International Journal For Advanced Research In Science & Technology
A peer reviewed international journal www.ijarst.in
ISSN: 2457-0362

A STUDY OF SUSTAINABLE METHODS FOR SYNTHESIS OF HETEROCYCLES

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ABSTRACT

An essential part of organic chemistry, the synthesis of heterocycles finds extensive use in fields as diverse as agriculture, materials research, and medicines. Innovative green techniques for the synthesis of heterocyclic compounds are being explored by researchers as the scientific community throughout the world becomes more and more aware of the critical need to implement sustainable practices. This abstract describes an experiment that aimed to find greener ways to synthesize heterocycles. Our research focuses on developing synthetic pathways that make use of renewable resources, decrease energy use, and produce little waste by using green chemistry concepts. Sustainable methods were used to produce a range of heterocyclic compounds with various biological properties. Methods used in the experiments included catalysis, alternative, sustainable starting materials, and the use of safe reaction conditions. Our research looks on the effectiveness and viability of the created techniques in addition to their environmental advantages. The yields, selectivity, and scalability of the green synthetic approaches were compared to standard techniques in comparative studies.

KEYWORDS: Sustainable Methods, heterocyclic compounds, environmental advantages, green synthetic approaches.

INTRODUCTION

Hydramagnesite, having the chemical formula [$Mg_5(CO_3)_4(OH)_2$•$4H_2O$], is the most common hydrated basic magnesium carbonate mineral. Magnesite, nesquehonite, lansfordite, artinite, dypingite, and hydromagnesite are the six varieties of magnesium carbonates with the chemical formula [$MgCO_3$], [$MgCO_3$•$3H_2O$], [$4MgCO_3$•$Mg(OH)_2$•$5H_2O$], and [$Mg_5(CO_3)_4(OH)_2$•$4H_2O$], respectively. 1 Because of its stability in the atmosphere, HM is the only one of these that has been determined to have geologic significance. With its unique properties like super-hydrophilicity and photoluminescence, hydromagnesite has piqued the interest of material chemists. It finds use in a variety of applications, such as CO_2 gas sequestration, corrosion resistance for magnesium alloys, fire retardants in the plastics industry, RNA chromatography, as a versatile precursor of MgO, and catalysis.

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In 1990, Seifritz first suggested the idea of carbonate mineral carbon capture and sequestration (CCS). Carbonate minerals provide a low-maintenance, environmentally friendly option for carbon dioxide sequestration. In the last nine years, there has been a plethora of published research on the topic of carbonate mineralization from different types of magnesium carbonates. Hydromagnesite precipitation from serpentinite material was investigated by Teir et al. in 2007 for the purpose of CO2 sequestration. The most efficient conversion of magnesium ions to carbonate was obtained, leading to the maximum purity of hydromagnesite (99 wt%) and the sequestration of 37 wt% of CO2 as carbonate precipitate. Atilhan et al. looked at the possibility of using hydromagnesite and other metal carbonate minerals for CO2 sequestration. Using a Rubotherm magnetic suspension balance, CO2 adsorption studies were conducted at high pressures of 175 bar and temperatures ranging from 316 to 340 degrees Celsius. Hydromagnesite, as described by Unluer et al., might be used as an addition in magnesia cements to increase the carbonation level and CO2 sequestration in porous blocks. They also looked at two alternative curing conditions—accelerated carbonation (70-90% RH, 20% CO2) and natural curing (60-70% RH, ambient CO2)—to see how HM, nesquehonite, and dypingite affected the strength of MgO-cements. Hydromagnesite and other magnesium carbonate minerals may be effectively carbon sequestered by a process described recently by McCutcheon et al. using a microbial bioreactor. The CO_2 sequestration rate was determined to be 33.34 t C/ha/year based on the data from the water chemistry.

