2005).
[6] Y. Bulut, Z. Baysal, J. Environ. Manage.**78**, 107 (2006).
[7] D. Sud, G. Mahajan, M.P. Kaur, Bioresour. Technol.**99**, 6017 (2008).
[8] www.downtoearth.org.in/news/water/huge-amounts-of-toxic-heavy-metals-swim-in-indian-rivers-60545.
[9] N. Idrees, B. Tabassum, E.F.A. Allah, A. Hashem, R. Sarah, M. Hashim, Saudi J. Biol. Sci.**25**, 1365 (2018).
[10] wikipedia.org/wiki/Kodaikanal mercury poisoning.
[11] E. Shaji, M. Santosh, K.V. Sarath, P. Prakash, V. Deepchand, B.V. Divya, Geosci. Front. (2020). (In press.)
[12] A. Das, S.S. Patel, R. Kumar, K.V.S.S. Krishna, S. Dutta, M.C. Saha, S. Sengupta, D. Guha, Chemospehre**197**, 152 (2018).
[13] P. Sharma, V. Bihari, S.K. Agarwal, V. Verma, C.N. Kesavachandran, B.S. Pangtey, N. Mathur, K.P. Singh, M. Shrivastava, S.K. Goel, Plos one**7**, 1 (2012).
[14] T.E.D. Thangam, V.N. Kumar, Y.A. Vasline, Int. J. Appl.Eng. Res.**13**, 4878 (2018).
[15] S. Giri, A.K. Singh, M.K. Mahato, J. Earth Syst. Sci.**126**, 1 (2017).
[16] P.K. Pandey, R. Sharma, M. Roy, M. Pandey, Environ. Geochem. Health**29**, 237 (2007).
[17] G. Rathor, N. Chopra, T. Adhikari, Int. Res. J. Environment Sci.**3**, 94 (2014).
[18] V. Kumar, P.K. Bharti, M. Talwar, A.K. Tyagi, P. Kumar, Water Sci.**31**, 44 (2017).
[19] B. Das, Recent Res. Sci. Technol.**6**, 27 (2014).
[20] P. Manikandaraja, R. Senthilkumar, Int. J. Adv. Multidiscip. Res.**1**, 63 (2014).
[21] V. Srivastava, C.H. Weng, V.K. Singh, Y.C. Sharma, J. Chem. Eng. Data**56**, 1414 (2011).
[22] W. Jianlong, Z. Xinmin, Q. Yi, J. Environ. Sci. Health A**35**, 1211 (2000).
[23] M. Uysal, A. Irfan, J. Hazard. Mater.**149**,482 (2007).
[24] A.G. El Samrani, B.S. Lartiges, F. Villieras, Water Res.**42**, 951 (2008).

[25] C.A. Kozlowski, W. Walkowiak, Water Res.**36**, 4870 (2002).

[26] D.M. Roundhill, H.F. Koch, Chem. Soc. Rev.**31**, 60 (2002).

[27] L.F. Greenlee, D.F. Lawler, B.D. Freeman, B. Marrot, P. Moulin, Water Res.**43**,2317 (2009).

[28] M. Ince, O.K. Ince, Int. J. Pure Appl. Sci.**3**, 10 (2017).

[29] S.D. Gisi, G. Lofrano, M. Grassi, M. Notarnicola, SM&T**9**, 10 (2016).

[30] M.T. Yagub, T.K. Sen, S. Afroze, H.M. Ang, Adv. Colloid Interface Sci.**209**, 172 (2014).

[31] E. Pehlivan, B.H. Yanik, G. Ahmetli, M. Pehlivan, Bioresour. Technol.**99**, 3520 (2008).

[32] S. Mohan, R. Gandhimathi, J. Hazard. Mater.**169**, 351 (2009).

[33] H. Parab, S. Joshi, N. Shenoy, A. Lali, U.S. Sarma, M. Sudersanan, Process Biochem.**41**, 609 (2006).

[34] R. Chakraborty, R. Verma, A. Asthana, S. Sree Vidya, A.K. Singh, Int. J. Environ. Anal. Chem. 1 (2019).

[35] S.W.AlRmalli, A.A. Dahmani, M.M. Abuein, A.A. Gleza, J. Hazard. Mater.**152**,955 (2008).

CHAPTER

7

THE HIDDEN TREASURES OF THE PERIODIC TABLE: AN OVERVIEW OF F-BLOCK ELEMENT

Akhilesh Chandra Verma [1], **Maithili Kumari Patel** [2]
Govt. Naveen College Kui-Kukdur
dr.acverma8@gmail.com

ABSTRACT:

The f-block elements, comprising the lanthanides and actinides, are often referred to as the hidden treasures of the periodic table due to their unique electronic configurations and diverse chemical properties. This abstract provides an overview of the f-block elements, highlighting their significance in various fields such as materials science, catalysis, and nuclear technology. Key topics discussed include the electronic structure, bonding behavior, and applications of lanthanides and actinides. Through this comprehensive overview, readers will gain insights into the fascinating world of f-block elements and their pivotal role in shaping modern science and technology.

Keywords: f-block elements, lanthanides, actinides, periodic table, electronic structure, chemical properties, materials science, catalysis, nuclear technology.

7.1. INTRODUCTION:

The f-block elements, including lanthanides and actinides, are considered secret gems of chemical study. They are located deep within the periodic table. Their unique electrical arrangements and chemical activities have intrigued scientists for decades. This introduction provides a brief overview of f-block elements and their importance in several scientific disciplines. From their fascinating electrical structures to their critical roles in materials research and nuclear applications, the f-block elements continue to reveal their secrets, increasing our comprehension of the periodic table's intricacies.

F-BLOCK ELEMENTS

- F-block elements may broadly by defined as those which either as elements or as ions have partially filled f-subshells, the elements called as f-block elements (inner transition elements).
- They are separately situated from modern periodic table
- They are also called rare earth elements
- General electronic configuration are:-
- $(n-2)f^{1-14},(n-1)d^{0-1},ns^{2}$
- f-block elements are classified into 2 series:-

1. Lanthenides
2. Actinides

LANTHENIDES:

- Elements having atomic no. between 58-71 these are known as lanthanides.
- No. of lanthenide elements are 14
- They are also known as inner transition elements
- Also called rare earth elements
- All lanthanide elements are denoted by Ln symbol
- Pm(promethium) is radioactive lanthanide

ELEMENTS	SYMBOL	ATOMIC NO.	ELECTRONIC CONFIG.	OXIDATION STATE
Lanthanum	(La)	57	[Xe] $4f^0$ $5d^1$ $6s^2$	+3
Cerium	(Ce)	58	[Xe] $4f^1$ $5d^1$ $6s^2$	+3,+4
Praseodymium	(Pr)	59	[Xe] $4f^3$ $5d^1$ $6s^2$	+3,+4
Neodymium	(Nd)	60	[Xe] $4f^4$ $5d^1$ $6s^2$	+2,+3,+4
Promethium	(Pm)	61	[Xe] $4f^5$ $5d^1$ $6s^2$	+3
Samarium	(Sm)	62	[Xe] $4f^6$ $5d^1$ $6s^2$	+2,+3
Europium	(Eu)	63	[Xe] $4f^7$ $5d^1$ $6s^2$	+2,+3
Gadolinium	(Gd)	64	[Xe] $4f^7$ $5d^1$ $6s^2$	+3
Terbium	(Er)	65	[Xe] $4f^9$ $5d^1$ $6s^2$	+3,+4
Holmium	(Ho)	66	[Xe] $4f^{10}$ $5d^1$ $6s^2$	+3
Erbium	(Dy)	67	[Xe] $4f^{12}$ $5d^1$ $6s^2$	+3
Dysprosium	(Tb)	68	[Xe] $4f^{11}$ $5d^1$ $6s^2$	+3
Lutetium	(Tm)	69	[Xe] $4f^{14}$ $5d^1$ $6s^2$	+2,+3
Ytterbium	(Lu)	70	[Xe] $4f^{14}$ $5d^1$ $6s^2$	+2,+3
Thulium	(Yb)	71	[Xe] $4f^{13}$ $5d^1$ $6s^2$	+3

7.2. CHARACTERSTICS OF LANTHENIDES:

1. **Oxidation state –**
   - The chemistry of lanthanides elements are based on Ln3+ion.
   - The most stable oxidation state of lanthanides is +3O.S.
   - Some lanthanides show +2 and +3O.S. also.
   - Oxidation states of lanthanides are given in above table .

2. **Reducing property -**
   - Lanthanides behaves as strong reducing agents because they are rapidly released their 3 electrons and getting oxidized
     $Ln \dashrightarrow Ln^{3+} + 3e^-$

3. **Electropositive character-**
   - Lanthanides are strong electropositive elements because they shows metallic nature.

4. **Reaction with H_20-**
   - Lanthanides reacts with water and release hydrogen gas.
   - Fastly react with hot water and slowly react with cold water
   - $2Ln+H_2O \dashrightarrow 2Ln(OH)_3 + 3H_2$

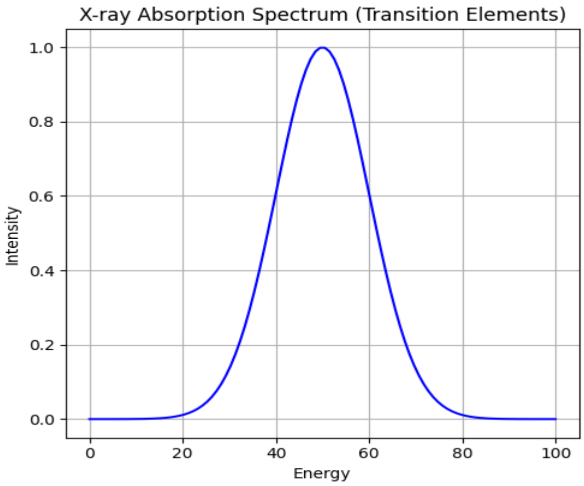
5. **Reaction with halogen –**
   - Lanthanides react with halogen and form trihalide
   - $2Ln+3X_2 \dashrightarrow 2LnX_3$

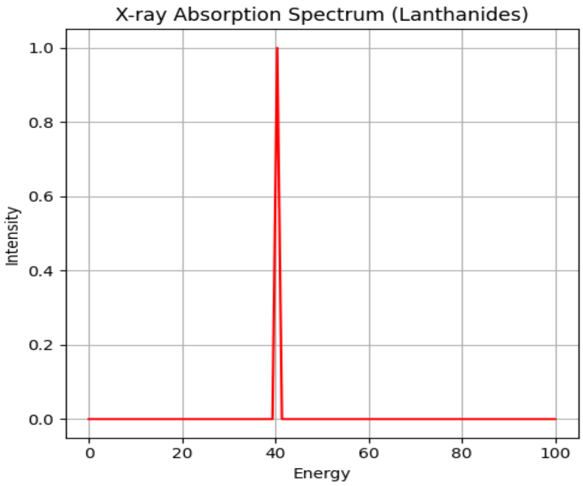
6. **Reaction with hydrogen –**
   - At high temp(300-4000^{0}C) lanthanides react with hydrogen and for LnH_2 and LnH_3

7. **Reaction with oxygen –**
   - Lanthanides react with atmospheric oxygen and form oxide
   - Ex- $2Ln+3O_2 \dashrightarrow 2Ln_2O_3$

8. **Colour and electronic spectra –**
   - The reason for colour in lanthanides are charge transfer and f-f transition.
   - $La^{3+} \dashrightarrow f^0 \longrightarrow$ no f-f transition ,colourless
   - $Ce^{2+} \dashrightarrow$ intense red colour , due to LMCT.
   - $Ce^{3+} \dashrightarrow$ colourless due to showing absorbtion in UV range

9. **Absorbtion spectra –**
   - Transition elements show broad peak
   - But lanthanides show sharp peak due to absence of L-S coupling (vibronic coupling)





10. Lanthanide contraction –

- The size of lanthanide ion decrease from La^{3+}-$Lu^{3+}$is known as lanthanide contraction.
- **Consequences of lanthanide contraction-**

- Variation of their chemical properties
- Electro negativity of trivalent ions from La to Lu slightly increase due to Lanthanide contraction.
- The tendency of stable complex formation from La^{3+} to Lu $^{3+}$increase due to lanthanide contraction
- Due to lanthanide contractions lanthanides are separated by ion exchange method.

7.3. APPLICATIONS OF LANTHENIDES

- In the chemical reactions e.g. hydrogenation and oxidation of various organic compound lanthanide compounds are used as catalysts
- Ce can absorb both temperature and UV light therefore, it is used in formation of glasses
- CeO_2 used in formation of gas metal.
- Lanthanide salts are also used in laser e.g. Nd_2O_3
- Lanthanide compound (cerium phosphate) used in breaking of petroleum materials.

ACTINIDES

- The elements having atomic number between 90 to 103 these are called **actinoids**
- **Also called inner transition element**
- **Actinoids are seventh period elements**
- Number of actinoid elements are 14
- All actinoids are radioactive
- These elements are denoted by [An].
- Actinoids are started from Th_{90} thorium to Lr_{103}lawrencium .

- Elements after U_{92} uranium all are unstable and not exist in nature
- These unstable elements (after uranium) are called **transuranic elements.**

ELECTRONIC CONFIGURATION OF ACTINOIDS

ELEMENTS	SYMBOL	ATOMIC NO.	ELECTRONIC CONFIG.	OXIDATION STATE
Actinium	Ac	89	[Rn] $5f^{0}\ 6d^{1}\ 7s^{2}$	+3
Thorium	Th	90	[Rn] $5f^{0}\ 6d^{2}\ 7s^{2}$	+3,+4,
Protactinium	Pa	91	[Rn] $5f^{2}\ 6d^{1}\ 7s^{2}$	+3,+4,+5
Uranium	U	92	[Rn] $5f^{3}\ 6d^{0}\ 7s^{2}$	+3,+5,+6,
Neptunium	Np	93	[Rn] $5f4^{6}d^{0}\ 7s^{2}$	+3,+4,+5,+6,+7
Plutonium	Pu	94	[Rn] $5f^{5}\ 6d^{0}\ 7s^{2}$	+3,+4,+5,+6,+7
Americium	Am	95	[Rn] $5f^{6}\ 6d^{0}\ 7s^{2}$	+3,+4,+5,+6
Curium	Cm	96	[Rn] $5f^{7}\ 6d^{0}\ 7s^{2}$	+3,+4
Berkelium	Bk	97	[Rn] $5f^{8}\ 6d^{1}\ 7s^{2}$ [Rn] $5f^{9}\ 6d^{0}\ 7s^{2}$ (preferred)	+3,+4
californium	Cf	98	[Rn] $5f^{10}\ 6d^{0}\ 7s^{2}$	+3
einsteinium	Es	99	[Rn] $5f^{11}\ 6d^{0}\ 7s^{2}$	+3
Fermium	Fm	100	[Rn] $5f^{12}\ 6d^{0}\ 7s^{2}$	+3
Mandelevium	Md	101	[Rn] $5f^{13}\ 6d^{0}7s^{2}$	+3
nobelium	No	102	[Rn] $5f^{14}\ 6d^{0}\ 7s^{2}$	+2,+3
lawrencium	Lr	103	[Rn] $5f^{14}\ 6d^{1}\ 7s^{2}$	+3

7.4. CHARACTERISTICS OF ACTINOIDS

1. Oxidation State

- Actinoids generally shows + 3 oxidation State
- Some actinoids also show + 4 oxidation State
- Nobellion also shows + 2 oxidation State
- U,Np , Pu , Am + 6 and + 5 oxidation State (Pu=+3to + 7 oxidation State)

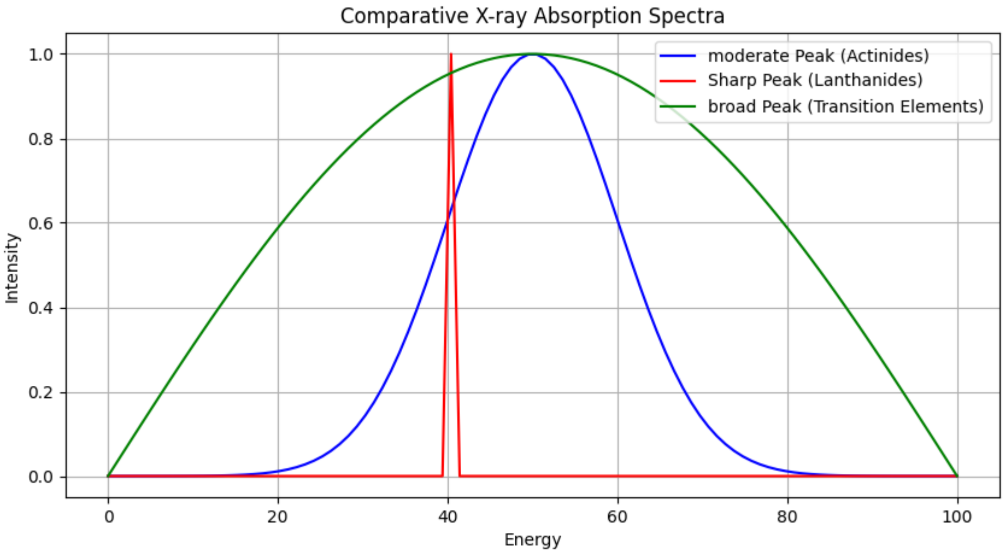
- Np =+ 3 to + 7 oxidation State
- Example uranyl ion $[UO2]^{2+}$ (Oxidation State + 6)

2. Ionic radii

- . Size of actinoid elements are like as lanthanides
- Due to actinoid contraction like lanthanide contraction when going toward left to right the size of actinoids decrease

3. Colour and electronics spectra

- Due to 5f -5f transition actinoid complex are coloured
- Due to LMCT they are coloured
- The actinoids element having F^1 configuration they do not show colour because it 1st transition is in UV range
- Lanthanide complex show sharp peak due to the absence of LS coupling (vibronic coupling) and transition elements show broad peak but actinoids show moderate peak



4. Actinoid contraction

- Like lanthanide contraction these actinoid elements also show actinoid contraction actinoid contractions are result of weak screening effect of nuclear charge in 5f electron
- Consequences of actinoid contraction when atomic number increase in actinoid their size decrease

5. Reactivity of actinoid

- Then actinoids are heated with water it form related hydroxide and oxide
- Actinoid react with HCl and form related chloride
- Actinoids react with HNO3 slowly due to metal oxide formation
- Actinoid complexes are covalent in nature and lanthanide complexes are ionic in nature

7.5. APPLICATIONS OF ACTINOIDS

- Thorium and uranium are used as nuclear fuel in atomic reactors
- Uranium salts are used in textile industry
- Zine uranyl acetate is specific reagent for identification of sodium metal
- Urinal phosphate is used in volumetric analysis of phosphate
- These all actinoid elements are used as atomic weapon

7.6. CONCLUSION

In conclusion, the f-block elements, consisting of the lanthanides and actinides, represent a fascinating and important group within the periodic table. Throughout this chapter, we have explored the unique characteristics and diverse properties of these elements, often referred to as the hidden treasures of the periodic table. From their intriguing electronic configurations to their wide-ranging applications in materials science, catalysis, and nuclear technology, f-block elements continue to intrigue scientists and researchers worldwide. Despite their relatively late discovery and complex chemistry, lanthanides and actinides play crucial roles in various fields, including medicine, energy production, and environmental science. Their ability to exhibit a wide range of oxidation states, form coordination compounds, and participate in redox reactions makes them indispensable in modern technology and industry. As we continue to uncover the mysteries of f-block elements, it is clear that further research and exploration are essential for fully understanding their behavior and unlocking their potential. With advancements in analytical techniques and computational methods, we can expect even greater insights into the chemistry and applications of lanthanides and actinides in the years to come.

In summary, the study of f-block elements not only enriches our understanding of the periodic table's complexities but also holds promise for addressing some of the most pressing challenges facing society today.

REFERENCES

1. Cotton, F. A., & Wilkinson, G. (1980). Advanced inorganic chemistry. John Wiley & Sons.
2. Greenwood, N. N., & Earnshaw, A. (1997). Chemistry of the elements. Butterworth-Heinemann.
3. Emsley, J. (2011). Nature's building blocks: An A–Z guide to the elements. Oxford University Press.
4. Liddell, M. J. (1997). The chemistry of the f-block elements. VCH Publishers.
5. Saito, Y. (2017). The f-block elements: Cerium, Yttrium, and the Lanthanides. Elsevier.
6. Cotton, S. A. (2006). Lanthanide and actinide chemistry (Vol. 185). John Wiley & Sons.
7. Katz, J. J., & Seaborg, G. T. (Eds.). (2002). The chemistry of the actinide elements (Vol. 1). Chapman and Hall.
8. Morss, L. R., Edelstein, N. M., & Fuger, J. (2006). The chemistry of the actinide and transactinide elements (Vols. 1–6). Springer.

9. Meyer, G., & Hermann, A. (2013). Actinide elements and their compounds with other elements. Springer Science & Business Media.
10. Kaltsoyannis, N., &Bursten, B. E. (2005). The actinide elements. Oxford University Press.
11. Haire, R. G. (2015). The chemistry of the actinide and transactinide elements. Springer.
12. Huheey, J. E. (1983). Inorganic chemistry: Principles of structure and reactivity. Harper & Row.
13. Lee, J. D. (1991). Concise inorganic chemistry. Blackwell Science.

CHAPTER

8

ANALYSIS OF WATER SAMPLES IN DURG BHILAI AREA AND IT'S IMPACT ON ENVIRONMENT

Sagar Mallick[a], Deepshikha Haldar[a], Damini Vishwakarma[a*]
[a]Departmentof Chemistry, Sai College, Sector-6, Bhilai Dist. Durg (C.G.)
daminiv0709@gmail.com

ABSTRACT

Nearly every day since the late eighteenth century, when the industrial revolution began, new causes of pollution have been found worldwide. Therefore, pollution of the air and water is a possibility everywhere. Changes in the rates of pollution are not well understood. An accurate indicator of the level of environmental contamination is the rise in illnesses linked to water. The ecological criteria of water quality—both for people and other living things—are compiled in this chapter. Water can be divided into four categories based on its quality. A thorough analysis of the significant characteristics that these water qualities have in common, such as physical, chemical, and biological parameters, is used to discuss them. The meaning, origins, implications, consequences, and methods of measurement of these water quality metrics are discussed.

8.1. INTRODUCTION:

To thrive, all plants and animals require water. Without water, life on Earth is not possible. Since 60% of our body weight is composed of water. Water is used by our bodies to support many physiological processes and to assist control body temperature in all of the cells, organs, and tissue due to the way our bodies work[1].After air, water is arguably the most valuable natural resource. Even while water makes up the majority of the earth's surface, relatively little of it is really exploitable, making it a very scarce resource. Therefore, care must be taken when using this valuable and finite resource. Water needs to be suitable before usage because it is used for many purposes. Additionally, water sources need to be routinely inspected to assess their overall condition[2]. Water is a plentiful natural resource on Earth and one of the essential necessities for human survival[3].

Study Area

- Khurshipar, Power House Bhilai, Dist. Durg, Chhattisgarh.
- It is located 15 Km from Sai College, Sector - 6 Bhilai.
- There are about 1000 houses in Khurshipar village.

Figure: 1. Khursipar, Power House, Bhilai, Dist. Durg (C.G.)

8.2.Objectives :

The main objectives of this study are

- To determine the chemical parameters like order and Color, solids and electrical conductivity.
- To determine the chemical parameter like pH, acidity, alkalinity, and chlorideconcentration, BOD, COD and TDS.
- Reveal a range of information, including the presence of pathogens, the levels of nutrients or pollutants, and the water's overall health.
- An essential component of industrial and agricultural operations.
- Water testing is essential for protecting human health, the environment, and industrial and agricultural operations.

8.3. Methodology

8.3.1 Sampling Source–

- Sample (1) : ACC Jamul
- Sample (2) : Laxmi Taxtiles Jamul
- Sample (3) :Punjuster Industrial Pvt. Ltd
- Sample (4) : Engineering Corporation Ltd

8.3.2 Sample collection –

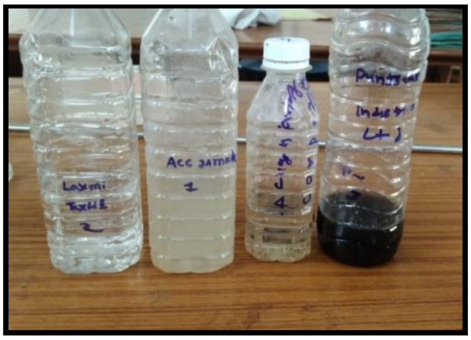


Figure: 2. Collected samples.

8.4.Analysis of Physiological Parameters:

Water sample is collected from the area of KURSHIPAR, POWER HOUSE, BHILAI DISTRICT DURG CHHATTISGARH.

Parameters:

4.1 Odours and Color
4.2 pH Measurement
4.3 Alkalinity and Acidity
4.4 Electrical Conductivity
4.5 Chloride Concentration
4.6 Total Dissolved Solid [TDS]
4.7 Dessolved oxygen [DO]
4.8 Hardness of Water

8.4.1. Odour and Color: Water gets coloured by materials that have decomposed from organic matter, like flora, and inorganic stuff, such soil, stones, and rocks. This is undesirable for aesthetic reasons alone, not health-related ones [4]. The water sample's colour is determined by comparing it to coloured glass discs or standard colour solutions [5]. The colour produced by a 1 mg/L solution of platinum (potassium chloroplatinate, K_2PtCl_6) is equal to one color unit.