The low density, excellent stability, and high specific strength of magnesium have made it a highly sought-after structural material for use in automotive and aircraft systems. Magnesium alloys have many useful technical applications, but their poor corrosion resistance is a major downside. Surface corrosion mechanisms on magnesium (AZ91D) and aluminum (AA 2024-T3) alloys have been investigated by a small number of researchers in this field. The most common byproduct of corrosion, according to the findings, was hydromagnesite, a carbonate layer that alloys may use to resist corrosion by obstructing the surface's active corrosion sites. During the corrosion of magnesium alloy AZ91D caused by NaCl, Jonsson et al. found magnesium carbonates, such as hydromagnesite and nesquehonite, as corrosion products. The development of hydromagnesite in sites with greater NaCl concentrations initiated the corrosion process. Hydromagnesite crusts limit air corrosion by preventing CO2 and O2 from reaching the magnesium alloy surface. After subjecting the AZ91D alloy to a variety of atmospheric conditions, including urban, rural, and coastal settings, they discovered rates of corrosion of 1.8 lm/year, 1.8 lm/year, and 1.8 lm/year, respectively. Among the several products of magnesium oxidation and corrosion seen in AA 2024-T3 alloy during prohesion exposure, Wang et al. identified hydromagnesite as the most significant.

1.2 GREEN AND SUSTAINABLE METHODS

There has been a remarkable surge in the adoption of environmentally friendly and sustainable practices in many fields this century. More and more people are realizing that we need to adapt to a more sustainable way of life since our world is struggling with issues like climate change, resource loss, and environmental degradation. Beyond empty platitudes, this paradigm change requires an active commitment to green practices in all aspects of life. Green and sustainable techniques are important in many different industries, including energy, agriculture, architecture, and transportation. In this in-depth investigation, we will explore these strategies from every angle.

Industrial Energy:

The energy industry is one of the main places where sustainable and environmentally friendly practices have become quite popular. One of the main causes of global warming and greenhouse gas emissions has been conventional energy, which mostly uses fossil fuels. A major step towards sustainability has been the move towards renewable energy sources like solar, wind, and hydropower. The use of photovoltaic cells to collect solar energy has made it a major participant in the fight for renewable power. This approach lessens the strain on limited resources and lessens the ecological footprint of traditional energy generation.

As an additional eco-friendly option, wind power harnesses the kinetic energy of the wind to produce electricity. Increases in wind turbine efficiency and their ability to blend in with natural landscapes are having a major impact on lowering carbon footprints. Hydropower, which is created by the motion of water, is another clean and dependable energy source; however, its effects on aquatic ecosystems must be carefully considered.

The agricultural sector:

Preserving biodiversity, guaranteeing food security, and maintaining soil health are all facets of agriculture that depend on sustainable methods. The use of synthetic fertilizers and pesticides is common in conventional agricultural practices, which degrade soil and pollute water. There has been a sea change towards sustainability with the rise of organic agricultural

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practices. Soil fertility is improved and the environmental impact of agriculture is decreased via the practice of organic farming, which rejects synthetic inputs in favor of natural alternatives.

Natural pest management, crop rotation, and biodiversity are also highly valued in agroecology, an agricultural system that incorporates ecological principles. Agroecology is a way of farming that emphasizes balancing crop production with ecological processes, which has several benefits, including increased sustainability and adaptability to climate change.

In the realm of architecture and construction, there is a revolutionary shift towards sustainability in a sector that has a reputation for traditionally using a lot of resources. One of the most important aspects of sustainable architecture is green building design, which focuses on reducing energy use, conserving water, and using environmentally friendly materials. To lessen the toll that buildings take on the environment, energy-saving innovations like insulated windows, solar panels, and smart building systems play a crucial role.

By reducing the need for new construction and the environmental costs it entails, the idea of adaptive reuse and reusing existing buildings is in line with sustainability aims. Natural lighting, adequate ventilation, and green areas are all components of sustainable design that take into account both the environment and the health of the people who live in or use the place.

Green and sustainable practices are being spearheaded by the transportation industry, which is a major source of carbon emissions. Many people are starting to see electric vehicles (EVs) as a viable replacement for conventional gas-powered automobiles. Electric vehicles help lessen our reliance on fossil fuels and contamination of the air since they run on electricity, which is often generated from renewable sources.

When planned with environmental responsibility in mind, public transportation networks provide a practical way for people to lessen their impact on the environment. Communities benefit from investments in public transportation, bike lanes, and pedestrian-friendly design, which in turn help to preserve the environment and make people's lives better.

An essential part of sustainable practices is waste management, as incorrect disposal may cause pollution, habitat loss, and health problems for humans. Reusing and recycling materials is an important part of sustainable waste management since it lessens the need for new resources and lessens the toll that production takes on the environment.