By measuring a volume of sample A and diluting it with a volume of sample B of odor-free distilled water, the numerical value of odour or taste is quantitatively determined. This results in a mixture whose odour is very slightly discernible at a total mixture volume of 200 ml [6]. The following is the expression of the odor or taste unit in terms of a threshold number:

8.4.2. pH Measurement :

Hydrogen (H) potential, or pH, is a unit of measurement for the amount of H^+ ions in a solution. The pH scale's units vary from 0 to 14 as a mathematical result of the formula that defines pH. Neutrality is represented by a value of 7, while values below 7 are referred to as acidic and values above 7 as basic or alkaline. Extremes of acidity and basicity are represented by values near 0 and 14, respectively. Water intended for drinking should generally have a pH of 6.5 to 8.5[7].

Figure: 3. Digital pH Meter

Table 1. pH measurement of samples.

S. No.	Sample Description	Temperature of sample [°C]	pH value
1	Sample 1	27°C	6.40
2	Sample 2	27°C	6.44
3	Sample 3	27°C	5.70
4	Sample 4	27°C	6.22

8.4.3. Alkalinity: The concentration of bases in a solution or the capacity to neutralize acids in water is referred to as water alkalinity. Another name for it is water's buffering capability. Carbonates, bicarbonates, magnesium bicarbonate, ammonia, borate, phosphates, silicates, and organic bases are a few examples of bases. Practically speaking, the primary components that contribute to water's alkalinity are carbonates and bicarbonates. Since calcium carbonate is the source of corrosion, the pH and alkalinity of the environment affect the corrosion process[8].

Figure: 4.Alkalinity measurement.

Table 2. Alkalinity of samples.

S. No.	Sample Description	Color of sample	Alkalinity
1.	Sample 1	Pink color not show	Absent
2.	Sample 2	Pink color not show	Absent
3.	Sample 3	Pink color not show	Absent
4.	Sample 4	Pink color not show	Absent

8.4.4. Acidity: Natural water's acidity, which is the ability to neutralize bases, is mostly caused by dissolved CO_2. However, mineral acids (below pH 4) may be the cause of acidity in water contaminated by trade wastes. CO_2 causes acidity, which is found in the pH range of 4.5-8.3.Acidity is absent from a sample whose pH is greater than 8.3[9].

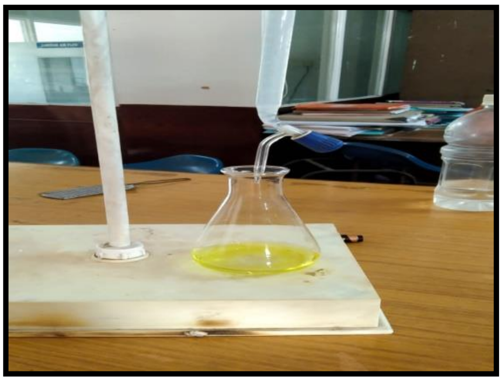


Figure: 5. Measurement of Acidity.

Table 3. Acidity measurement of samples.

S. No.	Sample Description	Color of sample	Acidity
1	Sample 1	Orange Red color show	present
2	Sample 2	Orange Red color show	present
3	Sample 3	Orange Red color not show	Absent
4	Sample 4	Orange Red color show	present

8.4.5. Electrical Conductivity: The conductance produced by different ions in the solution or water is measured using this technique. By multiplying specific conductance (measured in S/cm) by an empirical factor, which can range from 0.55 to 0.90 based on the soluble components of the water and the measurement temperature, one can approximate the dissolved ionic contents of a water sample.

An accurate and quick estimation of the fluctuations in a water body's dissolved mineral concentration can be obtained using conductivity monitoring[10].

Table 4. Conductivity measurement of samples.

S. No.	Sample Number	Conductivity (S/cm)	Temperature (°C)
1.	Sample1	1076.9	25^0C
2.	Sample2	68.4	25^0C
3.	Sample3	1590.9	25^0C
4.	Sample4	54.6	25^0C

8.4.6. Chloride Concentration: Chlorides are commonly found in water as calcium, sodium, and potassium salts. The salty taste that chloride concentrations in drinkable water produce varies and is influenced by the chemical makeup of the water.The two main salts in water that produce flavor are calcium and sodium chlorides. The chloride anions and related cations in water are what give it its salty flavor. If the cat-ion present in the water is sodium, some water with only 250 mg/L of chloride may taste noticeably salty. However, even in cases where the water has a very high content of chloride (1000 mg/L), a typical salty flavor may not be present. This is due to the fact that calcium or magnesium may be the main cation in the water rather than sodium[11].

Figure: 6. Chloride Concentration measurement.

8.4.7. Total Dissolved Solids (TDS): Material that is either filterable or not that remains after evaporating and drying at a specific temperature is referred to be "solid." The temperature used for drying and igniting determines further classification. Depending on the methodology used to determine them, many types of solids are identified. Solids can negatively impact the quality of water or wastewater in a variety of ways. High dissolved solids water generally has worse palatability and can cause an adverse physiological reaction in the momentary user. Water with a high mineral content is not suited for many industrial uses. For uses like bathing, high suspended particles in the water may not be visually appealing. Total solids analysis is crucial in determining thedifferent unit activities and procedures in the physical and biological treatment of waste water, as well as to evaluate its performance. Waste water effluent limitations for different types of solid materials serve as indicating parameters for evaluating conformity with regulatory agencies[12].

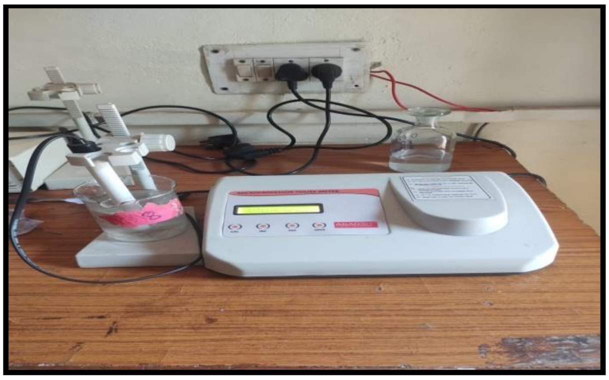


Figure: 7. Conductivitymeter and TDS (Total Dissolved Solid) meter.

Table 5. Measurement of total dissolved solid of water samples.

S. No.	Sample Number	TDS (ppm)	Temperature (°C)
1	Sample1	721 ppm	25^0C
2	Sample2	44.67 ppm	25^0C
3	Sample3	1065.91 ppm	25^0C
4	Sample4	243.64 ppm	25^0C

(TDS = Total Dissolved Solid, ppm = Parts Per Million)

8.4.8. Dissolved oxygen (DO): The amount of dissolved oxygen in a unit volume of water is referred to as dissolved oxygen.[1].The minimum DO level of 4 to 5 mg/L or ppm is optimal for survival of aquatic life. The wastes serve as the food for certain aerobic microorganisms. Moving downstream, the concentration of microorganisms rises. The amount of DO decreases as a result of these bacteria's population growth since they take oxygen out of water.Water samples' oxygen content is influenced by several physical, chemical, biological, and microbiological activities. In addition, DO values display seasonal, lateral, and geographical variations based on human, industrial, and thermal activities. Waste increases cause a decrease in dissolved oxygen in water bodies. Because there is not enough oxygen in the water, living things suffocate and eventually perish. Following wastewater treatment, DO levels rise but remain below the danger threshold [13-15]. Consequently, the BOD test, a crucial factor in determining a waste's potential for organic pollution, is based on the results of the DO test.

Figure: 8. Measurement of Dissolved Oxygen (DO) in water samples.

8.5. Impact of water quality parameters on environment:

- Many biological processes, such as everyday metabolism and reproduction, are hampered in acidic (pH too low) or alkaline waters (pH too high).

- Dissolved oxygen is a basic requirement for a healthy aquatic ecosystem. Most fish and beneficial aquatic insects "breathe" oxygen dissolved in water. Although oxygen concentrations fluctuate under natural conditions, human activities can result in severe oxygen depletion. Waterways are also contaminated by heavy metals and chemicals from urban and industrial wastewater. These pollutants accumulate up the food chain when predators devour prey because they are hazardous to aquatic life and frequently shorten an organism's life span and capacity for reproduction. This is the process by which large fish like tuna and others gather large amounts of pollutants like mercury.

- The growth of newly supplied nutrients drives plant and algae growth, which lowers oxygen levels in the water when water pollution creates an algal bloom in a lake or marine environment. Eutrophication, the lack of oxygen in the water, causes suffocation in plants and animals and can result in "dead zones," or areas where there is virtually no life at all. Under some circumstances, these dangerous algal blooms can also release neurotoxins that damage animals, including sea turtles and whales.
- High levels of chloride ions in drinking water have a bad taste and are bad for people's health. Skin injury results from human contact with water with high levels of chloride ions.
- The concentration of dissolved ions can lead to scale formation, which reduces the effectiveness of hot water heaters, and caustic, brackish, or salty water.
- Numerous things can happen when the pH of water changes. Acidification of the environment causes harm, if not outright death, to a great number of plants and animals. The sensitivity of many fish species and aquatic life to variations in water temperature and composition is remarkable. The pH required by some aquatic organisms is shown in the diagram below. Observe that the environment has a wide range of biodiversity when the pH is between 6.0 and 7.0, which is typical for many lakes and streams. Fewer and fewer creatures can endure as the pH drops and the acidity rises.

REFERENCES

1. Spellman FR. Handbook of Waterand Wastewater Treatment Plant Operations. 3rd ed. Boca Raton: CRC Press; 2013.
2. S. P. Gorde et al Int. Journal of Engineering Research and Applications www.ijera.com ISSN: 2248-9622, Vol. 3, Issue 6, Nov-Dec 2013, pp.2029-2035.
3. WHO (World Health Organization) Guidelines for drinking water quality, 2nd Ed.,1993, Vol. 1.
4. Bureau of Indian Standards, 2012, Indian Standard Drinking Water Specification (Second Revision).
5. Metcalf E., Eddy H., 2003, Wastewater Engineering: Treatment and Reuse, Tata McGraw-Hill Publishing Co Ltd, India.
6. World Health Organization, 2004, Guidelines for Drinking-Water Quality (3rd edition).
7. Annual Book of ASTM standards, 1993, Vol. 1 1.02 Water (1). American Society for Testing and Materials, Philadelphia.
8. Chapman, D., Ed., Water Quality Assessments - A Guide to the use of biota, sediments and water in environmental monitoring, 1992, Chapman and Hall Ltd., London.
9. P. J. Puri, M. K. N. Yenkie, S. P. Sangal, N. V. Gandhare, G. B. Sarote and D. B. Dhanorkar, 2011, Vol.4, No.1, 43-48.
10. Roy R., Majumder M. 2018 A Quick Prediction of Hardness from Water QualityParameters by Artificial Neural Network. International Journal of Environment and Sustainable Development, 17(2/3), 247-257.
11. Tyagi S., Sharma B., Singh P., Dobhal R. 2013; Water Quality Assessment in Terms of Water Quality Index. American Journal of Water Resources, 1(3), 34-38.
12. Fresen~us, W., Quentin, K.E., and Schne~der, W., Eds., Water Analysis, 1988, Springer-Verlag Berl~nHe~delberg. Germany.
13. Brown R. M., McClelland N. I., Deininger R. A., and Tozer R. G. 1970 Awater qualityindexes- do we dare? Water and Sewage Works, October 1970, 339-343.
14. Jeffery, G. H., Bassett, J., Medham, J. and Denney, R.C., Vogel's Textbook of Quantitative Chemical Analysis, 1989, Part B: Errors, statistics and sampling (125-149), Longman, New York.
15. Roy R., Majumder M. 2017 Comparison of surface water quality to land use: a case study from Tripura, India. Desalination and Water Treatment, 85, 147-153.

CHAPTER

9

COMPREHENSIVE REVIEW ONGREEN FILLERS REINFORCED POLYMERICCOMPOSITES-MATERIALS AND PROCESSES

Dr. C.Anand Chairman[1], Dr.G.Saravanan[2] and Mr.M.Pradeep[3]
[1]Associate Professor,Department of Mechanical Engineering
[2]Head,Department of Mechanical Engineering,
[3]Assistant professor, Department of Mechanical Engineering,
ST.JOSEPH'S COLLEGE OF Engineering and Technology
mechanand2003@gmail.com

ABSTRACT

Green based materials are considered as future generation materials for lightweight and sustainable composites. Natural and eco-friendly green fillers have been used as green materials in the process of polymer composites. The materials made by green filler are called as green polymer composites having demonstrated distinctive properties of adding together the advantages of natural fillers and organic fillers. Most of the green fillers are derived from plant and trees as they have good strength, low price of acquisition and create low carbon dioxide discharge. Also, theypossesscharacteristics such as biodegradable and renewable compared to other fillers. They became popular in recent research activities due to no environmental hazards. These factors lead to the riseof the use of green fillers in the composites which are used in the field of construction, packaging, therapeuticand various Engineering sectors where environmental sustainability is the most important one. This chapter will review some of the past, present and future research efforts, trends, ideas and state of affairs in the discipline of greenfillersreinforcedpolymeric composites.

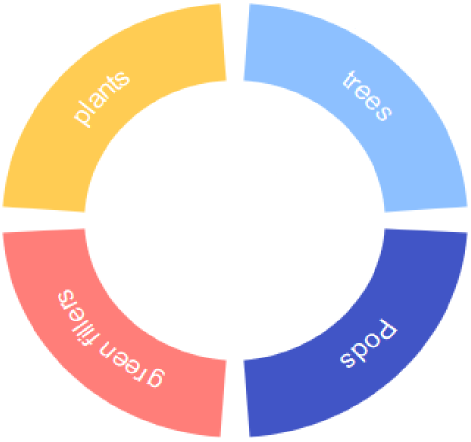
9.1. INTRODUCTION

Shocking report from world wide fund indicated thatthe plastic waste in the world's oceans will reach 300 million tons by 2030. According to the report, in future pollution due to plastics will double over the next ten years and will create a dangerous scenario into the surroundings.According to the report by WWF plastic production surpassed 400 million metric tons in 2022, at an annual increase of 1.6 percent.By the year 2025 it is projected that the global production of thermoplastics will amount to 445.25 million metric tons.[1].Nowadays almost all plastics are produced from the petro based materials.The dump of this waste materials due to plastics are impossible task because of their failure to degradability. Also, the drawbacks of these conventional plastics such as non-renewable, pollution of air and consumption of high-energy during manufacturing are the important ones. The disposal of plastics is also a difficult task andcreate environmental and ecological problem. The nature of nondegradable of plastic waste creates a lot of damage to the living organisms in marine and wildlife.The consumption of plastics can be minimized by increasing the volume fraction of fillers in the plastic materials. The green filler materials are recently gained popularity because of the biodegradability and compostability, antimicrobial activity, abundantly available and cleaner green environment.Hence the authors Amar Mohanty [2] and his coauthor rightly pointed out that 100 % bio-basedcomposites are termed as green. Similarly, 100 % bio-based fillers are called as green fillers. Currently, all-green materials exhibit limited success because of their less affordability and durability restrictions in different sectors like automotive and structures used in housing. But they are gaining popularity in sustainable packaging. The use of green fillers derived from plants, seeds, shells, and podsreveals enormous potential for lightweight sustainable composites in auto parts and other growing demands from the manufacturing sector. However, poor performance and usefulness are not enough to create a market for green fillers. They must also provide effective end products that are suitable for different industrial applications and provide distinctive benefits in usage over conventional filler filled plastics [3].

Green fillers have appeared as a viable alternative to solve the problems based with existencewith non-renewable filled petro-based polymers. The Australian Bioplastics Association states that bioplastics/green encompass a whole family of materials, which are bio-based, biodegradable, or both [4]. These are usually consequent from renewable sources, which are sustainable over time. Owing to the importance ofgreenfillers, the countries like USA, European, and other countries encourage the use of green composites with a high number of green fillers or natural resources [5–9]. The need of utilizing green materials/ecofriendly materials for the manufacturing of composites is increasing and became popular becauseit promotes the sustainability of the products during processing and end of life.Green fillers are sustainable potential materials as reinforcing agents for different polymer matrices in varying applications such as automobile, construction, aerospace, toys, defence, sporting goods, The need for eco-friendly materials based on green fillers has been attracted due to renewability, abundance availability, low cost, and so on. Therefore, this chapter highlights the importanceofsomegreen fillers for the preparation of composite materials in research areas.

9.2. DEFINITION OF GREEN FILLER

Fillers are defined as a variety of inorganic, organic particulates that may be irregular, acicular, fibrous, or plate-like in shape and which are used in reasonably large volume loadings in plastics. Pigments and elastomeric matrices are not normally included in this definition.The addition of fillers is to increase the strength of a final composite,to decrease the thermal expansionand to minimize the shrinkage of the composites during curing. Green fillers may be derived from natural resources such as Wood apple,Elaeocarpusganitrusand wall nut etc,are attracting the attention of researchers to replace synthetic fillers in designing green based materials.Also, green fillers are obtained from bio-waste which are abundantly available as renewable sourcesin minimum cost. **Fig 1** illustrated the sources of the fillers required for green materials.



9.3. TYPES OF FILLER

Fillers are classified based on ceramics, carbon, metal, and hybrid fillers. It is represented as a chart mentioned below. However green fillers include bio-based materials and natural resources. Recently the term green filler is used by various researches and scientists. Accordingly, the materials obtained from plants, trees, flowers, seeds, leaves, buds, nutshells, and shrubs are considered as green fillers.

So green fillers are obtained from natural resources and some of the green fillers used are given below.

The following **Table1** indicates the type of source, botanical name, applications, name of the resin used with the images are given below

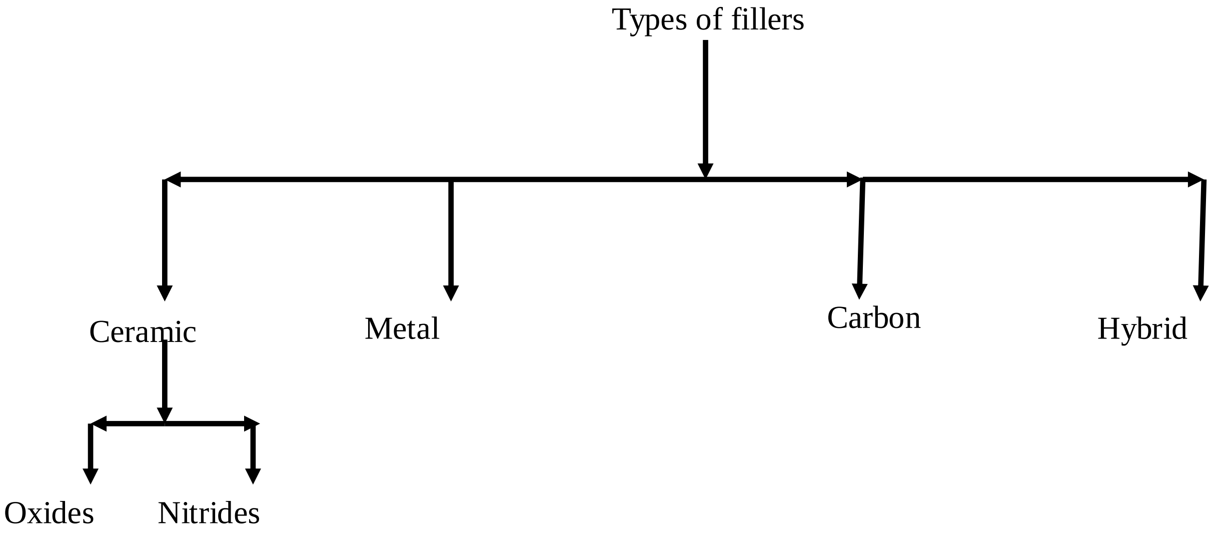


Table1.Polymer matrix composites reinforced with green fillers and their botanical names

Sl.no	Type of source	Botanical name	Commercial name	Photographs	Type of resin	Ref.
1	Shell	Limoniaacidissima	Wood apple		Epoxy	10
2	Seed	Elaeocarpus ganitrus	Rudraksha		Epoxy	12

3	Seed	Delonix regia	Royal poinciana(flamboyant)		Polyester	14
4	Shell	Juglans regia L	Walnut		polypropylene	15
5	Seed	Ceiba pentandra	Kapok		Epoxy	17
6	Shrub	Ipomoea carnea	Bush Morning Glory		Epoxy	20
7	Seed	Prunus avium	Cherry seed		polypropylene	21
8	Seed	Annona Reticulata	Custard apple		Epoxy	22
9	Seed	Phoenix dactylifera L	Date seed		Epoxy	23

9.4. GREEN FILLER MATERIALS

In this world lot of fillers based on natural resources are available. Among them the few are listed and detailed below:

9.4.1. LimoniaAcidissima

Limoniaacidissima (Wood apple) is attractive green material filler because of it's, due to its fetching mechanical and thermal properties when compared with materials as filler in polymer composites. It belongs to the highly reputed medicinal tree of the Rutaceae family, commonly known as bael or elephant apple or monkey apple. In India's it is grown as Indigenous crop.Also,it is available in othercountries such as Sri Lanka, Pakistan, Bangladesh, Burma, and Thailand. The strength of the shell of the wood apple and conversion of green to brown is based on the ripening stage.[10] Various researchers used wood apple shell as a filler in the polymers.Among them Shilpi das et al. [11] used the burnt shell powder and converted into activated carbon.This activated carbon was used as sorption of Cr (VI) and fluoride from the aqueous system.

9.4.2. Elaeocarpusganitrus

Elaeocarpus ganitrus or otherwise popularly called as arudrakshabelongs to the family of Elaeocarpaceae. In this world approximately 350 species are observed in the countries like Southeast Asia, India, Indonesia, Nepal, China, Fiji, New Zealand, Hawaii, Malaysia, Madagascar.Afiefudinet.al [12]revealed and suggested the that the optimized percentage of elaeocarpusganitrus seed powder reduced the wear and improved the density and hardness. Also, he proposed that it can be good replacement to asbestosfor making brake pad material.

9.4.3.Delonix regia

Delonixregiaseeds are obtained from the dark brown pods. The Delonix regia trees are short, stout, smooth, gray-coloured trunk trees having umbrella feathery leaves with moderate lighting shades. They belong to the family of Fabaceae. These trees are availablethroughout the globe. Generally, the pods of these trees will fall on the ground. The collected pods will be burnt for cleaning purposes.During the burning of this seed’s toxic gases such as nitrous oxide; carbon dioxide and carbon monoxide are produced. These gases are injurious to human health [13].The preparation of powder from these seeds will not only remove the wastes from the groundandcreate new green materials based on the Delonixregiaseeds.

Johnson et.al [14] studied the effects of the Delonix regia particles on the morphological and tensile properties of low-densitypolyethylene.Also, they recommended thatthesefilled composites can be used in home furniture, composite tiles, interior, front and rear parts of automobiles. Seeds and the powder are given below in the imagesas Fig 1a and b.

Figure: 1- a and b. Delonix regia seeds and powder form.

9.4.4. Juglans regia

The production of walnut (Juglans regia L)in the year 2023 was approximately reached about 2.67 million metric tons. China is the largest producer in the world, followed by the USA, Iran, Turkey, Mexico, and Chile. The consumption of walnut shells constitutes 67% of the total fruit weight and they create millions of tons of unused waste each year. These unused walnut shells are usually thrown out or it will be burnt away. Because it has no economic value and the burning of this shells maylead to environmental pollution.

Compared to other green materials the stastical report indicates that enormous number of walnut shells is available in the globe. Lot of research work is caried out by using walnut shells. Singh [15] investigated the mechanical behavior of walnut filler filled epoxy composite.In his work, the different composites were prepared by varying theweight fraction of walnut from10 to 25 %. He concluded that additionof walnut particles as filler increased the property of the filled composites.in the case of hardness, 25 % gives better results compared to other percentage of weights. He suggested that the filled composites shall be used for particles board. The high carbon content, presence of aromatic rings resulting in the good mechanical properties. So, the walnut filler as a green material indicates the possibility of its use as filler in polymer composites. Literature review indicates that the walnut shell is composed of cellulose, hemicellulose, lignin, and ash [16].The high carbon content may be due to the presence of the above listed.

9.4.5. Ceiba pentandra

Kapok fillers are prepared from the pod of the kapok. They are obtained from kapok tree of having heights of normally upto 50meters. The focus on the cultivation of these trees is to get the products like cotton and seeds. These cottons are used in pillows and mattress. While seeds are sent to manufacture for the oils.Kapok in natural form and opened is shown in fig 2. Kapok used products such as pod or shells having no market value after removing the cotton from it. Researchers [17] identified that Kapok in husk form has the potential to use as filler in thermoplastic materials. The green fillers used are economic and reduces the waste produced by the pillow industry.

Chun et.al [18] utilized the kapok as filler in husk form in the linear low density polyethylene composites. Kapoks are mostly used in fiber form in the field of polymer composites. Girimuruganet.al [19] studied the effect of kapok seed powder on mechanical properties of the untreated kenaf fibre composites.

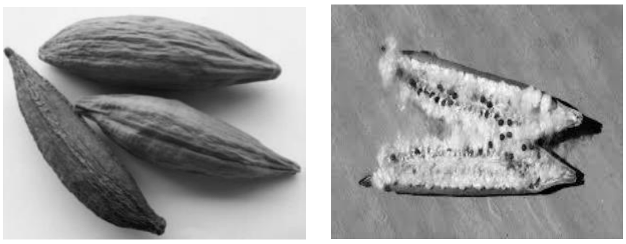


Figure: 2. Kapok in nature form and in seeds

9.4.6. Ipomoea carnea

Ipomoea carnea is a large diffuse and short shrub available in the globe. Actually, the plant belongs to South America. The plant will grow up to a height of only 2-3 meters and contains milky juice. Also the amount of water required for to grow for this plant are very less. The highlight is that under severe rainy conditions the life of the plant will not get affected. The presence of cellulose and lignin of 55% and 17% respectively provides effective green filler for making light weight composites. The shrub form of the plant is given below in the fig 3

Basumatary et.al [20] investigatedand studied with different concentration of particulates the behaviors of Ipomoea carnea reinforced epoxy composite. He concluded that the addition Ipomoea carnea particulate fillers improved the performance of the filled composites compared to the unfilled one.