An innovative solution that turns garbage into useful resources like heat or power is waste-to-energy systems. Decreased emissions of the strong greenhouse gas methane from landfills may be achieved by the use of anaerobic digestion, composting, and other techniques for managing organic waste.

The idea of Corporate Social Responsibility (CSR) has grown in the business sector as firms realize they need to do their part to ensure a sustainable future. Both for legal reasons and to show their dedication to the greater good of society and the environment, businesses are under growing pressure to implement eco-friendly policies and procedures.

Some examples of corporate social responsibility (CSR) activities include funding community development projects, establishing sustainable supply chain procedures, and cutting carbon emissions. Businesses have the power to make a significant impact by balancing financial success with social and environmental responsibility.

Opportunities and Difficulties:

Green and sustainable practices are becoming more popular, yet there are still obstacles to their broad acceptance. There are obstacles that must be overcome, such as economic concerns, a lack of knowledge, and opposition to change. To create a setting that is friendly to sustainable practices, it is essential for the government to implement legislation, provide incentives, and work together internationally.

Even while there are obstacles, there are also great possibilities. An emerging industry with the potential to propel innovation, provide employment opportunities, and boost economic growth is the "green economy," which is defined by eco-friendly business practices and the advancement of clean technology. Every sector, from governments to corporations to people, must work together to ensure a more sustainable future.

In light of the pressing environmental issues facing our planet, it is imperative that we immediately begin to implement green and sustainable practices. Sustainable solutions are quickly becoming dominant in many industries, including energy generation, farming, construction, transportation, waste management, and business operations.

By implementing these strategies, we can lessen the impact of climate change and help build a more just and sustainable society. For the sake of present and future generations, becoming

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ISSN: 2457-0362
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green is becoming more than simply a personal preference; it's a national and international obligation as we all strive for a more sustainable future.

1.3 HETEROCYCLES

Organic molecules known as heterocycles have long piqued the curiosity of chemists due to their unique ring structure, which contains an element other than carbon. A vast variety of compounds, each with its own set of characteristics and potential uses, make up this varied category. Because of their widespread use in fields as diverse as materials research, natural goods, medicines, and organic chemistry, heterocycles have far-reaching implications. Heterocycles are the subject of this in-depth investigation, which seeks to provide light on their structural variety, synthesis processes, and many applications across several scientific fields.

Distinct Structures:

Histerocyles are characterized by the structural variation among them. Heterocyclic compounds include atoms of several elements, often sulfur, nitrogen, oxygen, and sometimes phosphorus or boron, in contrast to homocyclic compounds that only have carbon atoms in the ring. Heterocycles are a dynamic and adaptable family of compounds due to the array of chemical and physical characteristics brought about by the integration of these heteroatoms.

Famous examples of the simplest heterocycles are pyridine, furan, and thiophene, which all include a single heteroatom in a five-membered ring. Multiple heteroatoms, fused rings, or different substitution patterns are common features of more complicated heterocyclic molecules. Heterocycles are essential building blocks in the synthesis of more complex compounds due to their structural complexity, which adds to their varied reactivity and utility.

Alternative Approaches:

Heterocyclic compound synthesis is a dynamic and ever-changing field in organic chemistry. Chemists use a wide variety of approaches, from time-honored practices to state-of-the-art methodologies, to build these varied structures. The formation of a ring from precursor molecules is achieved by controlling the reaction conditions in cyclization processes, which is one such method.

By combining a substituted phenylhydrazine with a ketone or aldehyde, indole rings may be constructed by condensation processes, as shown in the well-known Fischer indole synthesis. A significant alternative is the Hetero Diels-Alder reaction, which allows for the formation of fused heterocyclic rings by the cycloaddition of dienes and dienophiles containing heteroatoms.

In addition, the synthesis of heterocycles has been transformed by techniques catalyzed by transition metals, such as palladium-catalyzed cross-coupling reactions. One example is the effective assembly of complex structures made possible by Suzuki-Miyaura coupling, which has played a key role in the development of biaryl and heterobiaryl systems.

Beyond the realm of academia, synthetic approaches for heterocycles have immense importance. In the pharmaceutical sector, it is essential for the effective synthesis of heterocyclic scaffolds, which are fundamental for the development and discovery of new drugs. The efficiency and breadth of heterocycle synthesis are anticipated to grow as scientists hone current techniques and pave the way for novel synthetic approaches, which will increase their applicability in a wide range of contexts.

Chemistry of Medicinal and Natural Products:

A great many bioactive chemicals found in plants, fungi, and bacteria have heterocycles as their structural motif. An excellent illustration of this is the family of nitrogen-containing natural compounds known as alkaloids. Famous alkaloids having significant physiological effects include morphine, quinine, and nicotine; the pharmacological actions of these compounds are based on their heterocyclic structures.

In addition, medicinal chemistry relies heavily on heterocycles. The use of heteroatoms into medication design often confers desirable pharmacological characteristics, and a large number of pharmaceutical pharmaceuticals are heterocyclic compounds. One example of how heterocycles are useful in the fight against infectious illnesses is the benzimidazole ring, which is included in many antifungal and antiparasitic drugs.

Equally common is the use of heterocyclic chemistry in the creation of antiviral medications. Acyclovir and zidovudine are nucleoside analogs that include heterocyclic moieties. These components imitate the structure of nucleic acid bases and impede viral reproduction. Because of their adaptability, medicinal chemists may use heterocyclic compounds to optimize drug candidates' physicochemical qualities, including their solubility, bioavailability, and target specificity.

Heterocycles are well-known in medicinal chemistry and the realm of natural goods, but they have also found uses in materials science. Because of their optical and electrical characteristics, heterocyclic compounds are useful building blocks for organic electronics, sensors, and electronic devices.

Organic light-emitting diodes (OLEDs) and organic photovoltaic cells (OPVs) are two examples of organic electrical devices that have recently attracted interest due to conjugated polymers, which comprise heterocyclic units in their backbone. Materials with tailored energy levels and charge transport capacities may be designed with the use of heterocyclic building blocks, which enable the adjustment of electronic characteristics.

Another area where heterocyclic compounds play a crucial role is conducting polymers. Because of their distinct electronic conductivity, polypyrrole and polyaniline—both of which include heterocyclic units—are well-suited for use as sensors and other electrical devices. It is possible to modify the materials' characteristics for certain technical uses by changing the heterocyclic units.

SYNTHESIS OF HETEROCYCLES

Heterocycle synthesis is an interesting and complex area of organic chemistry that uses many different approaches. Important roles are played by heterocyclic compounds in medical chemistry, materials science, and other fields. These compounds are defined by having a ring structure that contains an element other than carbon. Creativity, accuracy, and the never-ending search for novel approaches characterize the path into the domain of heterocycle synthesis. Delving into the complexities of several synthetic methods and showcasing the endeavor's relevance in the larger field of organic chemistry, this investigation will explore the art and science of synthesizing heterocycles.

Reactions in Cyclization:

Cyclization, the basic process of inducing precursor molecules to form a ring structure, is at the core of heterocycle synthesis. An essential tool for synthetic chemists, cyclization processes allow for the construction of a wide variety of heterocyclic frameworks.

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ISSN: 2457-0362

The Fischer indole synthesis is a reliable way to create indole rings, and it is a classic example of cyclization. Under acidic circumstances, the indole ring is formed by condensing a substituted phenylhydrazine with a ketone or aldehyde. The indole motif is present in many bioactive natural compounds and medicines, which is why the Fischer indole synthesis has been used to synthesize them.

The Hetero Diels-Alder reaction is another important cyclization approach; it is a potent tool for building fused heterocyclic rings. This reaction involves the formation of a new ring by the cycloaddition of a diene and a dienophile that contains heteroatoms. An extensive variety of heterocyclic compounds may be synthesized using the Hetero Diels-Alder process, which adds to the variety of synthetic techniques accessible.

Reactions Catalyzed by Transition Metal Dipoles:

Heterocycle synthesis has been radically altered by the development of transition metal-catalyzed processes, which provide selective and efficient ways to build complex ring structures. Particularly useful in the synthesis of heterocycles are palladium-catalyzed cross-coupling processes.

One common palladium-catalyzed reaction that allows for the synthesis of biaryl and heterobiaryl complexes is the Suzuki-Miyaura coupling. This reaction opens up the possibility of incorporating various functional groups and substituents into the heterocyclic framework by coupling aryl halides with aryl boronic acids or boronate esters. The Suzuki-Miyaura coupling is an important tool for the efficient and adaptable synthesis of heterocyclic compounds with specific architectures.