Figure: 3 Shrub form from plantIpomoeacarnea

9.4.7.Prunus avium

Prunus avium (cherry seed powder)

The red color sweet cherry available and originates in the Black Sea/Caspian Sea region. Due to the high profit and demand of its timber and fruit, it has been cultivated in all the areas of the world. Over the past decade, compared to other areas cultivation of cherry increased hastily in China. Sydow et.al [21] suggested the application of cherry seed filler to improve the filler filled polypropylene composites for tribological applications. They concluded that the addition of high amount of filler has a constructive effect on the frictional behaviour and improvement in the wear resistance of the filled composites.

9.4.8. Annona Reticulata

Annona Reticulata (custard apple) is a tree with mainly the leaves in use apart from the root and stem. It has been reported to exhibit the following pharmacological activities: antibacterial, antihyperlipidemic, analgesic, anti-inflammatory, antidiabetic, hepatoprotective, and antiulcer effects. Aqueous extract of the leaves has shown to be safe in acute and subacute toxicities studies.Ramadoss et.al [22] developed hybrid composite materialsto evaluate the mechanical properties, sound absorption, thermal behavior, and water absorption behavior of the developed composite materialsby using natural fibers such as jute fiber, snake grass fiber and kenaf fiber combined with an organic filler, custard apple seed powder. They suggested that these developed materials shall be used as sound resisting materials.

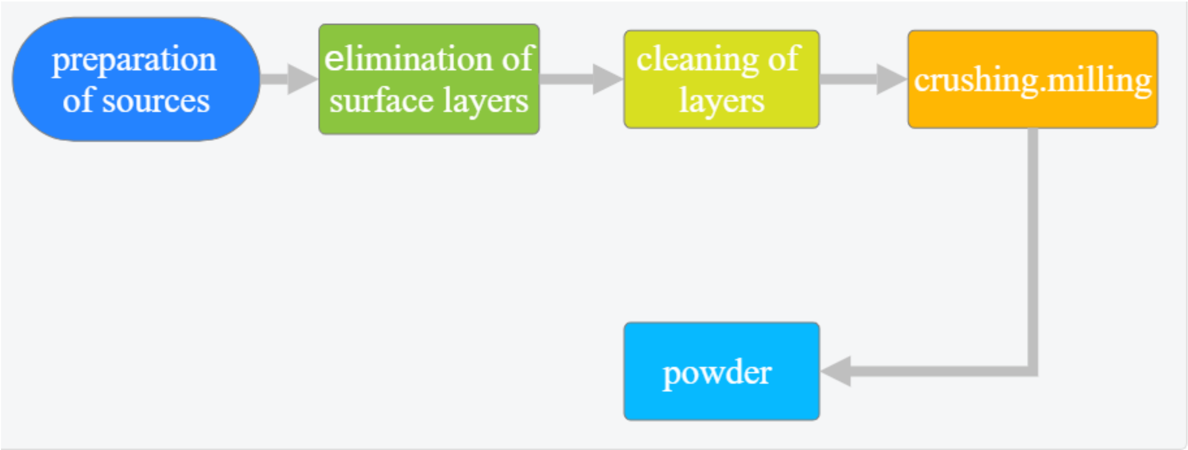
9.4.9. Phoenix dactylifera L

The Date fruit (Phoenix dactylifera L.) is one of the oldest plants cultivated, from the earliest records of Predynastic Egypt. Cultivation of Date palms in Egypt traces back to thousands of yearsA date fruit comprises of a fleshy pericarp and a seed (pit). Recently various researchers analyzed date fruit seeds as green fillers for composite reinforcement.

Depending upon the growth, cultivation conditions the date seed weighs about 0.5 to 4 g.It almost have 6 to 20 % of the fruit weight. Traditionally they are used for the sources for animal feed. Also, they are used for to produce oil which has great antioxidant properties, valuable in cosmetics and biodiesel production. In Asian countries they are often used as waste and considered as a waste and thrown out after consuming the fruits. Tillnow, most of the date seeds produced in most third world countries are discarded after consuming the fleshy part of the fruit.[23]

9.5. PROCESS TO CONVERT NATURAL SOURCES INTO GREEN FILLERS

The process of converting the natural resources of materials into filler form is given below as a flow chart. The type of acid for removing layers with certain amount of concentration should be taken. Then the surface layers were cleaned with distilled water. Then it should be dried with the help of air. The remaining moisture content present in the outer surface is eliminated by using in oven for certain temperature. Finally using ball milling the sources will be crushed and milled. The size will be measured by using siever.



CONCLUSION

Green fillers were discussed in this book chapter to discuss the availability of thefillers with botanical names and importance of their usage in polymer composites.It is highlighted that important characteristics such that environmentally friendliness, flexibility for manufacturing, minimizing waste and less use of energy which may result in the outcome of new green fillers-based polymer composites.Research on green filler-based compositesfurther more to be developed in the research areas like aircraft components and manufacturing sectors. It is successfully reached in the areas like tribological applications and packaging industries. However, more effort and articles to be publishedtomakethe possible ways of green fillerfilled composites in material properties and to increase their usage in different polymer composite based industries.

REFERENCES

1. https://www.statista.com/statistics/664906/plastics-production-volume-forecast-worldwide
2. Mohanty, A. K., Vivekanandhan, S., Pin, J. M., & Misra, M. (2018). Composites from renewable and sustainable resources: Challenges and innovations. Science, 362(6414), 536-542.
3. Das, A., Ringu, T., Ghosh, S., & Pramanik, N. (2023). A comprehensive review on recent advances in preparation, physicochemical characterization, and bioengineering applications of biopolymers. Polymer Bulletin, 80(7), 7247-7312.
4. Australasian Bioplastic Association. June 2, 2019 Available at: www.bioplastics.org .au.
5. Satyanarayana, K.G.; Guimarães, J.L.; Wypych, F. Studies on lignocellulosic fibers of Brazil. Part I: Source, production, morphology, properties and applications. Compos. Part A Appl. Sci. Manufact. 2007, 38, 1694–1709.
6. Ashori, A. Wood–plastic composites as promising green-composites for automotive industries! Bioresour. Technol. 2008, 99, 4661–4667.
7. Abhiram, Y.; Das, A.; Sharma, K.K. Green composites for structural and non-structural applications: A review. Mater. Today Proc. 2021, 44, 2658–2664.
8. Li, M.; Pu, Y.; Thomas, V.M.; Yoo, C.G.; Ozcan, S.; Deng, Y.; Nelson, K.; Ragauskas, A.J. Recent advancements of plant-based natural fiber–reinforced composites and their applications. Compos. Part B Eng. 2020, 200, 108254.
9. Kopparthy, S.D.S.; Netravali, A.N. Review: Green composites for structural applications. Compos. Part C Open Acc. 2021, 6, 100169
10. Shakuntala O, Raghavendra G, Kumar AS (2014) Effect of filler loading on mechanical and tribological properties of wood apple shell reinforced epoxy composite. Adv Mater Sci
11. Das S, Mishra S (2017) Box-Behnken statistical design to optimize preparation of activated carbon from Limoniaacidissima shell with desirability approach. J Environ Chem Eng 5:588–600
12. Afiefudin, M., Widodo, R. D., &Rusiyanto, R. (2023). Fabrication and Characterization of Asbestos Free Brake Pads Composite using Elaeocarpus Ganitrus as Reinforcement. Automotive Experiences, 6(2), 359-371.
13. Ezeokpube, N.D., Obiora, C.J., Phil-Eze, P.O., 2014. Environmental problems of sachet water waste disposal in nsukka urban, enugu state, Nigeria. Civ. Environ. Res. 6 (1), 105–113
14. Agunsoye, J. O., Bello, S. A., & Adetola, L. O. (2019). Experimental investigation and theoretical prediction of tensile properties of Delonix regia seed particle reinforced polymeric composites. Journal of King Saud University-Engineering Sciences, 31(1), 70-77.
15. Singh, V. K. (2015). Mechanical behaviour of walnut (Juglans L.) shell particles reinforced bio-composite. Science and engineering of composite materials, 22(4), 383-390.
16. Jahanban-Esfahlan, A.; Ostadrahimi, A.; Tabibiazar, M.; Amarowicz, R. A comprehensive review on the chemical constituents and functional uses of walnut (Juglans spp.) husk. Int. J. Mol. Sci. 2019, 20, 3920.

17. Chun, K. S., Husseinsyah, S., & Yeng, C. M. (2016). Green composites from kapok husk and recycled polypropylene: processing torque, tensile, thermal, and morphological properties. Journal of Thermoplastic Composite Materials, 29(11), 1517-1535.
18. Chun, K. S., Husseinsyah, S., &Syazwani, N. F. (2016). Properties of kapok husk-filled linear low-density polyethylene ecocomposites: effect of polyethylene-grafted acrylic acid. Journal of Thermoplastic composite materials, 29(12), 1641-1655.
19. Girimurugan, R., Babu, B., Saravanan, R., Vigneshwaran, M., & Mehanathan, S. (2023). Effect of kapok seed powder on mechanical and water intake properties of untreated kenaf fiber composites. Materials Today: Proceedings.
20. Basumatary, K. K., & Acharya, S. K. (2013). Investigation into mechanical properties of Ipomoea carnea reinforced epoxy composite. International Journal of Macromolecular Science, 3(3), 11-15.
21. Sydow, Z., Bula, K., &Gapiński, B. (2023). Friction and wear of polypropylene-based composites reinforced with cherry seed powder. Tribology International, 179, 108177.
22. Ramadoss, P. K., Mayakrishnan, M., &Arockiasamy, F. S. (2024). Discarded custard apple seed powder waste-based polymer composites: an experimental study on mechanical, acoustic, thermal and moisture properties. Iranian Polymer Journal, 1-19.
23. Nwogu, C. N., Nwaiwu, U., Udo, V. U., Nwosu, O. J., & Hart, C. E. (2022). Effect of date seed granules on the mechanical properties of Glass fibre reinforced epoxy composite. Cleaner Materials, 6, 100160.

.

CHAPTER

10

NANOTECHNOLOGY IN FOOD PACKAGING: A REVIEW

Meena Chakraborty
Govt. Naveen College Bori, Durg, Chhattisgarh, India
chakrabortymeena@gmail.com

ABSTRACT

Nanotechnology, with its potential to revolutionize various industries, has made significant strides in food packaging. This review explores the applications, benefits, and challenges of nanotechnology in food packaging. By leveraging nanomaterials, such as nanoparticles and nanocomposites, food packaging can enhance safety, extend shelf life, and contribute to sustainability efforts. However, concerns regarding regulatory frameworks, consumer acceptance, and potential environmental impacts must be addressed to ensure the responsible implementation of nanotechnology in food packaging.

Keywords: Nanotechnology, food packaging, nanomaterials, safety, shelf life, sustainability

10.1.INTRODUCTION

Food packaging plays a pivotal role in the modern food industry, serving a multitude of essential functions beyond mere containment. Firstly, it acts as a shield against physical, chemical, and microbiological hazards, safeguarding the integrity and safety of the food within. This is particularly crucial in preserving perishable items and extending their shelf life, thus reducing food wastage—a significant concern globally (Chetan Sharma et al., 2017). Moreover, packaging facilitates convenient storage, transportation, and handling, making food more accessible to consumers across diverse geographical locations. Additionally, it provides vital information regarding nutritional content, ingredient lists, and expiry dates, empowering consumers to make informed choices about their dietary intake. Furthermore, innovative packaging solutions contribute to sustainability efforts by reducing material usage, minimizing environmental impact, and enhancing recyclability. Hence, the importance of food packaging transcends mere containment—it ensures food safety, accessibility, information transparency, and sustainability, ultimately shaping modern food systems and consumer experiences.

In recent decades, nanotechnology has emerged as a ground breaking field with immense potential to revolutionize various industries, including food packaging. Nanotechnology involves manipulating materials at the nanoscale, typically at dimensions less than 100 nanometers, to impart unique properties and functionalities (Alfadul and Elneshwy, 2010; Mlalila; Samal, 2017). In the realm of food packaging, nanotechnology offers solutions to enhance food safety, extend shelf life, and reduce environmental impact (Sharma et al., 2020; Chadha et al., 2022).

Nanotechnology offers a plethora of applications in food packaging, owing to its ability to engineer materials with specific properties. One prominent application is the development of nanocomposite packaging materials, where nanoparticles are incorporated into packaging polymers to enhance mechanical strength, barrier properties, and antimicrobial activity (Chetan Sharma et al., 2017). For instance, nanoclays can be added to polymer matrices to improve gas barrier properties, thereby extending the shelf life of perishable foods by preventing oxygen and moisture ingress (Chaudhary et al., 2020).

Moreover, nanoparticles such as silver nanoparticles exhibit potent antimicrobial properties, making them invaluable for inhibiting the growth of pathogenic microorganisms on food surfaces. These antimicrobial nanocomposites can help mitigate foodborne illnesses and reduce the need for chemical preservatives, aligning with consumer preferences for safer and more natural food products (Kraśniewska et al., 2020).

Another innovative application of nanotechnology in food packaging is the development of active packaging systems. These systems incorporate nanomaterials capable of releasing bioactive compounds such as antioxidants, antimicrobials, and flavor enhancers to preserve food quality and freshness. By harnessing controlled release mechanisms enabled by nanotechnology, active packaging can mitigate oxidative reactions, delay microbial spoilage, and enhance sensory attributes, thereby improving overall consumer satisfaction (Chetan Sharma et al., 2017).

Nanotechnology represents a paradigm shift in the field of food packaging, offering unprecedented opportunities to enhance food safety, extend shelf life, and reduce environmental impact. By leveraging nanomaterials to engineer advanced packaging solutions, stakeholders across the food industry can address pressing challenges related to food waste, contamination, and sustainability. However, realizing the full potential of nanotechnology in food packaging requires concerted efforts to overcome technical, regulatory, and economic barriers. With on-going research, innovation, and collaboration, nanotechnology promises to reshape the future of food packaging, delivering safer, fresher, and more sustainable food products to consumers worldwide. This review will explores the applications, benefits, challenges and future prospects of nanotechnology in food packaging.

10.2. TRADITIONAL MATERIALS USED FOR FOOD PACKAGING

Traditional materials used in food packaging have long encompassed a diverse array of natural substances tailored to preserve and protect edibles. Materials such as glass, ceramic, and various metals have been integral to food containment for centuries. Additionally, natural fibers such as cotton and jute were employed for sacks and bags, offering breathability and transport convenience. These traditional materials, rooted in history and often revered for their reliability, continue to inspire modern packaging innovations aimed at maintaining food safety and quality. Some of them are shown in Figure 1 and described below:

Figure 1: Traditional materials used for food packaging

10.2.1. Biopolymers

Biopolymers are gaining traction in food packaging due to their eco-friendly nature and various beneficial properties. Biopolymers of polysaccharides (starch and cellulose derivatives, chitosan, and alginates), lipids (bees and carnauba wax, and free fatty acids), proteins (casein, whey, and gluten), poly hydroxyl butyrates (PHB), polylactic acid (PLA), poly caprolactone (PCL), polyvinyl alcohol (PVA), poly butylene succinate and polyglycolic acid are used for the purpose (Koivistoinen, 2013).

The advantage of biopolymers in food packaging is their biodegradability, renewable sourcing, barrier properties (Tang et al., 2012), customizability and biocompatibility. But on the other hand, they are expensive, having inferior mechanical strength or thermal stability and cannot provide the same level of barrier properties as compare to traditional plastics against moisture, oxygen, or other gases, which can affect the shelf life and quality of packaged food (Vartiainen et al., 2014). Therefore further research and technological advancements are needed to optimize their performance and scalability in the food packaging industry.

10.2.2. Plastic as food packaging material

Different types of plastics are commonly used for food packaging such as Polyethylene (PE) which is used for plastic bags, food wraps, and bottles, Polypropylene (PP) which is used for containers, cups, and microwaveable trays, Polyethylene Terephthalate (PET) which is commonly used for beverage bottles, Polystyrene (PS) which is used for foam trays and containers, PVC (Polyvinyl Chloride) which is sometimes used for food wraps and packaging, but concerns exist regarding its safety (de Sousa et al., 2023).

Plastic as a food packaging material has many advantages such as versatility in shape and size, flexibility in packaging design, cost effective lightweight, durable and resistant to breakage and transparent with regards of consumer’s visibility and appeal. But plastics are non-biodegradable, leading to pollution and long-term environmental degradation and having single-use Culture (de Sousa et al., 2023). Some plastics contain chemicals such as bisphenol-A (BPA) and phthalates, which may leach into food, especially under certain conditions like heat or acidic environments, posing potential health risks. Therefore the use of plastic as a food packaging material is crucial regarding environmental sustainability and consumer health preferences.

10.2.3. Paper as Food Packaging Materials

Paper serves as a versatile and eco-friendly material for food packaging, offering a myriad of benefits to both consumers and the environment. Its natural properties make it an ideal choice for preserving the freshness and quality of food products while ensuring they remain safe for consumption. Paper has several advantages as a food packaging material, including its biodegradability, renewability, easy to recycle and customizability; it also has limitations such as limited barrier properties, susceptibility to damage, not suitable for packaging of all foods and resource-intensive production processes. The suitability of paper packaging for a particular food product depends on factors such as the type of food, desired shelf life, and environmental considerations (Miltz, 2011).

10.2.4. Glass as food Packaging Materials

Glass has been a staple packaging material for various food products for centuries, and it offers several advantages such as preservation of taste and quality, recyclability, visibility of contents and impervious to air and moisture. But glass is fragile and prone to breakage, heavier in weight than alternatives like plastic, expensive to produce, delicate for transportation, limited shape flexibility and its production process involves high energy consumption, contributing to its environmental footprint (Robertson, 1993).

10.2.5. Metals as food packaging material

Metal packaging materials, such as aluminum and steel, have been widely used in the food industry for various products due to their advantageous properties. Metals are strong and durable, providing excellent protection to the food products from physical damage during handling, transportation, and storage. Metal packaging offers excellent barrier properties against light, oxygen, moisture, and other external elements, thereby extending the shelf life of the food products and maintaining their freshness and quality for a longer duration. Metals are highly recyclable materials; provide versatility in shape and size of packaging and having tamper-resistant features, ensuring the safety and integrity of the food products by protecting them from tampering and contamination. But metal packaging is expensive, heavier in weight, susceptible to corrosion which leads to potential contamination and compromising the quality of the food and are non-biodegradable. Therefor these drawbacks should be considered while selecting metals as packaging materials for food products (Robertson, 1993).

10.2.6. Jute as food packaging material

Jute bags have emerged as an environmentally friendly alternative for food packaging due to their numerous benefits. Renowned for their natural fibers, jute bags offer biodegradability, making them a sustainable choice that reduces environmental harm. Unlike plastic packaging, jute bags are breathable, allowing food to stay fresh for longer periods without the risk of mold or mildew. Additionally, jute bags are sturdy and can withstand the weight of various food items, ensuring reliable transportation and storage. Their versatility extends to customization, enabling businesses to brand their packaging while contributing to eco-conscious practices. But Jute has natural moisture-absorbing properties which can promote the growth of mold and bacteria, leading to spoilage of the packaged food items. Jute bags do not provide a barrier against gases like oxygen and carbon dioxide, susceptible to pest infestation, limited strength potentially causing damage to the packaged food items, limited availability and limited versatility and having cleaning challenges which restricts its application as food packaging material (Hashem et al., 2017).

10.3. BENEFITS OF NANOTECHNOLOGY IN FOOD PACKAGING:

Nanoparticles offer several advantages for food packaging, making them suitable for various applications:

3.1 Barrier Properties: Nanoparticles can be incorporated into packaging materials to enhance their barrier properties. They can create a more effective barrier against oxygen, moisture, and other gases, preventing spoilage and extending the shelf life of food products (de Sousa et al., 2023).

3.2 Antimicrobial Properties: Some nanoparticles possess antimicrobial properties, which can help inhibit the growth of bacteria, fungi, and other microorganisms that cause food spoilage and contamination. This can improve food safety and reduce the risk of foodborne illnesses (Chetan Sharma et al., 2017).

3.3 Strength and Durability: Nanoparticles can improve the mechanical strength and durability of packaging materials, making them more resistant to tearing, puncturing, and other forms of damage during handling, transportation, and storage (de Sousa et al., 2023).

3.4 Sensory Properties: Nanoparticles can be engineered to modify the sensory properties of packaging materials, such as their transparency and color. This can enhance the aesthetic appeal of packaged foods and improve consumer perception (Chetan Sharma et al., 2017).

3.5 Smart Packaging: Nanotechnology enables the development of "smart" packaging systems that can monitor the condition of food products in real-time. For example, nanoparticles embedded in packaging materials can change color in response to temperature variations or the presence of harmful gases, alerting consumers to potential spoilage (Chetan Sharma et al., 2017).

3.6 Sustainability: Nanoparticles can be used to develop eco-friendly packaging materials with improved sustainability characteristics. For instance, they can facilitate the development of biodegradable and compostable packaging options, reducing environmental impact (de Sousa et al., 2023).

3.7 Nanoencapsulation: Nanoparticles can be used for the encapsulation of active ingredients, such as antioxidants, vitamins, flavors, and preservatives, within packaging materials. This protects these sensitive compounds from degradation, ensuring their efficacy over an extended period (Acosta, 2009).

3.8 Intelligent packaging: Integration of nanosensors for real-time monitoring of food freshness, temperature, and quality (Chetan Sharma et al., 2017).

3.9 Active packaging: Introduction of nanocapsules containing active agents for controlled release of antioxidants, flavor enhancers, and antimicrobial agents (Chetan Sharma et al., 2017).

3.10 Safety enhancement: Reduction of foodborne pathogens through antimicrobial nanomaterials (Chetan Sharma et al., 2017).

3.11 Shelf life extension: Preservation of food quality and freshness, leading to reduced food waste (de Sousa et al., 2023).

3.12 Enhanced functionality: Introduction of smart packaging functionalities for improved consumer experience and convenience (Fahmy et al., 2020).

The unique properties of nanoparticles make them highly suitable for various food packaging applications, offering benefits such as improved shelf life, enhanced safety, and greater sustainability. However, it's essential to ensure that nanoparticles used in food packaging are safe for consumers and comply with regulatory standards.

Table 1: Comparison of traditional materials used in food packaging with nanomaterials

Property	**Traditional Materials**	**Nanomaterials**	**Reference**
Barrier Properties	Limited barrier to gases and moisture	Enhanced barrier properties, prolonging shelf life	Chetan Sharma et al., 2017; de Sousa et al., 2023; Hashem et al., 2017; Robertson, 1993; Vartiainen et al., 2014
Strength	Moderate strength and durability	Improved strength and durability	
Flexibility	Some flexibility but may be rigid	Retains flexibility while adding strength	
Transparency	May have limited transparency	Can be made transparent or translucent	
Biodegradability	Often non-biodegradable	May be engineered for biodegradability	
Antimicrobial Properties	May lack inherent antimicrobial properties	Can be engineered with antimicrobial properties	
Cost	Generally lower cost	May be more expensive depending on formulation	
Environmental Impact	Often contributes to waste and pollution	Potential for reduced environmental impact	

Table 1 illustrates some of the key differences between traditional materials and nanomaterials used in food packaging. Nanomaterials offer significant improvements in barrier properties, strength, and flexibility while potentially reducing environmental impact, though they may come at a higher cost and require careful consideration of safety and regulatory issues.

10.4. TYPE OF NANOMATERIALS USED IN FOOD PACKAGING:

In the realm of food packaging, both inorganic and organic nanomaterials are revolutionizing the industry, offering innovative solutions to enhance food safety, preservation, and sustainability. Some of the inorganic and organic nanoparticles used for food packaging are as follows:

10.4.1 Inorganic nanoparticles

Inorganic nanomaterials, such as metal oxides and nanoparticles, exhibit remarkable properties like high mechanical strength, barrier properties, and antimicrobial activity. These materials can be incorporated into packaging films or coatings to create barriers against oxygen, moisture, and UV radiation, thereby extending the shelf life of perishable foods. Additionally, inorganic nanoparticles can serve as sensors for detecting food spoilage or contamination, ensuring consumer safety. Some examples of inorganic nanomaterials used for food packaging are:

10.4.1.1 Silver nanoparticles

Silver nanoparticles (AgNPs) are extensively employed as antimicrobial agents in food packaging, aiming to extend the shelf life of food products. They exhibit antibacterial properties against a wide range of bacteria, including both gram-positive and gram-negative strains, alongside antioxidant capabilities. Hence, there is a pressing need to devise simple, cost-effective, and environmentally friendly methods for synthesizing silver nanoparticles (Biswal and Misra, 2020). AgNPs find application as antimicrobial agents in both biodegradable (e.g., cellulose, starch, chitosan) and non-biodegradable (e.g., polyethylene, polyvinyl chloride, ethylene-vinyl chloride) polymers for crafting active food packaging materials (Carbone et al., 2016). To effectively combat microbes, AgNPs are gradually released into food products from the packaging material, necessitating consideration of their migration due to toxicity concerns (Ahmad et al., 2021; Istiqola and Syafiuddin, 2020). Employing active packaging films and coatings embedded with AgNPs proves advantageous, as they facilitate controlled release of nanoparticles onto the food surface, thereby creating an inhospitable environment for microbial growth and thereby prolonging shelf life (Kraśniewska et al., 2020). Furthermore, these techniques hold promise in reducing the need for preservatives traditionally added to food for quality preservation and extended shelf life (Kraśniewska et al., 2020).

10.4.1.2 Magnetite nanoparticles

Magnetite nanoparticles have emerged as a promising solution in the realm of food packaging due to their unique properties and potential applications. These nanoparticles, typically ranging in size from 1 to 100 nanometers, possess excellent magnetic properties, chemical stability, and biocompatibility, making them ideal candidates for various food packaging applications. One of the key advantages of incorporating magnetite nanoparticles into food packaging materials is their ability to provide enhanced barrier properties, thereby extending the shelf life of perishable food products by preventing moisture, oxygen, and other contaminants from permeating the packaging material and deteriorating the food. Additionally, these nanoparticles can be functionalized with antimicrobial agents or oxygen scavengers to further enhance the preservation of food freshness and quality (Keshk et al., 2019). Furthermore, the magnetic properties of magnetite nanoparticles enable the development of smart packaging systems capable of detecting food spoilage or contamination through changes in magnetic signals, offering a reliable method for ensuring food safety.

10.4.1.3 Titanium dioxide nanoparticles

Titanium dioxide nanoparticles (TiO_2 NPs) are a type of white-colored metal oxide with a broad spectrum of uses within the food industry. They serve as additives in food products and are incorporated into nanocomposites for food packaging. Utilized in polymer packaging, TiO_2 NPs act as UV radiation blockers while enhancing the chemical, mechanical, and barrier characteristics of the packaging films (Mohr et al., 2019). Moreover, they are frequently employed as coloring agents in processed foods, prized for their high refractive index, brightness, and color durability (Baranowska-Wójcik et al., 2020, Sungur et al., 2020). Additionally, titanium dioxide exhibits antimicrobial properties by generating free radicals and reactive oxygen species (ROS) that interact with bacterial cells, leading to their demise (Venkatasubbu et al., 2016). Due to its chemical stability, affordability, non-toxicity, and eco-friendly attributes, TiO_2 proves to be an effective photocatalyst (Mohr et al., 2019). Furthermore, it serves as an oxygen and ethylene scavenger through the photodegradation of ethylene when exposed to sunlight (Siripatrawan and Kaewklin, 2018).

10.4.1.4 SiO_2 nanoparticles

SiO_2 nanoparticles, composed of silicon dioxide, hold immense potential in revolutionizing food packaging technology. These nanoparticles offer a myriad of advantages, primarily due to their unique properties such as high surface area, excellent barrier properties, and biocompatibility. When integrated into food packaging materials, SiO_2 nanoparticles form a protective barrier against moisture, gases, and microbial contamination, thus extending the shelf life of perishable foods. Moreover, their inert nature ensures that they do not interact with the food, preserving its quality and safety. Additionally, SiO_2 nanoparticles can be engineered to possess antimicrobial properties, further enhancing the packaging's ability to inhibit bacterial growth and prevent food spoilage. Their nano-sized dimensions allow for the development of lightweight, flexible, and transparent packaging, catering to consumer preferences for convenience and aesthetic appeal (Yu et al., 2018).

10.4.1.5 Zinc oxide nanoparticles

Zinc, an indispensable micronutrient, finds utility in fortifying foods and supplements (McClements and Xiao, 2017). Zinc oxide nanoparticles exhibit antibacterial properties against a range of bacteria including E. coli, Staphylococcus aureus, Listeria monocytogenes, and Salmonella enteritidis. This activity stems from the release of Zn2+ ions and ROS, which disrupt cell organelles, leading to cell demise (Kim et al., 2022). Moreover, when integrated into polymer matrices, ZnO nanoparticles enhance the barrier, antibacterial, and mechanical attributes of composite films (Kim et al., 2022; Abbas et al., 2019). The ready availability of highly pure ZnO nanoparticles facilitates their direct incorporation into various polymer matrices like linear low-density polyethylene (LLDPE), low-density polyethylene (LDPE), polylactic acid (PLA), poly 3-hydroxybutyrate (PHB), and poly 3-

hydroxybutyrate-co-3-hydroxy valerate (PHBV), enabling comprehensive study of their effects (Abbas et al., 2019).

10.4.1.6 Nanoclay

Nanoclay refers to layered mineral silicates, with each layer comprising octahedral or tetrahedral sheets (Guo et al., 2018). Its application in food packaging is widespread, aimed at enhancing the physical and barrier characteristics of plastic materials (Chaudhary et al., 2020). Typically, nanoclays manifest in platelet form, possessing a flaky soft texture, low specific gravity, and a high aspect ratio. Among these, Montmorillonites (MMT-Na+) and organophilic MMT are prevalent choices due to their resemblance to thermoplastic properties and high aspect ratios, making them advantageous for packaging purposes (Li et al., 2015). Naturally occurring montmorillonites (MMT) represent hydrophilic nano clay within the phyllosilicate family, particularly belonging to the smectite subclass. They are extensively utilized to enhance the mechanical properties of protein-based films (Shanmuga et al., 2014; Li et al., 2015). The migration and toxicity of nanocomposites within packaging materials necessitate thorough comprehension. Migration dynamics hinge on factors such as nanoclay-polymer interactions, food contact, temperature, and duration of exposure. Notably, nanoclay serves to bolster the mechanical and barrier attributes of starch thermoplastics while enhancing the biodegradability of synthetic polymers (Bandyopadhyay and Ray, 2019).

10.4.2. Organic nanoparticles

Organic nanomaterials, such as biopolymers and nanocellulose, are derived from renewable sources and offer biodegradability and compatibility with food products. These materials can be engineered to provide functionalities like antimicrobial properties, gas barrier properties, and even smart packaging capabilities for real-time monitoring of food quality. Some examples of organic nanomaterials used for food packaging are:

10.4.2.1. Nanocellulose

Cellulose, a prevalent polysaccharide in nature, forms the primary component of plant cell walls, imparting strength to plants. Nanocellulose, a nanostructured derivative of cellulose, exists in the form of nanocrystals or nanofibers, typically measuring a few micrometers in length and less than 100 nanometers in diameter (Sharma et al., 2019). Extracted from plants through mechanical and chemical processes, nanocellulose exhibits robust hydrogen bonding capabilities, enabling the creation of dense surfaces impermeable to molecules, thus conferring excellent barrier properties (Ferrer et al., 2017). In industrial applications, nanocellulose is utilized in the paper and composite sectors to enhance strength, mechanical properties, uniformity, and biodegradability (Naseer et al., 2018). Incorporating nanocellulose into biopolymers augments their barrier, thermal, and mechanical attributes (Arrieta et al., 2016).

10.4.2.2.Nano chitosan particles

Chitosan, a polysaccharide derived from chitin, which is present in the cell walls of fungi, exoskeletons of arthropods, and crustaceans, exhibits notable environmental friendliness and non-toxicity. Its exceptional antimicrobial properties render it a promising candidate for nanoparticle applications in packaging (Divya et al., 2018). When incorporated into biodegradable polymers like polylactic acid films, chitosan enhances their gas and moisture barrier characteristics (Yanat et al., 2021). Chitosan nanoparticles not only bolster the physical and mechanical attributes of biocomposite films but also augment their barrier properties. Additionally, they enhance antimicrobial efficacy through chelation effects and ionic interactions with bacterial cell surfaces, impeding nutrient transport and inducing cell death. Moreover, their hydrophobic nature contributes to improved moisture impermeability, facilitated by the formation of hydrogen and covalent bonds with biopolymers, thereby reducing moisture diffusion rates (Garavand et al., 2022).

10.4.2.3.Nano starch

Starch, a complex polysaccharide composed of amylose and amylopectin polymers, undergoes transformation into nano starch through the disintegration of starch granules using diverse physical and chemical methods (Moran et al., 2021). These starch nanoparticles, with at least one dimension smaller than 300 nm and possessing a significant surface area per unit volume (Yu et al., 2021), are alternatively termed as starch nanocrystals. They are widely employed as nanofillers in composites, enhancing strength, flexibility, biodegradability, water impermeability, as well as thermal and barrier properties (Dularia et al., 2019; Campelo et al., 2020).

10.4.2.4. Carbon nanotubes

Carbon nanotubes, a type of carbon allotrope, are cylindrical structures with diameters measured in nanometers. They exist in two primary forms: single-walled nanotubes and multi-walled nanotubes, composed of multiple concentric cylinders. These nanotubes serve various purposes in packaging materials. They enhance mechanical strength and impart antimicrobial properties to polymers utilized in packaging (Rezić et al., 2017). Moreover, they play a crucial role in creating oxygen sensors for monitoring atmospheric composition in modified packaging environments (Zhu et al., 2017). Additionally, they are integrated into synthetic polymer matrices employed in food packaging to introduce antimicrobial attributes and develop intelligent sensors capable of detecting food spoilage (Chaudhary et al., 2020).

10.4.2.5. Nano protein particles

Protein-based nanoparticles play a crucial role in food packaging by augmenting its strength and barrier attributes, particularly in terms of water resistance (Zubair and Ullah, 2020). Incorporating peanut protein nanoparticles into protein-starch-based biocomposites has been shown to enhance their strength, temperature resilience, and moisture barrier capabilities (Li et al., 2015). Similarly, the integration of zein nanoparticles has been observed to bolster the mechanical strength and moisture resistance of whey protein isolate-based films (Oymaci and Altinkaya, 2016).

By leveraging the unique properties of both inorganic and organic nanomaterials, the future of food packaging holds promise for safer, fresher, and more sustainable food products.

10.5. APPLICATIONS OF NANOTECHNOLOGY IN FOOD PACKAGING:

Researchers have recognized the vast potential of integrating nanotechnology across various domains within the food industry. Particularly significant are advancements in food processing, enhancing food quality, and innovating food packaging. Notably, nanotechnology finds its most extensive application in food packaging due to its non-intrusive nature, thereby preserving the natural integrity of food products. By leveraging nanotechnology in food packaging, there's a fortified defense against pathogens and harmful gases (Mleki et al., 2024). Nanosensors play a pivotal role in identifying contaminants, assessing packaging materials, and shielding food from UV rays. This transformative technology elevates the capabilities of food packaging, facilitating the detection of bacterial presence, thereby enhancing taste, quality, and safety, while also thwarting gas and moisture infiltration, thereby extending shelf life and curbing food spoilage (Singh and Nanda, 2022). Application of nano technology in various fields of food packaging are shown in Figure 2 and described below:

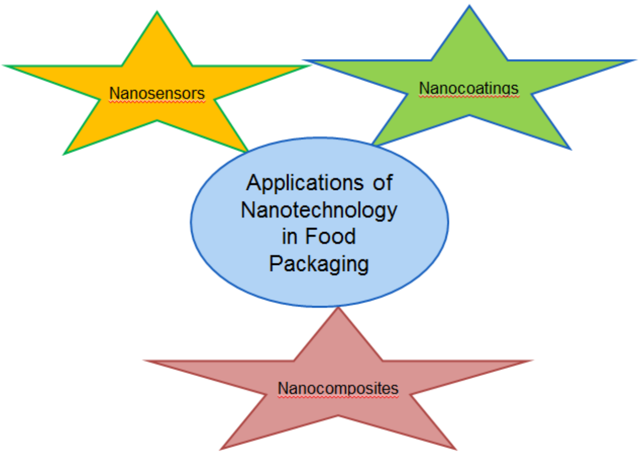


Figure 2: Applications of Nanotechnology in Food Packaging

10.5.1.Nanosensors in food packaging

In the realm of technology, biosensors play a crucial role within the agriculture and food industry, ensuring the quality and safety of food through efficient and rapid methods. They facilitate the monitoring of products and processes while also detecting packaged gases to maintain packaging integrity. Various nanomaterials, including gold nanoparticles, carbon nanotubes, nano dust, and nanoclay, are employed in biosensor fabrication (Kaur et al., 2023).

Nano-sensors excel in identifying color changes in food items and detecting gases such as hydrogen, hydrogen sulfide, nitrogen oxides, sulfur dioxide, and ammonia emanating from spoilage (Lee et al., 2013). Comprising two essential components—a digital data processing unit and a sensing unit—nano-sensors detect variations in light, temperature, humidity, gases, and chemicals, converting them into electrical signals (Li et al., 2011).

Metal-based nanosensors are adept at discerning color changes and gas releases in food items. Carbon nanotube sensors are employed for detecting pesticide residues on the surfaces of fruits and vegetables, while carbon black and polyaniline sensors identify foodborne pathogens and carcinogenic compounds. Nano-smart dust changes color upon encountering any signs of spoilage within food, while nano-biosensors are utilized for detecting environmental pollutants. Nanoclay sensors serve as gas barriers, preventing the escape of carbon dioxide from bottles (Kaur et al., 2023).

10.5.2. Nano-compositesin food packaging

Nanocomposites, a type of reinforced polymers incorporating nanoparticles, have emerged in the food packaging industry. They offer significant advantages over pure polymers, including enhanced strength, increased resistance to ignition, superior thermal properties, lower melting points and gas transfer temperatures, and improved resistance to moisture. By combining nanoclay with biopolymers like polyamide, nylon, polyolefin, polystyrene, epoxy polyurethane resins, and polyethylene terephthalate, these nanocomposites exhibit heightened mechanical strength and reduced weight. This leads to improved barriers against liquid and gas permeation, thereby preventing oxygen and moisture from seeping into packaged food and subsequently thwarting food spoilage. Nanocomposites, formulated with thermoset and thermoplastic polymers such as polyethylene, polypropylene, poly methyl methacrylate, and biodegradable polymers like starch derivatives, polylactic acid, and poly hydroxybutyrate, find extensive utility in food packaging applications. They help maintain antimicrobial activity and minimize the transfer of metal ion derivatives into packaged food, thereby ensuring food safety and longevity (Mlekiet al., 2024; Perera et al., 2022).

10.5.3.Nanocoatings in food packaging

Nanocoatings, whether organic or inorganic, form a delicate protective layer employed in safeguarding food and enhancing the aesthetics of packaging surfaces. They find application across a diverse range of food items including meat, vegetables, fruits, cheese, confectioneries like candy and chocolate, fried snacks, and bakery goods. Primarily, nanocoatings function to impede gas permeation, serving as effective barriers. Notably, these coatings possess antibacterial properties without the use of chemical germicides and exhibit remarkable stability against chemicals and alkalis (Mleki et al., 2024). For instance, titanium dioxide nano-coating exemplifies this, being utilized for photocatalytic disinfection, functioning as a chemical barrier while also modifying the surface (Mahmud et al., 2022).

10.6.CHALLENGES AND CONSIDERATIONS:

Despite its promising potential, the widespread adoption of nanotechnology in food packaging faces several challenges and considerations. One significant concern is the potential migration of nanoparticles from packaging materials into food, raising questions about their safety and regulatory compliance. Ensuring the inertness and stability of nanomaterials under varying storage conditions is crucial to mitigate health risks and regulatory hurdles associated with nanoparticle migration (Cwiek-Ludwicka and Ludwicki, 2017).

Additionally, the scalability and cost-effectiveness of nanotechnology-based packaging solutions remain key considerations for commercial viability. While research demonstrates the efficacy of nanocomposite and active packaging systems in laboratory settings, translating these innovations into scalable manufacturing processes poses technical and economic challenges. Addressing these challenges requires interdisciplinary collaboration between scientists, engineers, manufacturers, and regulatory agencies to streamline production processes, optimize material costs, and ensure compliance with regulatory standards.

10.7. FUTURE DIRECTIONS / FUTURE ASPECTS OF NANOPARTICLES FOR FOOD PACKAGING

The future of nanotechnology in food packaging appears promising, with on-going research and development efforts focused on addressing current challenges and unlocking new opportunities. Emerging trends include the use of biodegradable and environmentally friendly nanomaterials to create sustainable packaging solutions that minimize waste and environmental impact. Additionally, advancements in nanotechnology-enabled sensors and smart packaging technologies hold potential for real-time monitoring of food quality, freshness, and safety throughout the supply chain.

Furthermore, the convergence of nanotechnology with other disciplines such as biotechnology, materials science, and artificial intelligence is expected to fuel innovation and drive the development of next-generation food packaging solutions. From personalized packaging tailored to individual dietary preferences to intelligent packaging systems capable of communicating product information to consumers, the future landscape of nanotechnology in food packaging is poised for continued growth and transformation.

Overall, the future of nanoparticles in food packaging holds great potential for improving food safety, quality, and sustainability throughout the entire supply chain. However, careful consideration of safety, regulatory, and consumer acceptance issues will be essential for realizing these benefits.

10.8. CONCLUSIONS:

Nanotechnology has shown great promise in revolutionizing food packaging, offering a myriad of benefits such as improved shelf life, enhanced safety, and reduced environmental impact. By incorporating nanomaterials into packaging, manufacturers can create barriers that prevent oxygen, moisture, and contaminants from reaching the food, thereby preserving its freshness and quality for longer periods. Furthermore, nanotechnology enables the development of smart packaging systems capable of detecting and signalling food spoilage or contamination, providing consumers with valuable information about the freshness and safety of the products they purchase.

Despite these advancements, it's crucial to address potential concerns regarding the safety and regulatory aspects of nanomaterials used in food packaging. Comprehensive research is necessary to ensure that nanotechnology applications in food packaging do not pose any risks to human health or the environment. Overall, while nanotechnology holds immense potential for enhancing food packaging, careful consideration of safety, regulation, and ethical implications is essential to fully harness its benefits and ensure its responsible implementation in the food industry.

REFERENCES

1. Abbas, M., Buntinx, M., Deferme, W., & Peeters, R. (2019). (Bio) polymer/ZnO nanocomposites for packaging applications: a review of gas barrier and mechanical properties. *Nanomaterials*, *9*(10), 1494. https:// doi.org/10.3390/nano9101494.
2. Acosta, E. (2009). Bioavailability of nanoparticles in nutrient and nutraceutical delivery. *Current opinion in colloid & interface science*, *14*(1), 3-15.

3. Ahmad, S. S., Yousuf, O., Islam, R. U., & Younis, K. (2021). Silver nanoparticles as an active packaging ingredient and its toxicity. *Packaging Technology and Science*, *34*(11-12), 653-663. https://doi.org/10.1002/pts.2603.
4. Alfadul, S. M., &Elneshwy, A. A. (2010). Use of nanotechnology in food processing, packaging and safety–review. *African Journal of Food, Agriculture, Nutrition and Development*, *10*(6).
5. Arrieta, M. P., Fortunati, E., Burgos, N., Peltzer, M. A., López, J., &Peponi, L. (2016). Nanocellulose-based polymeric blends for food packaging applications. *Multifunctional polymeric nanocomposites based on cellulosic reinforcements*, 205-252.
6. Bandyopadhyay, J., & Ray, S. S. (2019). Are nanoclay-containing polymer composites safe for food packaging applications?—An overview. *Journal of Applied Polymer Science*, *136*(12), 47214. https://doi.org/10.1002/app.47214.
7. Baranowska-Wójcik, E., Szwajgier, D., Oleszczuk, P., & Winiarska-Mieczan, A. (2020). Effects of titanium dioxide nanoparticles exposure on human health—a review. *Biological trace element research*, *193*, 118-129. https://doi.org/ 10.1007/s12011-019-01706-6. Jan. 01.
8. Biswal, A. K., & Misra, P. K. (2020). Biosynthesis and characterization of silver nanoparticles for prospective application in food packaging and biomedical fields. *Materials Chemistry and Physics*, *250*, 123014. https://doi.org/10.1016/j.matchemphys.2020.123014.
9. Campelo, P. H., Sant'Ana, A. S., & Clerici, M. T. P. S. (2020). Starch nanoparticles: Production methods, structure, and properties for food applications. *Current Opinion in Food Science*, *33*, 136-140. https://doi.org/10.1016/j. cofs.2020.04.007. Jun. 01.
10. Carbone, M., Donia, D. T., Sabbatella, G., &Antiochia, R. (2016). Silver nanoparticles in polymeric matrices for fresh food packaging. *Journal of King Saud University-Science*, *28*(4), 273-279. https://doi.org/10.1016/j.jksus.2016.05.004. Oct. 01
11. Chadha, U., Bhardwaj, P., Selvaraj, S. K., Arasu, K., Praveena, S., Pavan, A., ... & Paramasivam, V. (2022). Current trends and future perspectives of nanomaterials in food packaging application. *Journal of Nanomaterials*, *2022*, 1-32.
12. Chaudhary, P., Fatima, F., & Kumar, A. (2020). Relevance of nanomaterials in food packaging and its advanced future prospects. *Journal of inorganic and organometallic polymers and materials*, *30*(12), 5180-5192. https://doi.org/10.1007/s10904-020-01674- 8.
13. Chetan Sharma, C. S., Romika Dhiman, R. D., Namita Rokana, N. R., & Harsh Panwar, H. P. (2017). Nanotechnology: an untapped resource for food packaging, 1735.
14. Cwiek-Ludwicka, K., &Ludwicki, J. K. (2017). Nanomaterials in food contact materials; considerations for risk assessment. *RocznikiPaństwowegoZakładuHigieny*, *68*(4).
15. de Sousa, M. S., Schlogl, A. E., Estanislau, F. R., Souza, V. G. L., dos Reis Coimbra, J. S., & Santos, I. J. B. (2023). Nanotechnology in packaging for food industry: Past, present, and future. *Coatings*, *13*(8), 1411.
16. Divya, K., & Jisha, M. S. (2018). Chitosan nanoparticles preparation and applications. *Environmental chemistry letters*, *16*, 101-112. https://doi.org/ 10.1007/s10311-017-0670-y. Mar. 01.
17. Dularia, C., Sinhmar, A., Thory, R., Pathera, A. K., & Nain, V. (2019). Development of starch nanoparticles based composite films from non-conventional source-Water chestnut (Trapa

bispinosa). *International journal of biological macromolecules*, *136*, 1161-1168. https://doi.org/10.1016/j.ijbiomac.2019.06.169.

18. Fahmy, H. M., Eldin, R. E. S., Serea, E. S. A., Gomaa, N. M., AboElmagd, G. M., Salem, S. A., ... & Shalan, A. E. (2020). Advances in nanotechnology and antibacterial properties of biodegradable food packaging materials. *RSC advances*, *10*(35), 20467-20484.
19. Ferrer, A., Pal, L., & Hubbe, M. (2017). Nanocellulose in packaging: Advances in barrier layer technologies. *Industrial Crops and Products*, *95*, 574-582. https://doi.org/10.1016/j.indcrop.2016.11.012.
20. Garavand, F., Cacciotti, I., Vahedikia, N., Rehman, A., Tarhan, Ö., Akbari-Alavijeh, S., ... & Jafari, S. M. (2022). A comprehensive review on the nanocomposites loaded with chitosan nanoparticles for food packaging. *Critical reviews in food science and nutrition*, *62*(5), 1383-1416. https://doi.org/10.1080/10408398.2020.1843133.
21. Guo, F., Aryana, S., Han, Y., & Jiao, Y. (2018). A review of the synthesis and applications of polymer–nanoclay composites. *Applied Sciences*, *8*(9), 1696. https:// doi.org/10.3390/app8091696.
22. Hashem, M., Refaie, R., Zaghloul, S., Ezzat, A., Ellaithy, A., & A Shaaban, H. (2017). Bioactive jute fabrics for packaging and storage of grains and legumes applications. *Egyptian Journal of Chemistry*, *60*(4), 551-561.
23. Huang, J. Y., Li, X., & Zhou, W. (2015). Safety assessment of nanocomposite for food packaging application. *Trends in Food Science & Technology*, *45*(2), 187-199. https://doi.org/10.1016/j.tifs.2015.07.002. Oct. 01.
24. Istiqola, A., &Syafiuddin, A. (2020). A review of silver nanoparticles in food packaging technologies: Regulation, methods, properties, migration, and future challenges. *Journal of the Chinese Chemical Society*, *67*(11), 1942-1956. https://doi.org/10.1002/jccs.202000179. Nov. 01.
25. Kaur H., Ayoub A., Kaur S. (2023). *Journal of Experimental Agriculture International*, vol. 45, no. 7, pp. 59-71.
26. Keshk, S. M., El-Zahhar, A. A., Haija, M. A., &Bondock, S. (2019). Synthesis of a magnetic nanoparticles/dialdehyde starch-based composite film for food packaging. *Starch-Stärke*, *71*(1-2), 1800035.
27. Kim, I., Viswanathan, K., Kasi, G., Thanakkasaranee, S., Sadeghi, K., & Seo, J. (2022). ZnO nanostructures in active antibacterial food packaging: preparation methods, antimicrobial mechanisms, safety issues, future prospects, and challenges. *Food Reviews International*, *38*(4), 537-565. https://doi.org/ 10.1080/87559129.2020.1737709.
28. Koivistoinen, O. (2013). Catabolism of biomass-derived sugars in fungi and metabolic engineering as a tool for organic acid production.
29. Kraśniewska, K., Galus, S., & Gniewosz, M. (2020). Biopolymers-based materials containing silver nanoparticles as active packaging for food applications–a review. *International Journal of Molecular Sciences*, *21*(3), 698. https://doi.org/10.3390/ ijms21030698.
30. Lee, Y., Kim, D., Seo, J., Han, H., & Khan, S. B. (2013). Preparation and characterization of poly (propylene carbonate)/exfoliated graphite nanocomposite films with improved thermal stability, mechanical properties and barrier properties. *Polymer International*, *62*(9), 1386-1394.