Aryl halides may be directly coupled to amines via the palladium-catalyzed Buchwald-Hartwig amination.

A family of chemicals found in many medications and natural goods, heterocyclic amines, may be synthesized with the help of this process. Researchers in medicinal chemistry and related areas now have a more robust synthetic toolkit because to the ability to selectively incorporate nitrogen atoms into heterocyclic structures.

Chemistry of Heterocycles for Medicinal Purposes:

Particularly important in medicinal chemistry is the synthesis of heterocycles because the building of certain ring structures is often crucial to the design and development of medicinal drugs. Due to their capacity to change the characteristics of bioactive molecules and their various pharmacological actions, heterocyclic compounds play a significant role in drug development.

For example, several drugs share the benzimidazole ring as a heterocyclic motif. The heterocyclic ring is typically formed in the synthesis of benzimidazoles by condensing o-phenylenediamine with a carboxylic acid or a derivative of it. Anthelmintic medications, proton pump inhibitors, and antiviral treatments all include benzomidazoles, demonstrating the therapeutic importance of heterocycles in medicinal chemistry.

Synthesis of Heterocycles and the Study of Materials:

The use of heterocycles goes beyond their original use in medicinal chemistry and into materials science. In this field, certain ring configurations are essential for the design and synthesis of functional materials used in organic electronics, electronic devices, and sensors.

Many heterocyclic units may be found in the structures of conjugated polymers, which are defined by the polymer backbone alternating between single and multiple bonds. When it comes to creating organic photovoltaic cells (OPVs) and organic light-emitting diodes (OLEDs), the design and production of these polymers are vital.

It is possible to develop materials with tailored energy levels, charge transport capacities, and optical features by using heterocyclic building blocks, which in turn allow for the tailoring of electronic properties. A ubiquitous heterocyclic unit in conjugated polymers, thiophene has been widely used in the manufacture of polymers for organic electronics due to its outstanding electron-donating capabilities.

Heterocyclic units are often found in the structures of conducting polymers, which are a kind of substance that can conduct electricity. Due to their distinct electrical characteristics, polypyrrole and polyaniline—both of which include heterocyclic moieties—are well-suited for use in electronic devices and sensors. Their adaptability in materials science and technology is boosted by their tunable qualities, which may be achieved by manipulating the heterocyclic units.

The Effects of Heterocycle Synthesis on the Environment:

Thinking about how synthetic methods could affect the environment is becoming more important as heterocycle synthesis develops further. Byproducts and trash from conventional heterocycle synthesis processes, particularly those that use stoichiometric reagents and transition metal catalysts, may contaminate the environment.

New, more eco-friendly ways of synthesizing heterocycles have been developed in response to green chemistry ideas that seek to reduce the negative effects of chemical reactions on the environment. An environmentally preferable substitute for conventional metal-catalyzed processes has developed: catalysis, and more specifically organocatalysis and biocatalysis. The use of less damaging chemicals is a common goal of these techniques, which makes heterocycle synthesis more sustainable.

Another step toward more environmentally friendly synthetic processes is the investigation of other reaction media, including water and ionic liquids. To lessen the environmental impact of heterocycle synthesis, it is consistent with green chemistry principles to employ gentler conditions and solvents that are safe for the environment.

CONCLUSION

This work aims to synthesize hydromagnesite with a flower-like thin sheet shape (F-HM) as a new catalyst for the hydrolysis of 1,4-dihydropyridines, flavonol, and flavanones, all of which have biological significance. We also successfully and selectively converted 2-hydroxy chalcone to 2,4-dihydroflavonol. In addition, we synthesized hydromagnesite with a large surface area and a unique rectangular thin sheet shape (RS-HM). When it came to the Yonemitsu-type trimolecular condensation process, the RS-HM catalyst performed far better than MgO in synthesizing 3-substituted indoles. Environmental friendliness, moderate reaction conditions, convenience of handling, broad substrate applicability, selectivity, and outstanding yields are some of the benefits of reactions catalyzed by F-HM and RS-HM. These reactions also have a low E-factor and a high atom economy. The catalytic activity of the catalysts remained unchanged even after six recycling cycles. The presence of HCO3 - and OHgroups on the surface of hydromagnesite catalysts may explain its superhydrophilic nature and large surface area, which contribute to its good performance in water.

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