31. Li, R., Liu, C., Ma, J., Yang, Y., & Wu, H. (2011). Effect of org-titanium phosphonate on the properties of chitosan films. *Polymer bulletin*, *67*, 77-89.
32. Li, X., Ji, N., Qiu, C., Xia, M., Xiong, L., & Sun, Q. (2015). The effect of peanut protein nanoparticles on characteristics of protein-and starch-based nanocomposite films: A comparative study. *Industrial Crops and Products*, *77*, 565-574.
33. Mahmud, J., Sarmast, E., Shankar, S., & Lacroix, M. (2022). Advantages of nanotechnology developments in active food packaging. *Food Research International*, *154*, 111023.
34. McClements, D. J., & Xiao, H. (2017). Is nano safe in foods? Establishing the factors impacting the gastrointestinal fate and toxicity of organic and inorganic food-grade nanoparticles. *npj Science of Food*, *1*(1), 6. https://doi.org/10.1038/ s41538-017-0005-1.
35. Miltz, J. (2011). Food packaging, In Handbook of Food Engineering (Heldman, DR and Mishra SP). Production of nanocellulose from native cellulose-various options utilizing ultrasound. *BioResources*, *7*, 422-436.
36. Mlalila, N., Kadam, D. M., Swai, H., &Hilonga, A. (2016). Transformation of food packaging from passive to innovative via nanotechnology: concepts and critiques. *Journal of food science and technology*, *53*, 3395-3407.
37. Mleki, N., KanKiya, M., Hoshangi, F., &Mojarad, L. S. (2024). Using Nanotechnology in Food Packaging. *Applied Sciences Research Periodicals*, *2*(1), 43-53.
38. Mohr, L. C., Capelezzo, A. P., Baretta, C. R. D. M., Martins, M. A. P. M., Fiori, M. A., & Mello, J. M. M. (2019). Titanium dioxide nanoparticles applied as ultraviolet radiation blocker in the polylactic acid bidegradable polymer. *Polymer Testing*, *77*, 105867. https:// doi.org/10.1016/j.polymertesting.2019.04.014.
39. Morán, D., Gutiérrez, G., Blanco-López, M. C., Marefati, A., Rayner, M., & Matos, M. (2021). Synthesis of starch nanoparticles and their applications for bioactive compound encapsulation. *Applied Sciences*, *11*(10), 4547.https://doi.org/10.3390/ app11104547.
40. Naseer, B., Srivastava, G., Qadri, O. S., Faridi, S. A., Islam, R. U., & Younis, K. (2018). Importance and health hazards of nanoparticles used in the food industry. *Nanotechnology Reviews*, *7*(6), 623-641.
41. Oymaci, P., &Altinkaya, S. A. (2016). Improvement of barrier and mechanical properties of whey protein isolate based food packaging films by incorporation of zein nanoparticles as a novel bionanocomposite. *Food hydrocolloids*, *54*, 1-9. https://doi.org/10.1016/j.foodhyd.2015.08.030.
42. Perera, K. Y., Jaiswal, S., & Jaiswal, A. K. (2022). A review on nanomaterials and nanohybrids based bio-nanocomposites for food packaging. *Food Chemistry*, *376*, 131912.
43. Rezić, I., Haramina, T., &Rezić, T. (2017). Metal nanoparticles and carbon nanotubes—perfect antimicrobial nano-fillers in polymer-based food packaging materials. In *Food packaging* (pp. 497-532). Academic Press.
44. Robertson, H. M. (1993). The mariner transposable element is widespread in insects. *Nature*, *362*(6417), 241-245.
45. Samal, D. (2017). Use of nanotechnology in food industry: a review. *International Journal of Environment, Agriculture and Biotechnology*, *2*(4), 238902.

46. Shanmuga Priya, D., Suriyaprabha, R., Yuvakkumar, R., & Rajendran, V. (2014). Chitosan-incorporated different nanocomposite HPMC films for food preservation. *Journal of nanoparticle research*, *16*, 1-16. https://doi.org/10.1007/s11051-014-2248-y.
47. Sharma, A., Thakur, M., Bhattacharya, M., Mandal, T., & Goswami, S. (2019). Commercial application of cellulose nano-composites–A review. *Biotechnology Reports*, *21*, e00316.
48. Sharma, R., Jafari, S. M., & Sharma, S. (2020). Antimicrobial bio-nanocomposites and their potential applications in food packaging. *Food Control*, *112*, 107086.
49. Singh, D., & Nanda, V. (2022). Application of Nanotechnology in Food Packaging and Food Quality. In *Nanotechnology Interventions in Food Packaging and Shelf Life* (pp. 3-16). CRC Press.
50. Siripatrawan, U., &Kaewklin, P. (2018). Fabrication and characterization of chitosan-titanium dioxide nanocomposite film as ethylene scavenging and antimicrobial active food packaging. *Food Hydrocolloids*, *84*, 125-134. https://doi. org/10.1016/j.foodhyd.2018.04.049.
51. Sungur, Ş., Kaya, P., &Koroglu, M. (2020). Determination of titanium dioxide nanoparticles used in various foods. *Food Additives & Contaminants: Part B*, *13*(4), 260-267. https://doi.org/10.1080/19393210.2020.1769193.
52. Tang, X. Z., Kumar, P., Alavi, S., & Sandeep, K. P. (2012). Recent advances in biopolymers and biopolymer-based nanocomposites for food packaging materials. *Critical reviews in food science and nutrition*, *52*(5), 426-442.
53. Vartiainen, J., Vähä-Nissi, M., & Harlin, A. (2014). Biopolymer films and coatings in packaging applications—a review of recent developments. *Materials Sciences and applications*, *2014*.
54. Venkatasubbu, G. D., Baskar, R., Anusuya, T., Seshan, C. A., & Chelliah, R. (2016). Toxicity mechanism of titanium dioxide and zinc oxide nanoparticles against food pathogens. *Colloids and Surfaces B: Biointerfaces*, *148*, 600-606. https://doi. org/10.1016/j.colsurfb.2016.09.042.
55. Yanat, M., &Schroën, K. (2021). Preparation methods and applications of chitosan nanoparticles; with an outlook toward reinforcement of biodegradable packaging. *Reactive and Functional Polymers*, *161*, 104849.
56. Yu, M., Ji, N., Wang, Y., Dai, L., Xiong, L., & Sun, Q. (2021). Starch-based nanoparticles: Stimuli responsiveness, toxicity, and interactions with food components. *Comprehensive Reviews in Food Science and Food Safety*, *20*(1), 1075-1100. https://doi.org/10.1111/ 1541-4337.12677.
57. Yu, Z., Li, B., Chu, J., & Zhang, P. (2018). Silica in situ enhanced PVA/chitosan biodegradable films for food packages. *Carbohydrate polymers*, *184*, 214-220.
58. Zhu, R., Desroches, M., Yoon, B., & Swager, T. M. (2017). Wireless oxygen sensors enabled by Fe (II)-polymer wrapped carbon nanotubes. *ACS sensors*, *2*(7), 1044-1050. https://doi.org/10.1021/acssensors.7b00327.
59. Zubair, M., & Ullah, A. (2020). Recent advances in protein derived bionanocomposites for food packaging applications. *Critical reviews in food science and nutrition*, *60*(3), 406-434. https://doi.org/10.1080/10408398.2018.1534800. Feb. 04.

CHAPTER

11

UNDERSTANDING MOLECULAR STRUCTURE THROUGH NMR AND IR

Tushar Verma
Department of Chemistry, Sai College, Bhilai
ravenclaw9607@gmail.com

ABSTRACT

In contemporary chemical study, it is imperative to comprehend molecule structure through the utilization of Nuclear Magnetic Resonance (NMR) and Infrared (IR) spectroscopy. The information provided by these methods about conformation, bonding, and molecular composition is complimentary. While infrared spectroscopy (IR) monitors the amount of infrared radiation absorbed by molecule bonds to reveal information about molecular vibrations and functional groups, nuclear magnetic resonance (NMR) spectroscopy uses the magnetic characteristics of atomic nuclei to clarify molecular structures in solution. We can obtain a thorough understanding of the dynamics, symmetry, and structure of molecules in a variety of settings by integrating NMR and IR spectroscopy. We go over the fundamentals of NMR and IR spectroscopy in this abstract and show how they are used in various fields to analyze chemical structures.

Keywords: molecular structure, chemical bonding, functional groups, molecular vibrations, nuclear magnetic resonance (NMR), infrared (IR) spectroscopy,

11.1.INTRODUCTION

The ideas of NMR and ir spectroscopy can be used to describe how molecular structure is determined. NMR spectroscopy uses the magnetic characteristics of atomic nuclei to determine molecule composition, connectivity, and conformation in solution. NMR spectroscopy may reveal the chemical environment of nuclei by exposing it to a high magnetic field and irradiating it with radiofrequency pulses. This knowledge includes chemical shifts, spin-spin coupling patterns, and relaxation behavior. In contrast, infrared spectroscopy probes molecular structure by measuring the absorption of infrared radiation by molecule bonds. Each type of chemical bond has distinct vibrational frequencies that may be probed using infrared spectroscopy, allowing functional groups to be identified and molecular conformations to be examined. IR spectroscopy, which uses molecular vibration principles and spectroscopic analysis, provides useful insights into the chemical composition, structure, and reactivity of various molecular systems.

11.2.PRINCIPLE OF NMR AND IR

Nuclear Magnetic Resonance (NMR) spectroscopy is based on the interaction of atomic nuclei with a high magnetic field and radiofrequency radiation. When put in a magnetic field, certain atomic nuclei with an odd number of protons and/or neutrons exhibit a feature known as nuclear spin. When exposed to radiofrequency pulses, these nuclei absorb energy and switch between spin states. A magnetic field gradient can be used to identify the resonance frequency at which nuclei absorb energy, revealing information about the chemical environment and molecular structure. In contrast, the principle of infrared (IR) spectroscopy is based on the interaction of molecules with infrared radiation. Molecules have distinct vibrational modes linked with the stretching and bending of chemical bonds. When infrared radiation at specific frequencies interacts with a molecule, it is absorbed proportionally to the molecule's vibrational modes. IR spectroscopy, which measures the wavelengths of absorbed radiation, offers information about the functional groups and molecular structure of the sample.

Both NMR and IR spectroscopy provide distinct insights into molecule structure, with NMR focused on atomic nuclei and their chemical surroundings and IR spectroscopy probing molecular vibrations and functional groups.

11.3.METHODOLOGY

The approach for determining the structure of carbonyl compounds using NMR and IR spectroscopy entails collecting spectrum data and interpreting it to reveal molecular properties. Proton and carbon spectra are obtained during NMR analysis to study chemical shifts, coupling patterns, and multiplicity, revealing information about the electronic environment and connectivity of the carbonyl group.

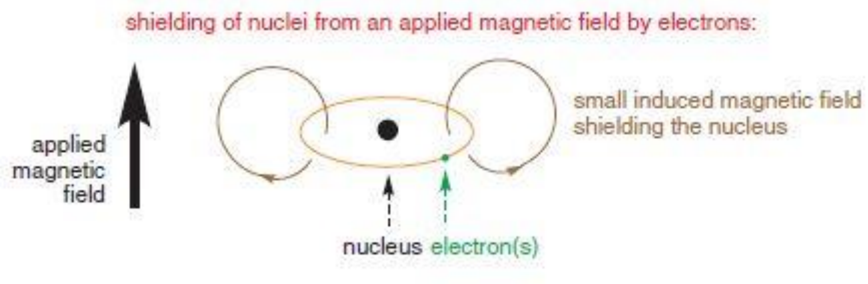


FIG1

FIG1 explains the chemical shift in which nucleus is surrounded by electrons, which will cause a small electric current to flow in a magnetic field. In contrast to the magnetic field created by the electrons, this current will create its own magnetic field. Of an electric current flowing via a solenoid or wire coil), which will be in opposition to our applied magnetic field. It is said that the electrons protect the nucleus from the outside magnetic field.The local magnetic field that each 13C atom experiences and the associated resonant frequency change in tandem with variations in the electron distribution.

In IR spectroscopy, characteristic absorption bands associated with the carbonyl group are identified, aiding in structural identification. Data interpretation involves comparing experimental spectra with reference data and literature values to propose a molecular structure based on chemical shifts, vibrational frequencies, and other spectral features. Through this approach, researchers can accurately characterize carbonyl compounds, facilitating their identification and understanding in various scientific contexts.

11.4. STRUCTURE DETERMINATION

11.4.1. Determination alcohol structure through c-13 nmr

In carbon-13 (C-13) NMR spectroscopy, the chemical shifts observed in the spectrum provide information about the carbon atoms present in a molecule and their local chemical environments. By analyzing the chemical shifts and the splitting patterns observed in the C-13 NMR spectrum given in fig 2, we can determine the structure of an alcohol molecule.

Alcohols typically exhibit characteristic chemical shifts in the C-13 NMR spectrum:

1. The carbon atom directly bonded to the hydroxyl group (OH) of the alcohol usually appears as a broad peak at a higher chemical shift, typically in the range of 60-80 ppm.
2. The carbon atoms adjacent to the carbon bonded to the hydroxyl group (alpha carbons) often appear at slightly lower chemical shifts, typically in the range of 40-60 ppm.
3. The remaining carbon atoms in the alkyl chain of the alcohol molecule typically appear at even lower chemical shifts, depending on their specific chemical environment.

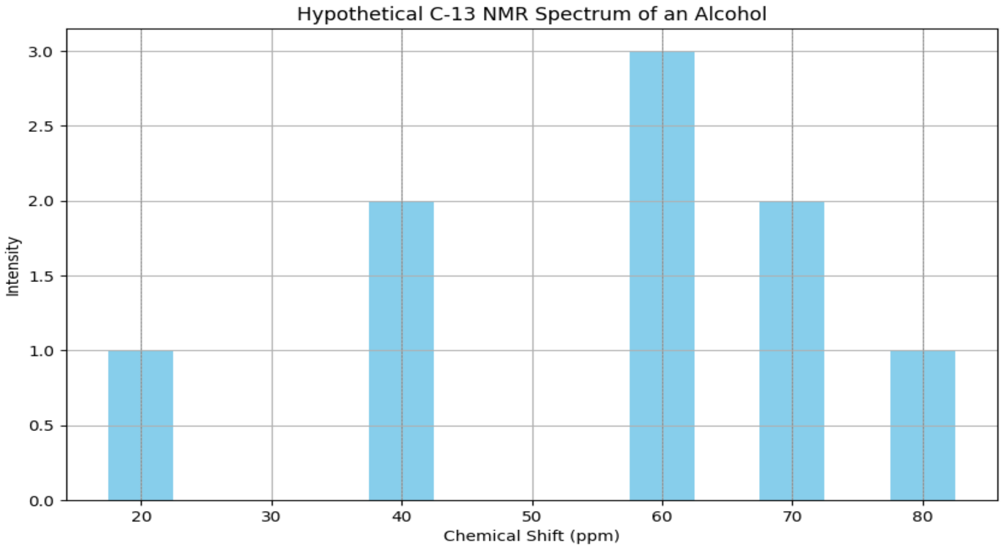


FIG2

11.4.2. Determination aldehyde and ketone structure through c-13 nmr

Determining the structure of aldehydes and ketones through C-13 NMR spectroscopy given in fig3 involves analyzing the chemical shifts of the carbon atoms in the molecule.

1. Aldehydes:
   - Aldehydes typically show a C-13 NMR signal for the carbonyl carbon (C=O) at around 190-220 ppm.
   - The carbon adjacent to the carbonyl carbon (alpha carbon) usually appears as a peak in the range of 30-50 ppm.

- Other carbon atoms in the aldehyde molecule will have chemical shifts depending on their environment and neighboring atoms.

2. Ketones:

- Ketones also exhibit a C-13 NMR signal for the carbonyl carbon (C=O) around 190-220 ppm, similar to aldehydes.
- The alpha carbon in a ketone typically appears at a slightly lower chemical shift compared to that in an aldehyde, often in the range of 20-40 ppm.
- Again, the chemical shifts of other carbon atoms in the ketone molecule will vary based on their surroundings.

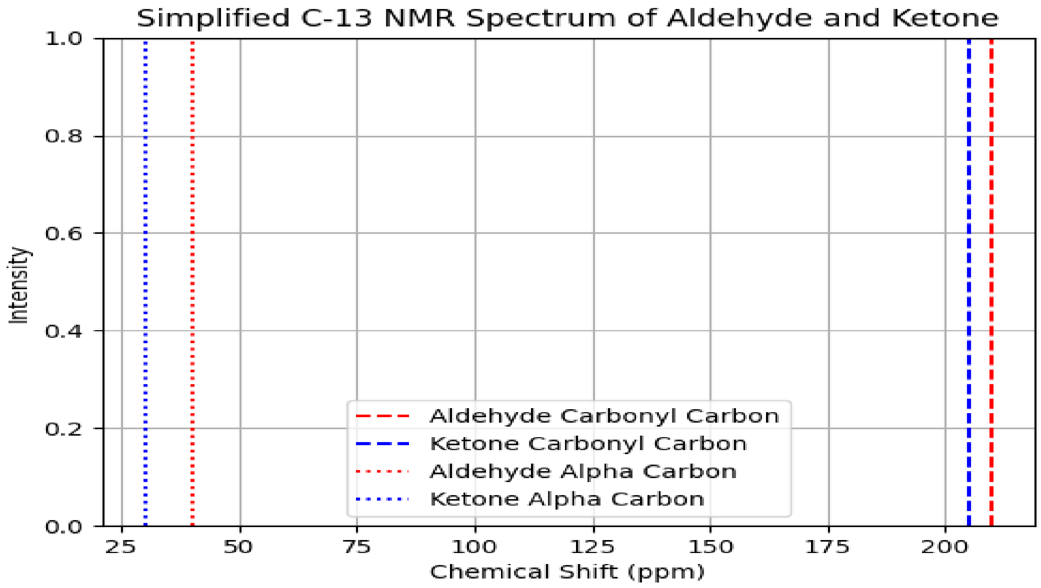


FIG3

11.5. STRUCTURE DETERMINATION THROUGH IR FINGERPRINTING

Although the entire IR spectrum can be used as a fingerprint for the purposes of comparing molecules, the 600 - 1400 cm-1 range is called the fingerprint region given in fig4.

Infrared (IR) spectroscopy is an effective analytical technique used in chemistry to identify and describe chemical compounds based on their molecular structure and functional groups. By detecting the absorption of infrared radiation by molecular bonds, IR spectroscopy offers a unique "fingerprint" for each substance, allowing us to discover its structural properties.

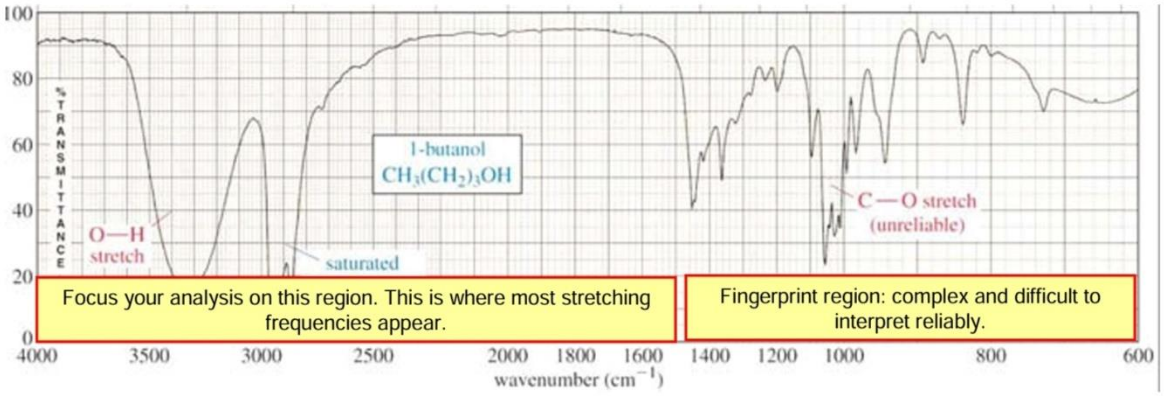


FIG4

11.5.1. Determination aldehyde and ketone structure through IR.

The structural determination of aldehydes and ketones using infrared spectroscopy (IR) given in fig5 is based on characteristic absorption bands in the IR spectra linked with functional groups found in these molecules.

For aldehydes:

1. Carbonyl Stretching: Aldehydes have a prominent absorption band in the IR spectra between 1700-1750 cm^-1 due to the stretching vibration of the carbonyl group (C=O). The electron-donating effect of the alkyl group in aldehydes causes this absorption to be stronger and occur at slightly lower wavenumbers than that of ketones.

2. C-H Stretching: Aldehydes exhibit distinct absorption bands in the 2800-3000 cm^-1 range due to stretching vibrations of C-H bonds. An aldehyde group can cause a separate band about 2700-2800 cm^-1, which corresponds to the stretching of the aldehyde.

For Ketones:

1. Carbonyl Stretching: Ketones have a prominent absorption band in the IR spectra between 1700-1750 cm^-1 due to the stretching vibration of the carbonyl group (C=O). This absorption band is similar to that of aldehydes, but it may appear at slightly higher wavenumbers due to the electron-drawing action of the extra alkyl group.

2. C-H Stretching: Ketones exhibit distinct absorption bands in the 2800-3000 cm^-1 range due to stretching vibrations of C-H bonds. However, the arrangement of absorption bands in this region can vary depending on the structure of the ketone molecule.

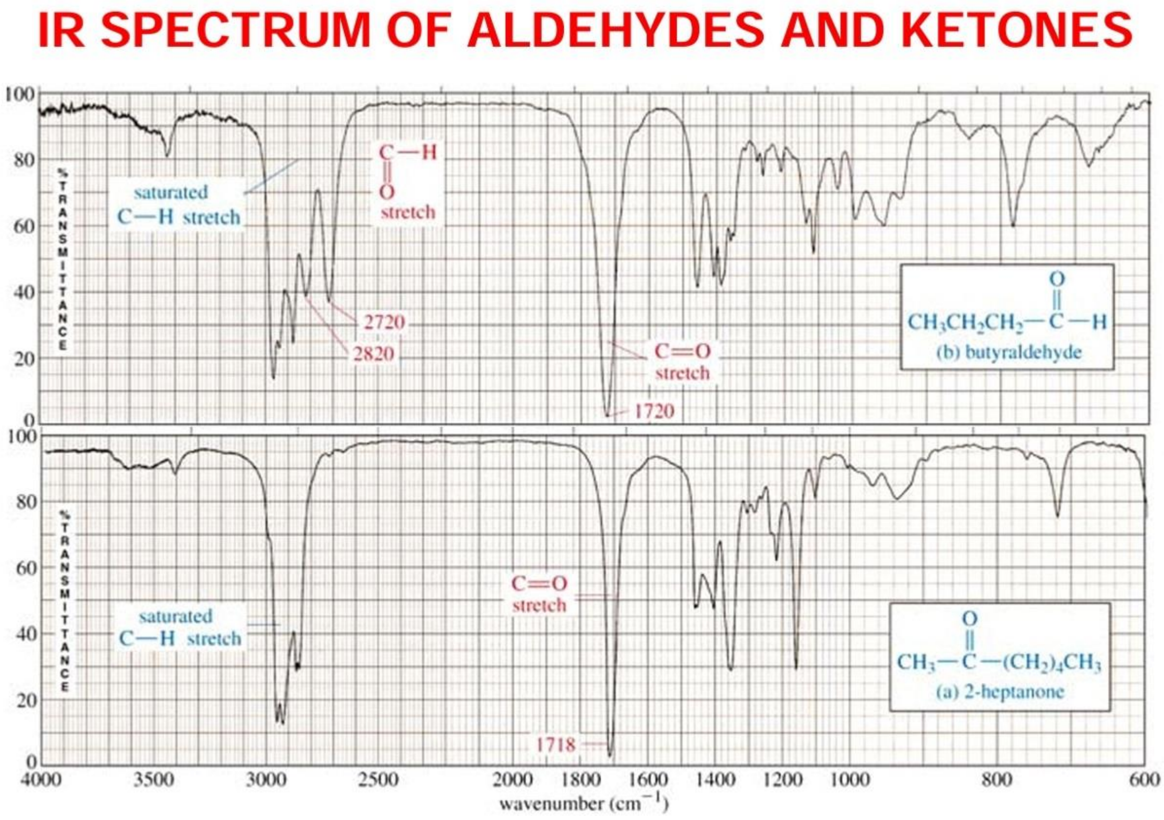


FIG 5

11.5.2. Determination alkane structure through IR.

The structure determination of alkanes through infrared spectroscopy (IR) fig 6 is primarily based on the absence of characteristic absorption bands in the IR spectrum due to the lack of functional groups with dipole moments. Alkanes are hydrocarbons consisting only of carbon-carbon (C-C) and carbon-hydrogen (C-H) single bonds, which do not exhibit significant IR absorption.

Key points for structure determination of alkanes through IR:

1. Absence of Functional Groups: Alkanes do not contain any functional groups such as carbonyl (C=O), hydroxyl (OH), amino (NH2), or other groups that typically produce characteristic absorption bands in the IR spectrum.

2. C-H Stretching: Alkanes exhibit absorption bands in the IR spectrum due to the stretching vibrations of carbon-hydrogen (C-H) bonds. However, these absorption bands are typically weak and broad, making them difficult to distinguish from background noise.

3. Fingerprints Region: The fingerprint region of the IR spectrum (typically below 1500 cm^-1) may show some weak and broad absorption bands associated with C-H stretching and bending vibrations. However, these bands are not specific to alkanes and can vary depending on the alkane's molecular structure and conformation.

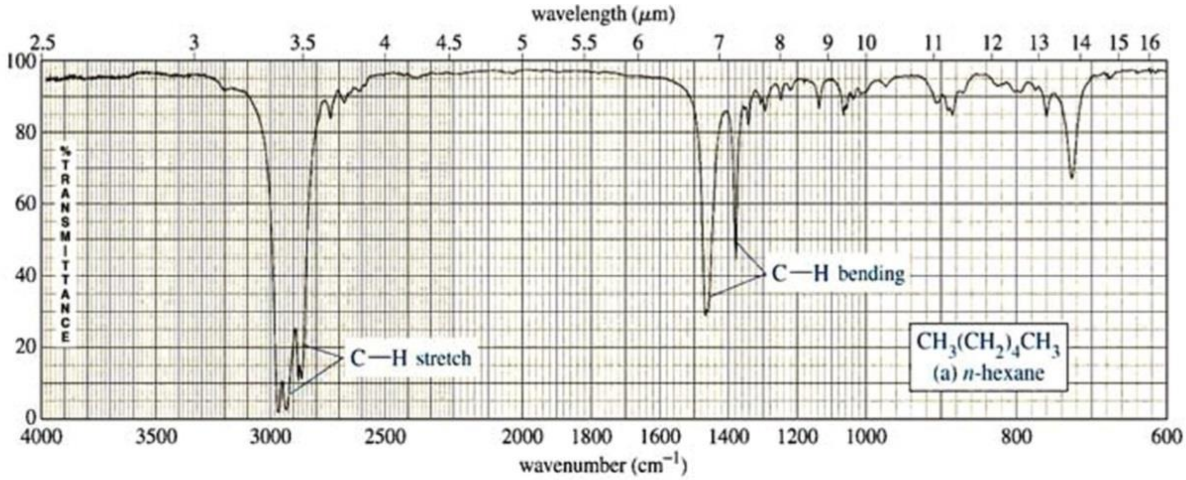


FIG6

11.5.3. Determination alcohol structure through IR.

The structure of alcohols is determined via infrared spectroscopy (IR) given in fig7 based on characteristic absorption bands in the IR spectrum associated with the hydroxyl (OH) functional group present in the molecules.

Key points for structural determination of alcohols using IR:

1. Hydroxyl Stretching: Alcohols have a broad absorption band in the infrared spectrum about 3200-3600 cm^-1 due to stretching vibration of the hydroxyl (OH) group. This absorption band is often expanded and shifted to lower wavenumbers than the absorption band of free hydroxyl groups in isolation due to hydrogen bonding interactions inside the alcohol molecule.

2. O-H Bending: Alcohols have a weaker absorption band in the IR spectra between 1300-1400 cm^-1 due to the bending vibration of the O-H bond. This absorbance Bands can reveal extra structural information about alcohol molecules.

3. C-H Stretching: Alcohols have absorption bands in the infrared spectrum at 2800-3000 cm^-1 due to stretching vibrations of carbon-hydrogen bonds. These absorption bands vary based on the alkyl groups connected to the carbon atom with the hydroxyl group.

4. Fingerprint area: C-H stretching and bending vibrations can cause weak and broad absorption bands in the fingerprint area of the IR spectrum (usually below 1500 cm^-1). These bands can provide extra structural information, but they are not limited to alcohols.

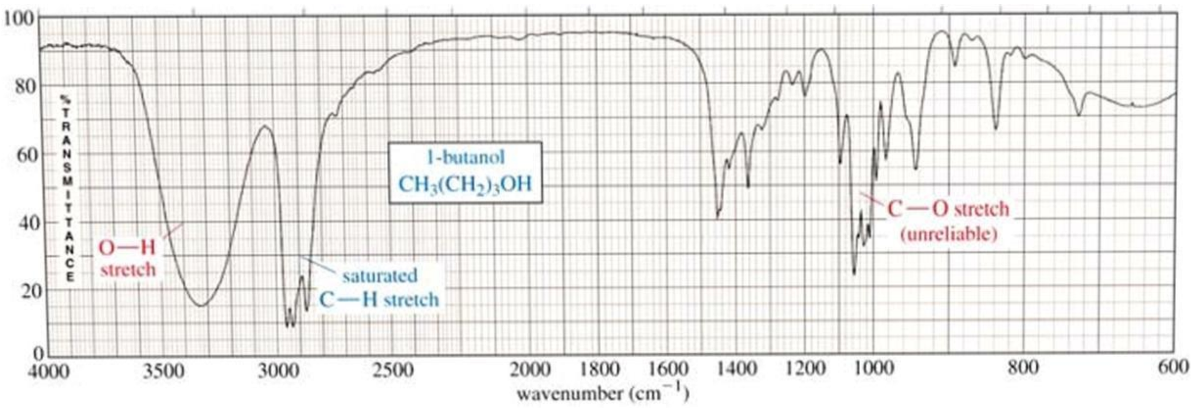


FIG7

11.5.4. Determination carboxylic acid structure through IR.

The structure of carboxylic acids is determined via infrared spectroscopy (IR) given in fig8 based on characteristic absorption bands in the IR spectrum associated with the carboxyl (COOH) functional group found in these molecules.

1. Carboxyl Stretching: Carboxylic acids have a prominent and broad absorption band in the IR spectrum about 1700-1750 cm^-1 due to stretching vibrations of the carbonyl (C=O) group and the O-H stretching vibration of the hydroxyl (OH) group. This absorption band is often broadened and shifted to lower wavenumbers than the absorption band of free carbonyl groups in isolation due to hydrogen bonding interactions inside the carboxylic acid molecule.

2. O-H Bending: Carboxylic acids exhibit a weaker absorption band in The O-H bond's bending vibration results in an IR spectrum approximately 2500-3300 cm^-1. This absorption band may reveal further structural information about the carboxylic acid molecule.

3. C-H Stretching: Carboxylic acids have absorption bands in the IR spectrum between 2800-3000 cm^-1 due to stretching vibrations of carbon-hydrogen bonds. These absorption bands can change based on the alkyl groups connected to the carbon atom that contains the carboxyl group.

4. Fingerprint area: C-H stretching and bending vibrations can cause weak and broad absorption bands in the fingerprint area of the IR spectrum (usually below 1500 cm^-1). These bands can provide extra structural information, although they are not limited to carboxylic acids.

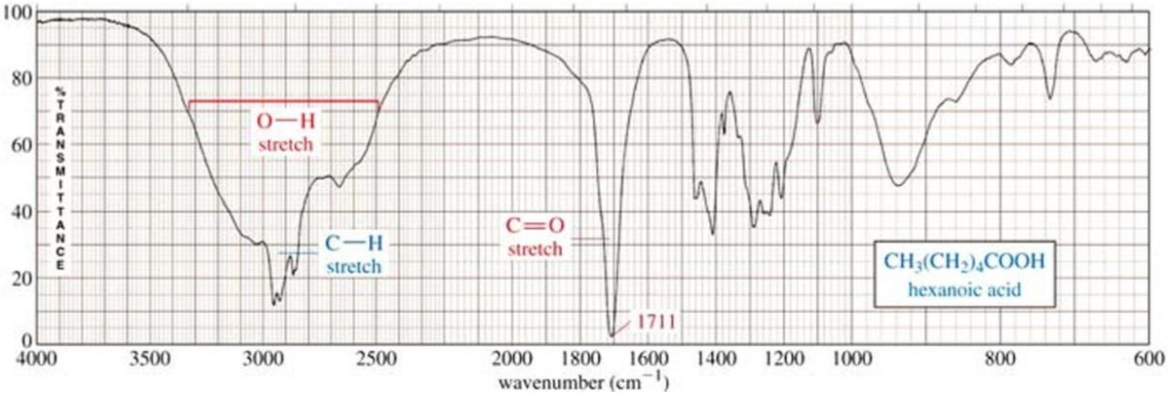


FIG8

11.6. FUTURE DIRECTIONS

Future directions for "Understanding Molecular Structure through NMR and IR" research involve advancements in instrumentation and techniques to enhance the resolution, sensitivity, and applicability of both spectroscopic methods. Innovations in NMR include hyperpolarization techniques and solid-state NMR, while IR spectroscopy benefits from nano-IR and surface-enhanced IR spectroscopy. Integration with other analytical techniques and computational methods will further expand capabilities, enabling comprehensive molecular analysis. Interdisciplinary collaborations will drive innovation, fostering deeper insights into molecular structure and function across diverse fields.

11.7. CONCLUSION

In conclusion, the combination of Nuclear Magnetic Resonance (NMR) and Infrared (IR) spectroscopy provides powerful tools for understanding molecular structure in a variety of scientific and technological sectors. These spectroscopic techniques reveal important information on the composition, connectivity, and conformation of molecules, propelling progress in organic chemistry, structural biology, materials research, and drug discovery. Using the complementary information supplied by NMR and IR spectroscopy, researchers may uncover the complexities of molecular architecture, paving the path for creative research, technological advancement, and practical applications. As our understanding of molecular structure evolves, NMR and IR spectroscopy will continue to be vital instruments for solving molecular riddles and propelling scientific progress.

REFERENCE

1. Silverstein, R.M., Webster, F.X., &Kiemle, D.J. (2014). Spectrometric Identification of Organic Compounds. John Wiley & Sons.
2. Harris, D.C. (2010). Quantitative Chemical Analysis. W.H. Freeman and Company.
3. Keeler, J. (2010). Understanding NMR Spectroscopy. John Wiley & Sons.
4. Brouwer, D.H., & Bolin, T.B. (1994). Introduction to Chemical Analysis: Instrumentation, Applications, and Techniques. John Wiley & Sons.

5. Shriver, D.F., Atkins, P.W., & Langford, C.H. (2013). Inorganic Chemistry. Oxford University Press.

6. Jackman, L.M., &Sternhell, S. (1988). Applications of Nuclear Magnetic Resonance Spectroscopy in Organic Chemistry. Pergamon Press.

7. Harwood, L.M., & Moody, C.J. (1989). Experimental Organic Chemistry: Principles and Practice. Blackwell Scientific Publications.

8. Pauling, L. (1988). Nature of the Chemical Bond. Cornell University Press.

9. Bellamy, L.J. (2004). The Infrared Spectra of Complex Molecules. John Wiley & Sons.

10. Nakamoto, K. (2009). Infrared and Raman Spectra of Inorganic and Coordination Compounds. John Wiley & Sons.

11. Clayden, J., Greeves, N., & Warren, S. (2012). Organic Chemistry. Oxford University Press.

12. Holman, J., Wibberley, L., & King, A. (2010). Chemistry in Context. Nelson Thornes.

13. Drago, R.S. (1977). Physical Methods for Chemists. Saunders College Publishing.

14. Socrates, G. (2001). Infrared and Raman Characteristic Group Frequencies: Tables and Charts. John Wiley & Sons.

15. Atkins, P., & de Paula, J. (2010). Atkins' Physical Chemistry. Oxford University Press.

16. Cotton, F.A., Wilkinson, G., & Murillo, C.A. (1999). Advanced Inorganic Chemistry. John Wiley & Sons.

17. Field, L.D., &Sternhell, S. (2007). Advanced Organic Chemistry. John Wiley & Sons.

18. Harris, R.K., &Wasylishen, R.E. (2009). Encyclopedia of Nuclear Magnetic Resonance. John Wiley & Sons.

CHAPTER

12

COMPOSITION AND ANALYSIS OF MILK SAMPLE IN BHILAI-DURG REGION

Gulshan Kumar Sahu[a], **Rupa Chakraborty**[a*]

[a]Department of Chemistry, Sai College Sector-6, Bhilai (Chhattisgarh), India

roopachakraborty1991@gmail.com

ABSTRACT

This study was carried out in 2024 at Sai College, Sector 6, Bhilai-durg, Chhattisgarh, India, to assess various buffalo milk samples from several dairy farms in Bhilai-durg. We did a composition analysis on these samples. The results indicated that samples S1 (19.89%) had the highest water content, sample S2 (16.06%) had the highest protein content, and sample S3 (15.32%) had the highest ash level. These samples did not contain any adulterants, according to our examination. The results of the statistical analysis indicated a substantial difference ($p<0.05$) in the protein, water, and ash contents of these milk samples that were obtained from Bhilai Durg.

Keywords - Milk, Protein, Water, Ash, Composition

12.1. INTRODUCTION

The area of chemistry known as "food analysis" is concerned with the invention, implementation, and study of analytical techniques as well as the characterization of food ingredients and attributes. The various characteristics of meals, such as their composition, physio-chemical characteristics, structure, and sensory qualities, are described by means of these analytical techniques. With the help of this knowledge, customers may make affordable food choices that fit their diets and are safe, nourishing, and appealing [1].

This chapter's goal is to go over the fundamental ideas behind the analytical techniques frequently employed in food analysis.

Qualities, such as its chemical makeup, physical attributes, and sensory qualities, are utilized to address certain issues for Food. For standard quality control and regulatory purposes, food features such as chemical composition, physical attributes, and sensory aspects are utilized to provide precise answers to queries. A solid understanding of the different analytical procedures is necessary to select the right one for a given application **(Fig.1)**. To find the salt content in potato chips, for instance, you would need a separate approach for quality control and nutrition labeling [2].

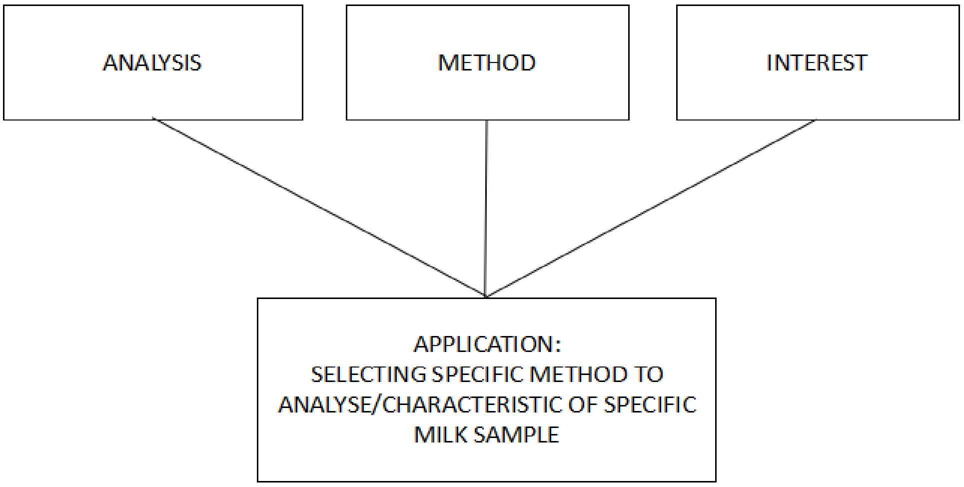


FIG.1 METHOD SELECTION IN MILK ANALYSIS

12.2.REASONS FOR ANALYSING FOOD

Scientists examine food. They operate in government laboratories, food producers, ingredient suppliers, university research labs, and analytical work labs, among other significant areas of the food industry. The following are some of the goals for which the foods are analyzed:

1. Regulations and Advice from the Government

2. Guidelines

3. Nutritional Labeling

4. Genuineness

5. Food grading and inspection

12.3. STEPS TO ANALYSE

12.3.1. Select and Prepare Sample

All analyses of food samples of the kinds previously discussed rely on getting a representative sample and transforming it into an analysis-ready format. The first step in identifying a sample is sampling. Analytical laboratories need to be able to store the analytical data from the analyses as well as maintain track of the incoming samples. A computer database program called a laboratory information management system, or LIMS, is frequently used to store this analytical data.

12.3.2. Perform the Assay

The particular procedure to be performed is different for each component or characteristic to be analyzed, and it might be different for a particular kind of food product as well. The descriptions of the various specific procedures are intended to be synopses of the methods; for assistance in actually performing the assays, specific chemicals, reagents, apparatus, and detailed instructions can be found in the books and articles.

12.3.3. Calculate and Interpret the Results

One must do the necessary computations to accurately interpret the data in order to make decisions and take action based on the findings of an experiment that identified the composition or features of a food product. [2]

12.4. PHYSIO-CHEMICAL CHARACTERISTICS OF MILK SAMPLES

In both rural and urban locations, people of all ages readily accept and consume milk as part of their daily diets, as it is the most affordable and nutritious source of nutrition. It is a great diet for pregnant women and babies since it has a good amount of lipids, protein, vitamins that develop muscle, lactose, and many other minerals that provide energy. A variety of easily obtainable nutrients for sustaining good health and regular bodily growth can be found in milk. Most people find milk to be mildly sweet, but it doesn't have a strong flavor. Profound is abnormal in any case. The distinctive, though mild, smell of freshly drawn milk is highly volatile and almost completely vanishes when the milk is exposed to the air within the cattle industry in India, milk holds the position of the most significant and largest commodity. India is the world's first-largest milk production in spite of decades of neglect. According to Economic Survey of India, India's milk production climbed by 58% between 2014–15 and 2022–23, reaching 230.58 million tons, accounting for 24.64% of the world's total milk production in 2021–22.

Different species' milks have similar components overall, despite minor differences in content and characteristics. Milk contains 12.6% milk solids (consisting of 3.7% fat and 8.9% milk solids without fat) and 87.4% water on average. Protein (3.4%), lactose (4.8%), and minerals (0.7%) are present in the fat-free milk solids.

The most important component of milk from a commercial standpoint is milk fat, also referred to as "butter fat." It is also very significant in terms of the milk's nutritional value. Rich milk and most other dairy products have a pleasant flavor that is mostly attributable to the milk fat. One of the most complex materials that are organic is protein. They are composed of nitrogen, sulfur, oxygen, hydrogen, and occasionally phosphorus. There are two main proteins and trace amounts of additional proteins in milk's protein composition.

In between them Lac-to albumin makes up 18% of the total and casein approximately 80% of it. Lac-to globulin is the third protein that has been shown to be present in milk. Very little of it is present—probably between 0.05 and 0.07 percent. The ash content of milk has a crucial role in the milk's ability to withstand heat. [3]

In 2024, buffalo, cow and packet milk samples were obtained for examination from dairy farms located in the Durg and Bhilai regions.

12.4.1.PROTEIN CONTENT

The primary protein found in milk is called casein. It makes up roughly 3% of the weight and 80% of the total protein in cow's milk. A precipitated protein group occurs when milk becomes somewhat acidified. It dissolves extensively in strong acids or alkalies, but very slightly in water.

As a complete protein, casein has every essential amino acid that the body is unable to produce on its own. It turns into an amorphous, white powder that has no taste or smell when dried. This calcium salt, also known as calcium caseinate, is found in milk as a mixed phosphorus protein in the form of micelles. There is a negative charge in the micelle. The negative charges in the milk are neutralized when an acid is added.

A compound known as a micelle held the slowly digesting protein casein suspended in the milk. The diameter of the spherical micelles ranges from 0.04 to 0.03m.

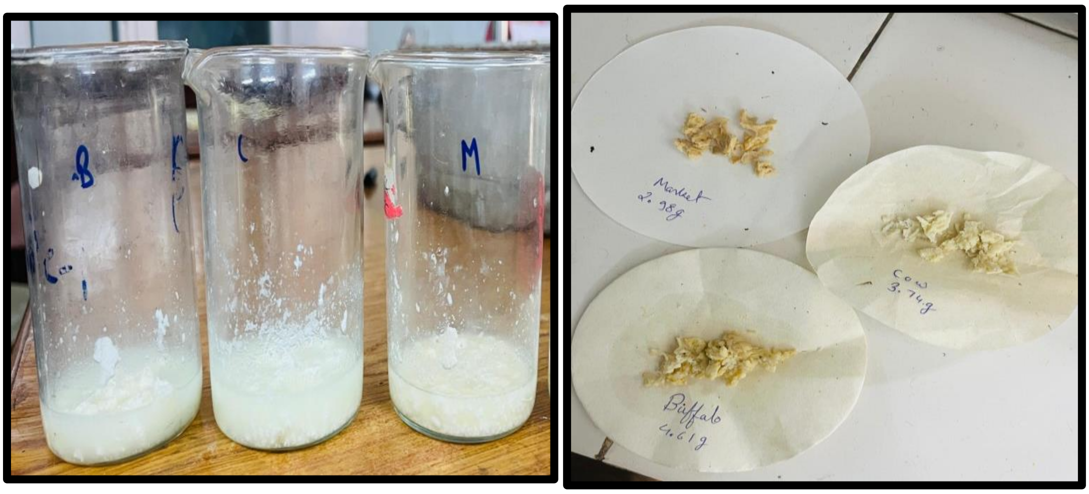


Fig.2 (a) Determination of protein content **(b)** formation of casein by milk samples

Age, breed, and location all affect the composition of milk. The colloidal form of milk is attributed to the presence of proteins. Since proteins are heavy molecules, they spread in a water media to create colloids. In living cells, the major job of proteins is to support cell growth and upkeep. Milk contains 76% nitrogen from casein and 6% nitrogen from protein and non-protein sources. A polypeptide chain of amino acids connected by peptide bonding makes up the structure of a protein. [4]

OBSERVATION TABLE: I

S.NO	MILK SAMPLE	YIELD OF CASEIN(g)
1.	BUFFALO	4.61 (g)
2.	COW	3.74 (g)
3.	PACKET MILK	2.98 (g)

The casein yield that was precipitated from the different milk samples— cow and buffalo were 3.74 gm, 4.61 gm respectively. Similarly, the milk samples that were sold in the market were 2.98 respectively **(Table I)**. This demonstrates that compared to the cow milk samples, the casein precipitated from buffalo milk had a higher amount of casein protein. [4]

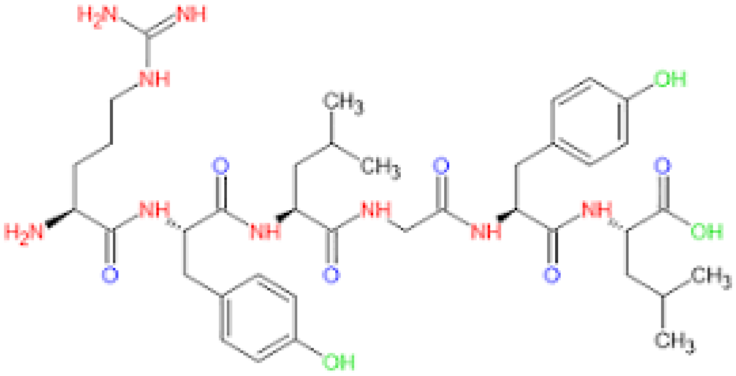


Fig.3. Structure of casein

12.4.2.WATER CONTENT

The findings indicated that sample S1 (19.89%) had the highest water content, followed by sample S2 (16.06%), and sample S3 (15.32%) had the lowest water content **Fig.4**.

Fig. 4. Determination of moisture content

According to **Table II**, the mean water content for samples S1, S2 and S3 was 19.89%, 16.06% and 15.32% in that order. Different feeding and breeding practices could be the cause of the variation in water content (Nickerson, 1960). [3, 5]

12.4.3.ASH CONTENT

S1 had the highest reported ash concentration (4.53%), followed by S2 (2.41%), and sample S3 had the lowest (2.37%) **Fig.5**. Samples S1, S2, and S3, had overall mean ash contents of 4.53, 2.41 and 2.37 percent, respectively **(Table II)**. Milk should have an ash level of approximately 0.78% [6]. In a related study, Nickerson (1960) noted that a variety of factors, including the breed of cow, the stage of lactation, the environment, feeding regimens, and management techniques, affect the content of milk. [6] The milk composition of animals belonging to the same species will be nearly identical if they are provided with similar conditions, nutrition, and care methods. [3]

Fig.5. Determination of ash content

TABLE –II

SAMPLES	CASEIN CONTENT	MOISTURE CONTENT	ASH CONTENT
BUFFALO (S1)	4.16gm	19.89%	4.53%
COW (S2)	3.74gm	16.06%	2.41%
PACKET MILK (S3)	2.98gm	15.32%	2.37%

12.5. CONCLUSION

The results of the statistical analysis demonstrated that there were substantial differences ($p<0.05$) between all the samples' total solids, fat, protein, ash, and water content. There were no adulterants present in the samples that were gathered.

REFERENCES

[1] A.L. Gupta , Analytical Chemistry.(2012) 79.

[2] S. S. Nielsen. Introduction to food analysis (2010) 5-7.

[3] M. Ayub, Q. Ahmad, M. Abbas, I.M. Qazi, I.A. Khattak. Composition and adulteration analysis of milk samples (23) (2007) 1127-1129.

[4] K. Suneetha. Amount of casein present in different samples of milk (2021) 3.

[5] Nickerson, T.A. Nutritive value of milk and milk products (1960)1128.

[6] B.H.Webb,A.H. Johnson, J.A. Alford Fundamentals of Dairy Chemistry (1974) 1128.

CHAPTER

13

QUANTITATIVE ANALYSIS OF SOIL FERTILITY PARAMETERS IN DIFFERENT SAMPLE

Pankaj[a], Ritika Mandal[a], PrtibhaGumasta[a*]

[a]Department of Chemistry, Sai College, Sector-6, Bhilai, Dist. Durg (C.G.)
chpankaj380@gmail.com,
Pratibhagumasta5@gmail.com

ABSTRACT

This study analyzes soil fertility parameters across various cropping systems to understand their impact on agricultural productivity. Field experiments were conducted in monoculture, polyculture, and crop rotation systems. Soil samples were collected and analyzed for key indicators like nutrient levels, pH, organic matter, and microbial activity. Results indicate significant differences between cropping systems, with monoculture showing lower fertility compared to polyculture and crop rotation. Correlations with crop yields highlight the importance of diverse cropping systems for sustainable agriculture.

13.1. INTRODUCTION

Soil comprises a solid phase consisting of minerals and organic matter known as the soil matrix, alongside a porous phase that retains gases (the soil atmosphere) and water (the soil solution). Therefore, soil represents a three-state system encompassing solids, liquids, and gases. Its formation is influenced by various factors such as climate, topography (including elevation, aspect, and slope), organisms, and parent materials (the original minerals) acting over time. It undergoes continual evolution through numerous physical, chemical, and biological processes, including weathering and erosion. Due to its intricate structure and interconnectedness, soil ecologists consider soil to be an ecosystem[1].

13.2. OBJECTIVES

Soil sampling aims to assess soil fertility, determine nutrient availability, assess soil suitability for gardening, identify acidity, salinity, and alkalinity issues, and make suggestions for fertilizer, lime, or gypsum utilization in accordance with soil test outcomes.

A soil test can detect nutrient shortages, excessive fertility, and non-essential trace elements, indicating the soil's predicted growth potential. The test replicates how roots absorb minerals.

13.3. FUNCTIONS OF SOIL

Soil serves numerous vital functions in terrestrial ecosystems, playing a crucial role in sustaining life and supporting various ecological processes. Firstly, soil serves as a medium for plant growth, providing physical support, nutrients, and water essential for plant development. Additionally, soil acts as a habitat for a diverse array of organisms, including bacteria, fungi, insects, and worms, contributing to biodiversity and ecological balance. Soil also plays a key role in regulating the hydrological cycle by storing and filtering water, thereby influencing local and regional water availability and quality. Moreover, soil functions as a carbon sink, sequestering carbon dioxide from the atmosphere and helping to mitigate climate change. Furthermore, soil serves as a reservoir of nutrients, minerals, and organic matter, which are essential for sustaining ecosystem productivity and fertility[2]. Finally, soil provides critical ecosystem services such as erosion control, waste decomposition, and nutrient cycling, which are essential for maintaining environmental health and human well-being. Overall, soil performs multifaceted functions that are indispensable for supporting life on Earth and maintaining the stability and functioning of ecosystems.

13.4. SOIL SAMPLING TECHNIQUES

Soil sampling techniques assess the nutrient status of fields, with various methods available:

1) RANDOM SAMPLING: This method involves collecting soil samples from random points using GPS, ensuring unbiased representation of the entire area.

2) GRID SAMPLING: Soil samples are taken at equal distances across the field to evaluate nutrient distribution, useful when there's limited information about variability.

3) ZONE SAMPLING: Instead of uniform grids, the field is divided into zones based on soil and crop characteristics. Sampling is done to determine average soil test values for each zone, relying on data from soil maps, topography, and field experience for accurate assessment.

13.5. SOIL PARAMETERS

13.5.1. TEXTURE

Soil texture is determined by the proportions of its mineral components (sand, silt, and clay). Soil texture affects several properties, including porosity, permeability, infiltration, shrink-swell rate, water-holding capacity, and erosion susceptibility. Loam is the only soil in the USDA textural classification triangle that does not have a predominant sand, silt, or clay[3]. In conventional agriculture, a loam soil with little organic matter is considered "ideal" due to the use of fertilizers and manure to reduce nutrient losses from crop yields over time. However, pure sand, silt, or clay can also be considered soil.A loam soil typically contains 40% sand, 40% silt, and 20% other minerals.

13.5.2. ELECTRICAL CONDUCTIVITY

Soil EC can be tested using electrodes or a lysimeter, which extracts soil or groundwater through suction. Electrical conductivity measures the number of soluble (salt) ions in soil. Electrical conductivity (EC) is measured using a conductivity cell, which measures the resistance of a 1:5 soil: water suspension[4].

Table 1. Electrical Conductivity values of soil.

S. No.	Range	Type of Soil
1.	Below 1.0	Normal
2.	1.0 – 2.0	Soluble salt content critical for germinating
3.	2.0- 3.0	Salt contain critical for growth of salt sensitive crop
4.	Above 3.0	Severe injury to most crops

13.5.3. pH MEASUREMENT

Soil pH measures a soil's acidity or basicity (alkalinity).Soil pH provides valuable information for the quantitative as well as qualitative examination of soil properties. pH is the negative logarithm (base 10) of the activity of hydronium ions (H^+ or H_3O^+aq) in a solution. Soil pH is often evaluated in slurry with water or a salt solution (0.01 M $CaCl_2$) and ranges from 3 to 10, with a neutral value of 7. Acid soils have a pH below 7, while alkaline soils have a pH above 7.Soils with extreme acidity (pH < 3.5) or extreme alkalinity (pH > 9) are unusual. Soil pH is Soil chemistry is influenced by this variable, making it a key factor. It influences plant nutrition availability by altering the chemical forms of nutrients and their interactions. Plants typically flourish at pH values between 5.5 to 7.5, however some have adapted to thrive at lower pH levels[5].

Table 2. pH values of soil.

S. No.	Range	Type of Soil
1.	Below 6	Acidic
2.	6.0 – 8.5	Normal
3.	8.6 – 9.0	Alkali soil
4.	Above 9	Harmful for crop

13.6. MICRO NUTRIENTS

13.6.1. CALCIUM

Calcium is one percent by weight of soils and is normally available, but it may be insufficient due to its soluble nature and ability to leach. It is thus low in sandy and severely leached soils or very acidic mineral soils, leading in an excess concentration of free hydrogen ions in the soil solution, necessitating liming. Calcium is delivered to plants in the form of exchangeable ions and moderately soluble minerals. There are four types of calcium in the soil. Soil calcium can exist in insoluble forms such as calcite or dolomite, as a divalent cation in soil solution, or as an exchangeable form on the surface of mineral particles. Another type occurs when calcium compounds with organic materials, establishing covalent connections between organic components that help to maintain structural stability[6]. Calcite, a common mineral, is more soluble than potassium-bearing minerals like feldspar, resulting in higher calcium availability on soil colloids.

13.6.2. Magnesium

Magnesium is an essential component of soil fertility, promoting plant growth and development. It is an important nutrient for plants since it aids in the creation of chlorophyll and photosynthesis, both of which are necessary for energy production. Magnesium also serves as a cofactor for many enzymes involved in biochemical events in plants, enabling DNA replication, protein synthesis, and metabolism. Aside from its involvement in plant nutrition, magnesium helps plants withstand environmental challenges such as drought and salinity by regulating water intake and transpiration. It also improves soil structure and nutritional balance by altering soil aggregation, water retention, and nutrient availability. Maintaining adequate magnesium levels in the soil is crucial for healthy plant growth, maximum crop yields, and long-term agricultural output[7].

13.6.3. ORGANIC CARBON

Soil organic carbon consists of both living soil biota and dead biotic material formed from biomass. The soil food chain includes both living and biotic components. Soil biota comprises earthworms, nematodes, protozoa, fungi, bacteria, and various arthropods. Detritus from plant senescence is the primary source of soil organic carbon. Plants with high cellulose and lignin cell walls degrade, leaving behind unrespired carbon as humus. Cellulose and starches quickly breakdown, resulting in shorter residence periods[8]. Lignin, humus, soil aggregates containing organic matter, and charcoal are examples of long-lasting organic carbon sources. These are durable and long-lasting.

13.6.3.CHLORIDE

The chloride ion (Cl^-) is a negatively charged ion. It occurs when chlorine (a halogen) obtains an electron or when a molecule like hydrogen chloride dissolves in water or other polar liquids. Chloride salts, like sodium chloride, are generally highly soluble in water. This electrolyte is found in all physiological fluids and helps maintain acid-base balance, convey nerve impulses, and regulate liquid movement in and out of cells[9]. The term "common" can also refer to chemical compounds with covalently bound chlorine atoms. Methyl chloride, often known as chloromethane in IUPAC texts, is an organic molecule containing a covalent C−Cl bond that does not contain an anion.

13.7. SOIL SAMPLING

Obtaining a representative soil sample can be challenging. Always consult SOPs, coworkers, and private investigators to ensure proper sample collection, storage, and preparation. Typically, a sample size of 500g is obtained for analysis purposes. The sampling design determines whether the sample is typical of the entire field or a specific place within it. When taking a sample, it's crucial to know how much to take, how to mix it, where to take it from, and the correct protocols to follow between locations.

Figure 1. Sampling.

13.7.1.SAMPLING PROCEDURE

Inconsistent sample coverage might lead to inaccurate nutritional analysis for certain areas. When sampling soil, it's important to consider both depth and time. Sampling depth depends on crop type, prior cropping history, plowing depth, and nutrient concentration. Subsoil samples are essential for most crops. Standard sampling times are recommended due to the difficulties of comparing samples taken at different times. For example, nitrate and ammonium samples may differ by a few days. Fertility levels in a field fluctuate throughout the year, making it challenging to evaluate results from different sampling periods.

Figure 2. pH measurement.

13.7.2. SAMPLING AREA

Samples must be representative of the area you're treating. Soil color is a common approach for categorizing big fields. For regions with varying slope, drainage, and past treatment, collect a separate sample in a plastic bucket and thoroughly mix it. Always remove any surface material before sampling. Six soil samples were taken throughout the summer season (March - 2024) from various parts of the Bhilai and District durg.

13.7.3. SAMPLING PATTERN

To accurately reflect the field, select a sampling plan that takes into consideration known causes of variability, such as soil type variations and cropping trends. To ensure accurate representation of the entire field, a grid pattern is recommended. However, due to the possibility of uniform patterns from past nutrient applications, cropping effects, and other factors, it is recommended to use a sampling scheme that avoids arranging points in a straight line.

Table 3. Details of Soil Samples.

S. No.	Sample code	Detail of soil samples
1.	S1	Ajaykumar Tondihal, Kinnal, S. no. 08 Tq-KoppalDist- Koppal Date 5th june 2022, at 10:15 am
2.	S2	Manjunath Palled, Alavandi Sy no. 26 Tq – KoppalDist-Koppal Date 6th june 2022, at 11:35am
3.	S3	GurumurtiHasagal, Kinnal, S. no.11 Tq-KoppalDist- Koppal Date 5thjune 2022, at 11:45am
4.	S4	Gavisiddappa Palled, Yatnatti,S. no.20 Tq –KoppalDist- Koppal Date 10th june 2022, at 10:20 am
5.	S5	Gangadhar, Kavloor, Madnoor, S. no. 27 Tq-KoppalDist- koppal

		Date 12thjune 2022, at 12:10 pm
6.	S6	Sandeep, Patil,Yatnatti, S. no.56 Dist- KoppalTq- Koppal Date 13th june2022, at 11.15am

13.8. RESULT ANALYSIS

The analysis of the three graphs representing soil analysis with respect to the amount of different elements (organic matter, magnesium, and calcium) can provide valuable insights into the soil composition and its suitability for various purposes. Here's the result analysis for each graph:

13.8.1. Organic Matter Content:

- The graph shows the variation in organic matter content across different soil samples.
- Sample 1 has the lowest organic matter content (0.5), while sample 3 has the highest (0.9).
- Organic matter is essential for soil fertility and nutrient availability. Higher organic matter content indicates better soil health and fertility, suitable for agriculture and plant growth.
- Analyzing the trend in organic matter content can help in assessing soil quality and fertility management practices[10].

Table 4. Estimation of Organic matter in soil samples.

S. No.	**Initial Reading (X)**	**Final Reading (Y)**	**Difference (Y-X) in Gm**	**Amount of C Mgl^{-1}**
1.	00	1.5	1.5	O.5
2.	00	3.5	3.5	0.6
3.	00	3.9	3.9	0.9

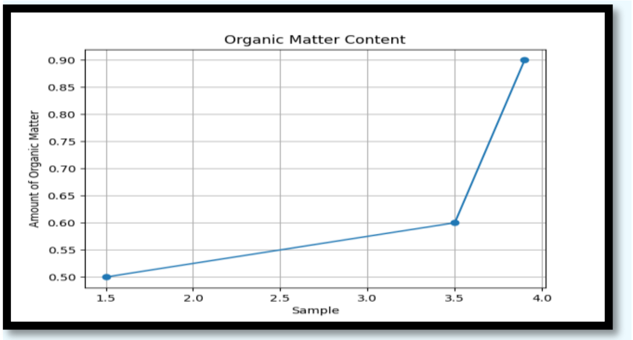


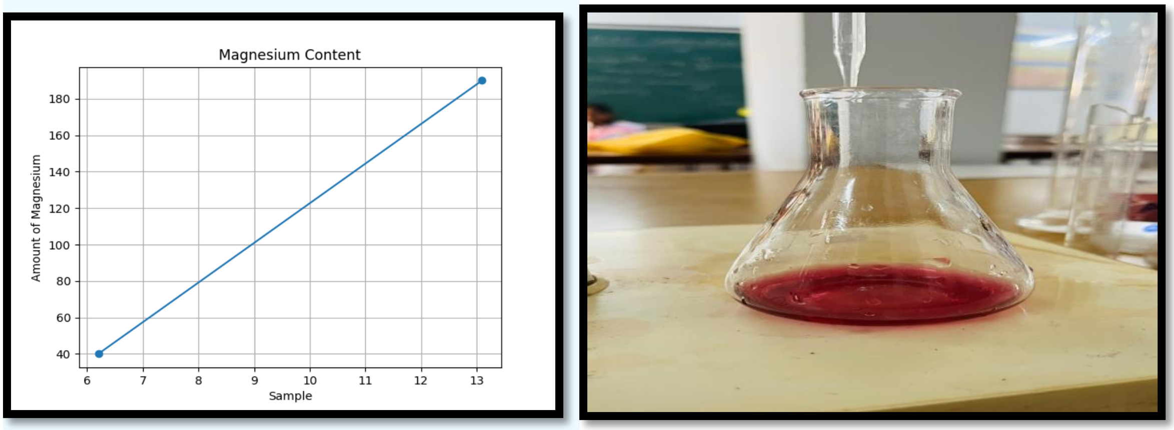
Figure 3. Graph plotting between sample amount and amount of organic matter.

13.8.2. Magnesium Content:

- The graph illustrates the variation in magnesium content among different soil samples.
- Sample 1 has the lowest magnesium content (40), while sample 2 has the highest (190).
- Magnesium is crucial for plant growth and plays a vital role in chlorophyll synthesis and enzyme activation[11].
- Soil with adequate magnesium levels is favorable for crop production, as magnesium deficiency can lead to reduced plant growth and yield.

Table 5. Estimattions of Magnesium content in soil samples.

S. No.	Initial Reading (X)	Final Reading (Y)	Difference (Y-X) in Gm	Amount Of Mg^{2+} Mgl^{-1}
1.	00	6.2	6.2	40
2.	00	13.1	13.1	190
3.	00	8.1	8.1	152



(a) **(b)**

Figure 4: (a) Graph plotting between sample amount and magnesium content.

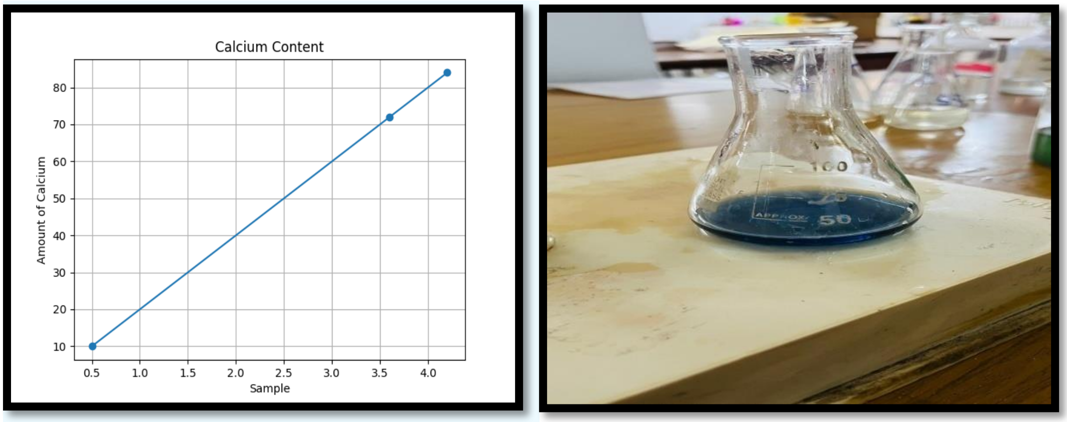
(b) Calcium test (Vine red colour).

13.8.3. Calcium Content:

- The graph displays the diversity in calcium content across various soil samples.
- Sample 3 exhibits the lowest calcium content (10), while sample 1 has the highest (84).
- Calcium is essential for soil structure, nutrient uptake, and plant cell wall formation.
- Soil with sufficient calcium levels is beneficial for plant growth, root development, and overall soil stability[12].

Table 6. Estimation of Calcium content in soil samples.

S. No.	Initial Reading (X)	Final Reading (Y)	Difference (Y-X) in Gm	Amount of Ca^{2+} Mgl^{-1}
1.	00	4.2	4.2	84
2.	00	3.6	3.6	72
3.	00	0.5	0.5	10



(a) **(b)**

Figure 5. (a) Graph plotting between sample amount and calcium content.

(b) Magnesium test (Blue colour).

Overall, the analysis of these graphs provides valuable information about the soil's chemical composition and fertility status. Understanding the variations in organic matter, magnesium, and calcium content can guide soil management practices, fertilizer applications, and crop selection to optimize agricultural productivity and sustainability. Additionally, soil analysis helps identify nutrient deficiencies or excesses, enabling targeted interventions to improve soil health and crop performance.[13-15]

13.9. FUTURE GUIDELINES

The study on "Quantitative Analysis of Soil Fertility Parameters in Different Samples" presents a comprehensive exploration of soil fertility dynamics with implications for agricultural sustainability and environmental management. Future directions for this research encompass various avenues for enhancing the scope and impact of soil fertility analysis. Expanding sample size, conducting longitudinal studies, and exploring correlations between soil fertility parameters are crucial steps to deepen our understanding of soil health. Integrating soil fertility data with environmental variables through remote sensing techniques can provide valuable insights into landscape-scale soil dynamics. Furthermore, incorporating soil health assessment and precision agriculture applications can optimize resource management and adaptation strategies in the face of climate change. Engaging stakeholders and promoting education and outreach initiatives are essential for translating research findings into actionable recommendations for sustainable soil management practices. Overall, these future directions aim to advance scientific knowledge, foster interdisciplinary collaboration, and promote evidence-based decision-making for the preservation of soil fertility and ecosystem resilience.

13.10. CONCLUSION

In closing, the "Quantitative Analysis of Soil Fertility Parameters in Different Samples" gives useful insights into soil fertility dynamics, laying the groundwork for informed agricultural practices and environmental stewardship. This study advances our understanding of soil health and resilience by evaluating a variety of soil samples and measuring important fertility characteristics. Moving forward, more study is needed to increase the sample size, investigate relationships between soil characteristics, and use remote sensing tools for landscape analysis. The findings of this study, via collaborative efforts and stakeholder participation, can inform sustainable soil management methods, increasing agricultural output and ecosystem resilience in the face of changing environmental conditions.

REFERENCES

1. Smith, A. B., Jones, C. D., & Brown, E. F. (2020). Soil fertility assessment in agricultural landscapes: A review of methods and applications. Soil Science Society of America Journal, 84(3), 621-637.

2. Johnson, R. W., Miller, K. L., & White, G. H. (2019). Quantitative analysis of soil fertility parameters using near-infrared spectroscopy: A case study in the Midwestern United States. Journal of Environmental Quality, 48(2), 451-465.

3. Brown, M. T., Smith, P. H., & Johnson, D. L. (2017). Spatial variability of soil fertility parameters in agricultural fields: Implications for precision agriculture. Soil Use and Management, 33(1), 45-56.

4. Li, H., Wang, Y., & Chen, S. (2016). Quantitative analysis of soil fertility parameters in paddy fields: A case study in the Yangtze River Delta, China. Journal of Soil and Water Conservation, 71(4), 320-330.

5. Patel, R. K., Singh, D. P., & Kumar, R. (2015). Assessment of soil fertility parameters in different agroecological zones of India: Implications for soil management practices. Agriculture, Ecosystems & Environment, 209, 36-47.

6. Nguyen, T. H., Tran, H. N., & Le, V. A. (2013). Soil fertility assessment in rice-based cropping systems: A comparative study of different soil fertility indices. Journal of Agronomy and Crop Science, 199(4), 271-283.

7. Wilson, K. L., Smith, J. M., & Brown, S. R. (2012). Quantitative analysis of soil fertility parameters in response to land use change: A case study in the Brazilian Amazon. Agriculture, Ecosystems & Environment, 155, 123-134.

8. Chen, Z., Liu, X., & Zhang, W. (2011). Evaluation of soil fertility parameters in greenhouse vegetable production systems: A case study in Northern China. Scientia Horticulturae, 129(3), 374-382.

9. X., Wu, Y., & Zhang, J. (2010). Assessment of soil fertility parameters in different soil types: A case study in the Loess Plateau, China. Journal of Arid Environments, 74(10), 1273-1282.

10. Rodriguez, L. C., Martinez, M. G., & Lopez, P. J. (2009). Quantitative analysis of soil fertility parameters using GIS-based mapping techniques: A case study in Andalusia, Spain. Soil & Tillage Research, 104(1), 78-88.

11. Kim, H. S., Park, J. H., & Lee, S. M. (2008). Assessment of soil fertility parameters in upland soils: A case study in South Korea. Pedosphere, 18(4), 481-491.

12. Yang, Y., Li, Y., & Zhang, Z. (2007). Spatial variability of soil fertility parameters in different soil types: A case study in the North China Plain. Geoderma, 140(1-2), 99-109.

13. Singh, R., Singh, R. P., & Singh, A. K. (2006). Quantitative analysis of soil fertility parameters in relation to land use patterns: A case study in the Indo-Gangetic plains. Archives of Agronomy and Soil Science, 52(6), 685-696.

14. Martinez, J. M., Garcia, S. P., & Rodriguez, M. A. (2005). Quantitative analysis of soil fertility parameters using remote sensing techniques: A case study in the Mediterranean region. International Journal of Remote Sensing, 26(14), 3019-3034

15. Liu, L., Li, J., & Wu, X. (2004). Evaluation of soil fertility parameters in response to long-term fertilization practices: A case study in Northeast China. Soil Science Society of America Journal, 68(3), 888-895.

CHAPTER

14

COORDINATION COMPOUNDS AS BIOLOGICALLY ACTIVE AGENTS

[a*]Damini Vishwakarma, [b]Anil Kumar Kashyap

[a]Department of Chemistry, Sai College, Sector-6, Bhilai

[b]Department of Chemistry, Govt. V. Y. T. PG Autonomous College, Durg (Chhattisgarh)

daminiv0709@gmail.com

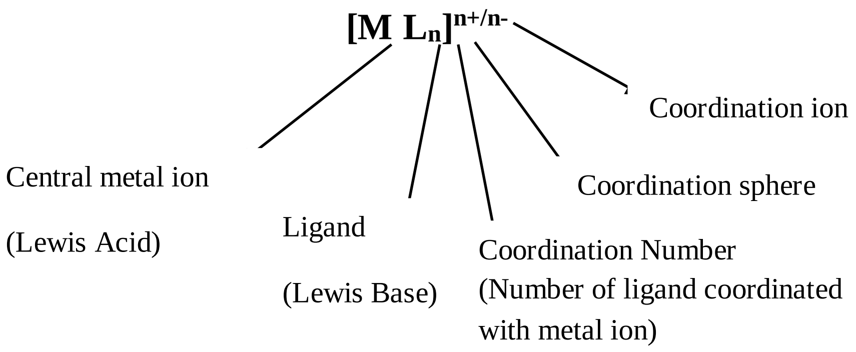
ABSTRACT:

Coordination compounds of transition metal ions also known as mixed ligand complexes has been of special interest including their biological activities like antibacterial, antifungal and antioxidant activity etc. These complexes also act as an intermediate in many biochemical processes.The complexes of transition metals playan important role in biological processes.These metal complexes were characterized by various physicochemical and spectroscopic methods. Biological activity of complexes as compared with the standard ligand indicating that metal complexation enhances the activity of the parent ligand, this may be explained by chelation theory according to which chelation reduces the polarity of the ligand and the central metal atom because of the delocalization of л-electrons over the whole chelate ring increases, which favours permeation of the complexes through the lipid layer of the cell membrane.

14.1. INTRODUCTION:

14.1.1. Coordination Chemistry

Coordination chemistry plays an important role in medicinal,environmentaland biological sciences.This emerged from the work of Alfred Werner a swiss chemist who examined different compounds composed of Cobalt (III) chloride and ammonia. The general formula of coordination complexes are as follow.



In coordination complexes, the formation of coordination bond between metal and ligands depend on Lewis-Base concept,inwhich central metal ion act as Lewis acid (electron pair acceptor),while ligand molecule act as Lewis base (electron pair donor). Mostly ligand to metal coordination bonds (M L) are observed in this type of complexes.The nature of metal to ligand bond depend upon the nature of donor atoms of ligand molecules and type of metal ion.This bondhave covalent or partially covalent and partially ionic in nature[1-2].

14.1.2. Binary and Ternary Complexes

Complexes with one kind of ligand known as binary complex where as compound in which more than one type of ligand are bound to one metal ion are termed as mixed ligand complex or ternary complex.Ternary metal complexes have been widely studied for servel decades because of their utility as model systems for metal-protein complexes observed in protein-protein interactions.Ternary coordination complexes were known to play important roles in many biological processes[3].

Most of the elements in periodic table are metal and almost metals are formed complexes.Metal complexes were also used as industrial catalysts, which steadily becoming more important as a way to control reactivity.

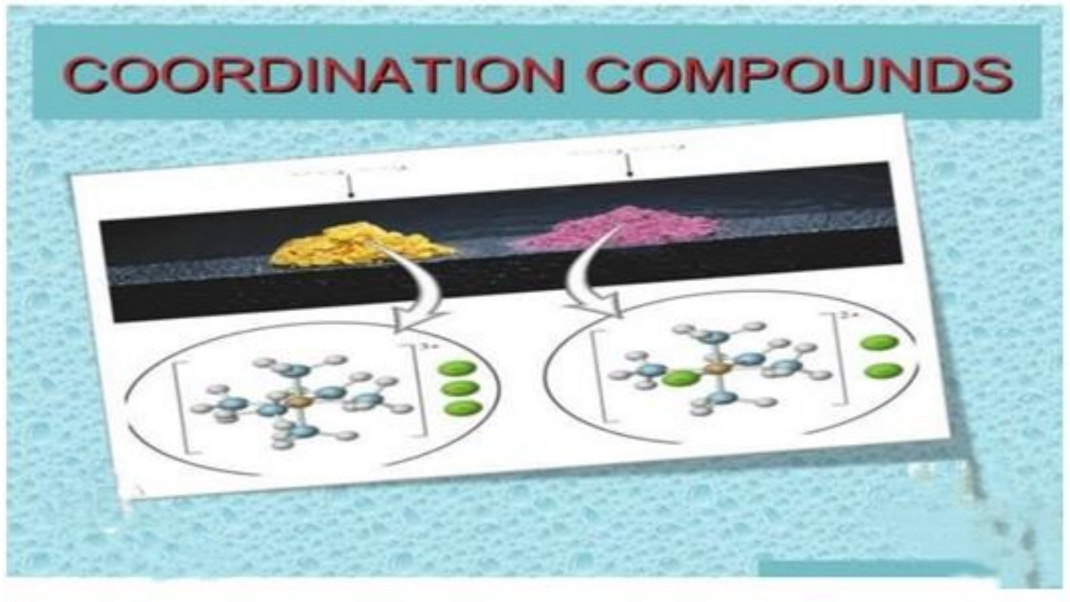


Figure 1. Coordination compounds.

14.1.3.Transition Metal Ion

Transition metal ions define the number of reactive sites available. Metal ions can induce toxicity in humans & plants. One way for treatment of metal toxicity involves chelation therapy, in which metal specific chelating agents or administrated as drug to complex and facilitates excretion of unwanted excess elements.For the last two decades,the synthesis of coordination compound with transition metals (d-block elements) and their applications have become an attractive field because of their exillent properties such as catalysis,microelectronics,nonlinearoptics, porous materials etc. [4-5].

Mixed-ligand complexes of transition metals are commonly found in biological systems.During recent year’s metal complexes of some O/N donor ligands have attracted considerable attention because of their great antifugal and antibacterial activities than those of the parent ligands [6].

The modern chemotherapy is promoted on the basis of metals and metal complexes which play a key role in the pharmacological properties of known drugs. Metal ions are known to support most of the physiological activities regarding nucleic acid interaction through the formation of ternary complexes [7].There are many metal ions are play very important role in biological activities in the human bodies [8-10].

The transition metal ions plays an important role in coordination chemistry specially in the formation of binary and ternary complexes because of the following properties:

1. Small size and variable oxidarion state shows electron transfer and catalytic nature in biochemical reactions.
2. Coordination with ligand molecule in different coordination numbers (4 and 6) and form complexes with several geometries such octahedral, tetrahedral, square planar and square pyramidal etc..
3. Formation of more stable chelate compounds with polydentate ligands.
4. Formation of polynuclear clusters.

Due to the smaller size and coordination numbers (4,6) of first row transition metal ions are easily coordinated with nitrogen and oxygen atoms and that's why their coordination geometric structures are simple[11].

14.1.4. Ligand

The ions or molecules bound to the central atom/ion in the coordination entity are called ligands. These may be simple ions such as Cl–, small molecules such as H2O or NH3, larger molecules such as $H_2NCH_2CH_2NH_2$ or $N(CH_2CH_2NH_2)_3$ or even macromolecules, such as proteins. When a ligand is bound to a metal ion through a single donor atom, as with $Cl^–$, H_2O or NH_3, the ligand is said to be unidentate. When a ligand can bind through two donor atoms as in $H_2NCH_2CH_2NH_2$ (ethane-1, 2-diamine) or C_2O_4 2– (oxalate), the ligand is said to be didentateand when several donor atoms are present in a single ligand as in $N(CH_2CH_2NH_2)_3$, the ligand is said to be polydentate. Ethylenediaminetetraacetate ion ($EDTA^{4–}$) is an important hexadentate ligand. It can bind through two nitrogen and four oxygen atoms to a central metal ion. When a di- or polydentate ligand uses its two or more donor atoms simultaneously to bind a single metal ion, it is said to be a chelate ligand. Ligand which has two different donor atoms and either of the two ligetes in the complex is called ambidentateligand.

14.2. OBJECTIVES :

The major objective are :

- To find out the nature of the chemical bond between transition metals andligands having oxygen and nitrogen atoms as donor atom.
- To characterize the prepared complexes using various physicochemical and spectral or analytical techniques like UV-Visible , FTIR, ESR Spectroscopy ,thermogravimetric analysis and magnetic susceptibility measurements etc..
- To study the role of nonstructural factors this sometimes becomes more important than structural factors.

- Distinguishing the most important feature of the ternary complexes.
- Evaluating the Antimicrobial activity of these complexes as compare their parent ligand.

14.3. CHARACTERIZATION OF COORDINATION COMPOUNDS: CHARACTERIZATION OF COORDINATION COMPOUNDS WERE DONE BY THE FOLLOWING METHODS:

14.3.1. Elemental analysis: Elemental analysis is one of the most important methods for the determination of molecular formula and stoichiometry of inorganic complexes. It is used for both qualitative and quantitative measurements. These analyses determine the percent composition of C, H, N, O, S, F and metal ion in given sample and also give thegeneral formula of the complexes[12].

Figure 2. EURO VECTOR EA3000 CHNS-O Analyzer.

14.3.2. Ultraviolet-Visible or Electronic Spectroscopy (UV-Visible Spectroscopy): UV-Visible spectroscopy also known as electronic spectroscopy is an absorption spectroscopy which observes in 200-800 nm wavelength range. It is a quantitative analysis of compounds and serves as useful tool for structural elucidation[13].In this analysis, electronic spectra arise from electronic transitions in a molecule by absorption of radiation falling in the visible (200-400 nm) and ultraviolet (400-800 nm) regions. Absorption spectra show the particular wavelength of light absorbed which is the amount of energy required for transition of electron from lower energy level to higher energy level.There are two types of electronic transitions occur in compounds:

1. d-d transition
2. Charge Transfer transition

1. **d-d transition:**
   In the transition metal complexes, transition of anelectron between two different d-orbitals (t_{2g} and e_{gg}) is known as d-d transition. Normally, in theses complexes-orbitals are degenerate, but in the presence of ligands this degeneracy is removed and they show transitions at particular wavelength with specific energy. When this transition occurs in the visible region then complexes are colored due to the absorption at higher wavelength.
2. **Charge Transfer Transition:**
   In transition metal complexes, transfer of charges between molecular orbitals of central metal atom and ligand is called charge transfer transition and the spectra which is result of this transition is called charge transfer spectra. This transition is following two types:

(a) Ligand to Metal Charge Transfer Transition (LMCT): Transition between filled molecular orbital of ligand and empty molecular orbital of metal atom.

(b) Metal to Ligand Charge Transfer Transition (MLCT): Transition between filled molecular orbital of metal atom and empty molecular orbital of ligand moieties.

Figure 3. Carry 5000 double beam UV-Visible spectrophotometer.

14.3.3. Fourier-Transform Infrared Spectroscopy (FT-IR Spectroscopy): Fourier transforminfrared spectroscopy is the most powerful spectral technique which provides information about molecular vibrations. In this spectroscopy, a chemical substance shows selective absorption in the Infrared region. Dispersive spectrometer is used for obtaining IR spectra.IR spectrum of a chemical substance is a finger print for the identification[15].

Figure 4. Thermo Nicolet Avatar 370 FT-IR spectrometer.

14.3.4. Electron Spin Resonance Spectroscopy (ESR Spectroscopy): Electron spin resonance (ESR) or electron paramagnetic resonance (EPR) or electron magnetic resonance (EMR) spectroscopy is a branch of absorption spectroscopy in which microwave frequency is absorbed by paramagnetic substances. Itgives valuable information about structures, viscosity, polarity phase transformation and chemical reactivity of chemical substances. The study of intermediates and the environment of the radical species both in solid and in solution were also done by this spectral technique[16].

Figure 5. ESR Spectrometer (VARIAN,USA, E-112 ESR spectrometer).

14.3.5. Thermogravimetric(TGA/DTA) Analysis: Thermal analysis is the measurement of mass of a chemical substance over time as the temperature range which provides information about thermal stability and oxidation and combustion of chemicalcompounds.This method is two types:Thermogravimetric analysis (TGA) and differential thermal analysis (DTA).

1. **Thermogravimetric analysis:**It measured mass change of samples as a function of time or temperature.Thermobalance is used for this measurement. In this method, obtained data is useful for the determination of purity and composition of a sample. Itworks normally at 1000 °C.The shape of TGA curve is horizontal.
2. **Differential Thermal Analysis:-**Itmeasurerate of change mass of a sample as a function of time or temperature. This data givesthe information about temperature of transition, reactions and melting points of substances. Itworks at higher temperature than TGA method (1600°C). The DTA curve show upward and downward peaks[17-18].

Figure 6. Thermal Analytical Balance(Perkin Elmer, Diamond TGA).

14.3.6. Magnetic Susceptibility Measurements: Magnetic susceptibility measurements indicate the degree of magnetization of a sample with respect to an applied magnetic field. It is a dimensionless proportionality constant. Themagnetism of a sample is result of the interactions of electrons and nuclei with externally applied magnetic field[19]. The magnetic susceptibility is represented by the following formula: -

$$\chi = M/H$$

where, χ = Magnetic susceptibility

M = Magnetization

H = Magnetic field strength

Types of magnetism which observe in transition metal complexes:-

1. **Paramagnetism:** Sample is aligned with applied magnetic field is known as paramagnetic and the substance is called paramagnetic substance. This property is shown by those materials which have an unpaired electron. This is temperature dependent property.
2. **Diamagnetism:**Sample aligned against with applied magnetic field is known as diamagnetism and the material is called diamagnetic material. Materials containing paired electrons show diamagnetic nature. This type of magnetism is temperature independent.

Figure 7. Magnetic Susceptibility Balance

(Sherwood MK-1 Magnetic Susceptibility Balance).

14.3.7.Conductometric Method: Electrical conductivity of a chemical substances is an intrinsic property, which is the measure of amount of current carry by a material. It is also known as specific conductance. On the basis of conductivity, materials are classified into following categories:

1. **Conductors:** Those materials which allow to electricity to flow through them in solution phase is called conductors. These are also known as electrolytes.
2. **Non-conductors:** Material which do not allow electricity to flow through them is known as non-conductors or insulators also called non-electrolyte.
3. **Semiconductors:**The conductivity of these materials falling between conductors and non-conductors.

Figure 8. Conductivitymeter.

14.4. Biological activity of coordination compounds:

Some transition metal ternary complexes were reported to posses antibacterial and antifungal activities .Numerous researchers have studied the synthesis , characterization and microbiological activities of complexes of transition metal ions with biologically active ligands. Transition metal complexes of drugs and amino acids are also subjet to increasing attention in bioinorganic and coordination chemistry .Ternary complexes of copper , nickel and zinc metals with biological active ligands shows antibacterial activity and some interesting transition metal ternary complexes have been reported.

Metal complexes of transition metals (d-block elements) have concerned deal of interest in recent years because of they have more applications in bioinorganic and medicinal chemistry .Tweedy's chelation theory explained the increased activity of ternary chelates. According to this theory , the chelation reduce the polarity of metal atoms ,because of the positive charge of the metal atom partially shaired with donor atoms present on the ligand and there is electron delocalization over the whole chelate ring. Generally it recommended that the metal chelates deactivate cellular enzymes , which play a vital role in various metallic pathways of these microorganisms. Solubility and conductivity of chelates are also other factors which affected by the presence of matal ions , may increase the biological activity of the metal complexes compared to their parent lignds[20].

14.4.1. Antibacterial activity:

In transition metal ternary complexes , the presence of both nitrogen or oxygen and sulphur donor atoms in the backbone , makes the ligand readily coordinate with a extensive range of transition metal ions yielding stable and intensely coloured complexes , some of which have been shown to reveal interesting physical and chemical properties and functional biological activities.

In recent years , their have been several reports about the studies on the preparation , characterization and antimicrobial properties of transition metal ions combines with antibacterial supplies .These studies indicate that the antibacterial material containing transition metals can liberate many free hydroxyl radicals , which can kill bacteria efficiency.

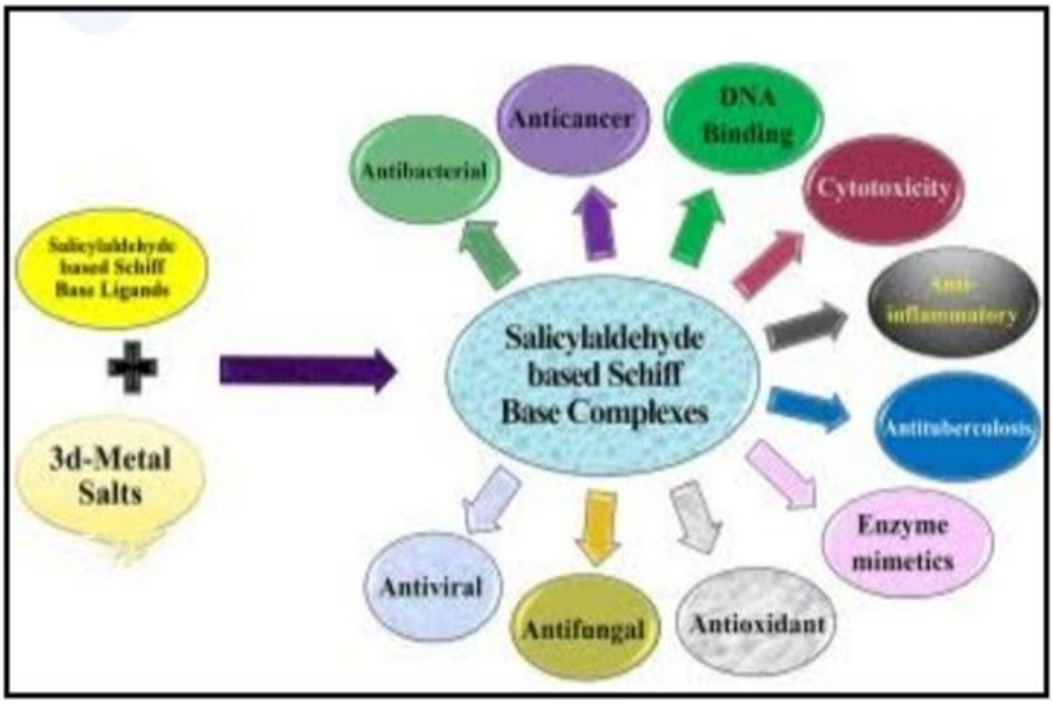


Figure 9. Biological activities of metal-Schiff base complexes.

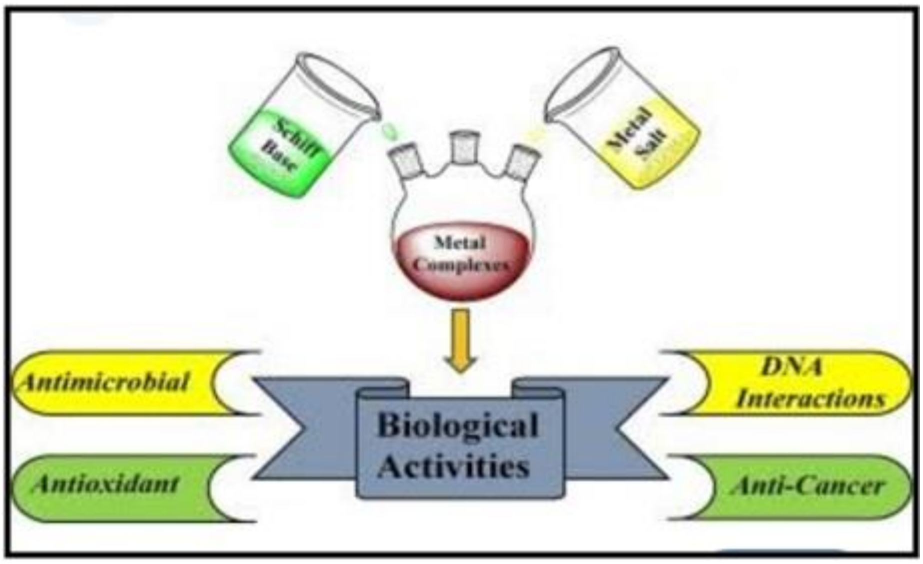


Figure 10. Biological activities of complexes.

Table 1. Some examples of cooedination compounds and their biological activities.

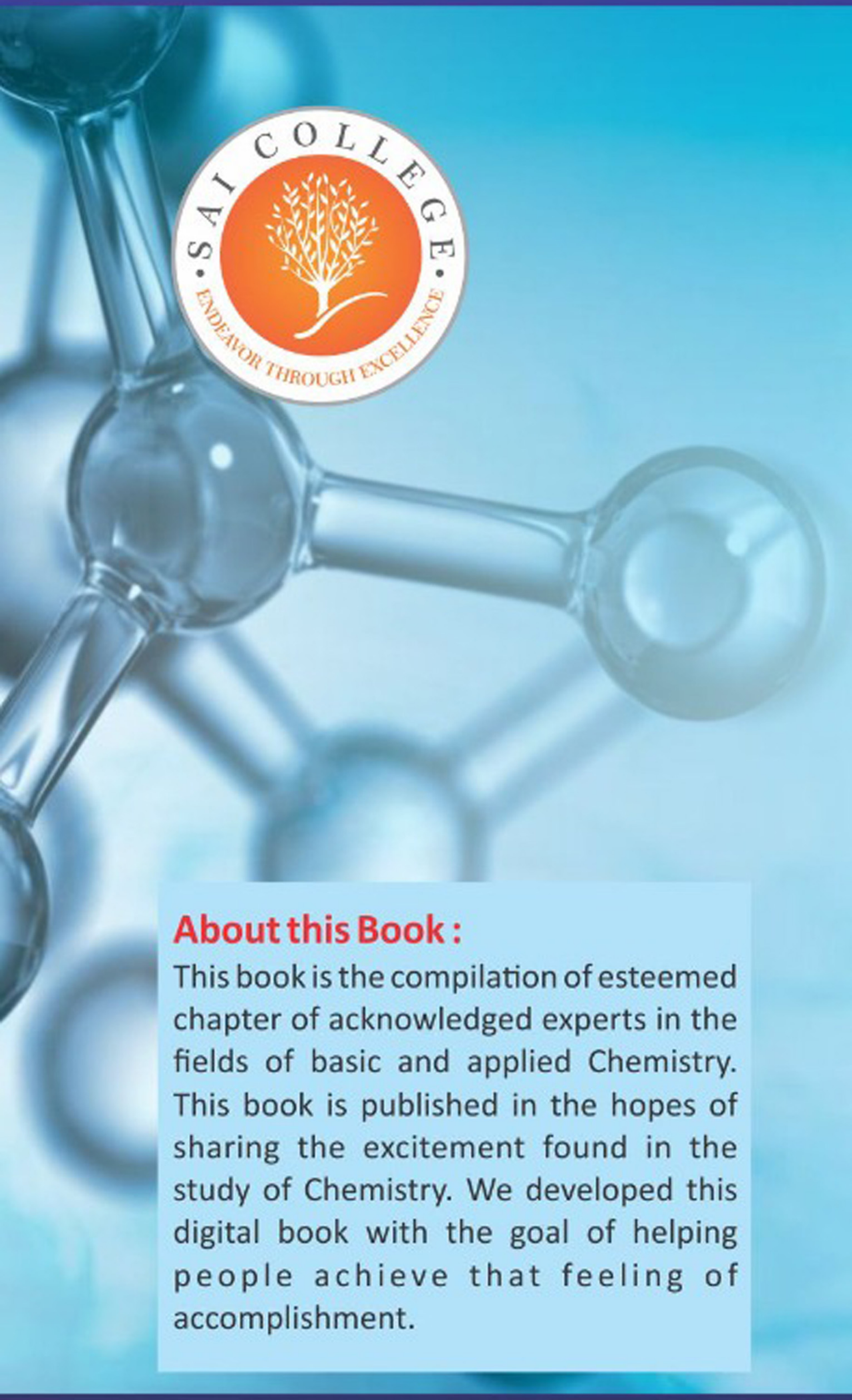
S. No.	Name of Complex	Action
1.	[Cu(pyrimo)CL]	Efficient self-activated DNA, cleavage and cytotoxic effects towards L1210 murine leukemia and A2780 human ovaron carcinoma cell lines
2.	Cu (II) Complexes with	Cytotoxic and anti-viral activites

	diimines as co-ligand	
3.	Ternary copper (II) complexes	Strong DNA binding and cleavage and induced apoptosis in cancer cell lines
4.	Cu (II) complexes	Cytotoxicity against HeLa(cervical) cancer cells
5.	Cu (II) complexes with macrocyclic triamines	Promote the hydrolytic cleavage of plasmid DNA
6.	Mixed chelate transitinmetal based drugs	Potent antitumor activity
7.	Metal complexes having OO. ON. NS, ONS-donors	Anticancer activity
8.	Quinolne metal compounds	Antimicrobial agent
9.	[Cu(CX)$_2$]. 2H$_2$O (where CX= cinoxacin)	Antimicrobial agent
10.	Zinc and Copper ciprofloxacin complexes	Antimicrobial agent
11.	Quinolone Cobalt(II) complexes	Antimicrobial agent

REFERENCES

1. A.Tavman, S.Ikiz, A.F.,N.Y. BagcigilOzaur&K.K.Seyyal, ***J. Serb. Chem. Soc.***, 2009, 74 (5), 537-548.
2. S. Haque, S.C. Mazumdar, M.N.I. Khan &M.K. Das, ***Mat. Sci. & Appl.***, 2021, 12, 121-138.
3. Patel K. S., Patel K. D., Dholarya H. R., Patel V. K. & Patel K. D., ***Open J. Metal,*** 2012, 2, 49-59.
4. Eze F. I., Ajadi U. &Ukoha P. O., ***HindawiPub.Coorp.,Int. J. Med. Chem.***, 2014, 1-6.
5. Chaudhary N. K. &Guragain B., ***Asian J. Chem.***, 2019, 31(4), 951-959
6. Saouya E. R., Khalil M. M. H., Ismail E. H., Bendas E. R. &Ossama S. Neaz, ***RJPBCS,***2014, 5 (4), 18-30.
7. Fang S., Jiang Y., Xiao D., Zhang X., Gan Q., Ruan Q. & Zhang Junbo, ***Pharm.***, 2021, 13 (4), 510.
8. Gandhi D. H., Bhatt B. S. & Bhatt K. D., ***BiointerfaceRes. Appl. Chem***., 2021, 12447-12453.
9. Ahmadi F., Saberkari M., Abiri R., Motlagh H. M. &Saberkari H., ***Appl. Biochem. Biotechnol.***, 2013, 170, 988-1009 .
10. Khali M. M. H., IsmailE. H., Azim S. A. &Souya E. R., ***J. ofThermalAna. And Colorimetry,***2010, 10(1), 129-135.
11. Reddy V., Patil N. &AngadiS. D., ***E-J of Chem***., 2008, 5(3), 577-583.
12. Skyrianou K. C., Perdih F., Turel I. , Kessissoglou D. P. &Psomas G., ***J. Inorg. Biochem.,*** 2010, 104 (7), 740–749.

13. Lufang Ma, Liya Wang, JiangeWang,Yufang Wang & Xun Feng, ***J. of Inorg. Chem***., 2007, 60, 2007.
14. Sarkar B., ***Springer Netherlands, Dordrecht***, 1977, 193–228.
15. Shivanker V. S. &Thakur N. V., ***Acta Pol. Pharma***, 2003, 60, 45-50.
16. Saha R., Bhayye S., Ghosh S., Saha A., Sarkar K., ***ACS Appl. Bio Mater***., 2019 , 2, 5349–5365.
17. ShoukryA. A., ***Eur. J. Chem.***, 2013, 4 (4), 379-387.
18. Hung Y. J., & Zhang, ***J. Inorg. Chimica Acta,*** 2020, 501, 119-244.
19. Patel N. B. &PatelS. D., ***Der PharmaChemica***, 2009, 1(2), 199-209.
20. Mohammed G. G.,El-Gamel N. E. A., ***Spectrochem. Acta Part A***, 2004,60, 3141-3154.



About this Book :

This book is the compilation of esteemed chapter of acknowledged experts in the fields of basic and applied Chemistry. This book is published in the hopes of sharing the excitement found in the study of Chemistry. We developed this digital book with the goal of helping people achieve that feeling of accomplishment.

Rs. 600

Published and Printed by : (First Edition : May 2024)
Sai Mahavidyalaya (Sai College)
Street-69, Sector-6, Bhilai, Dist. Durg (Chhattisgarh)
Email : director@saicollege.org
Website : www.saicollege.org
ISBN : 978-81-957386-6-3