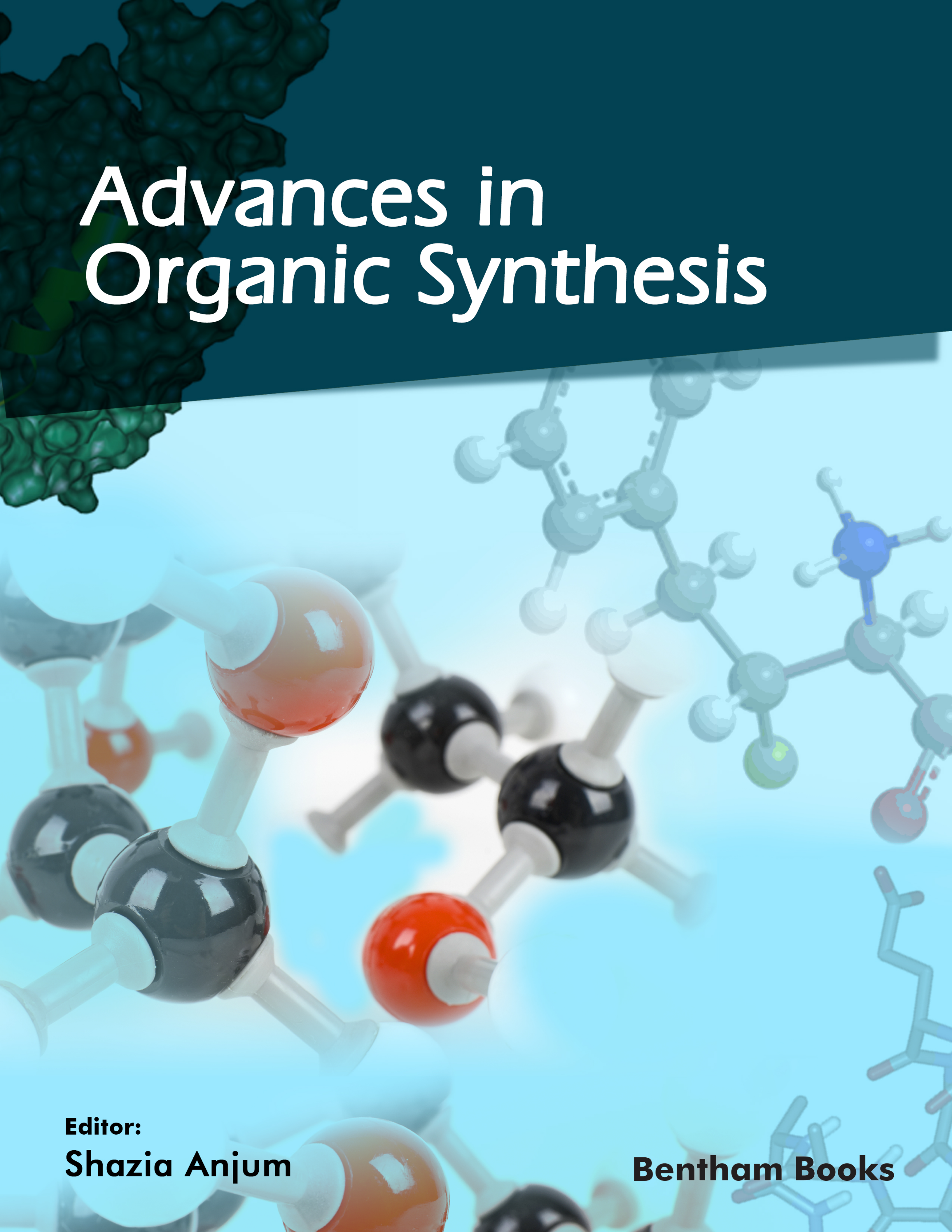

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Shazia Anjum

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(*Volume 18*)

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PREFACE

The series ‘Advances in Organic Synthesis’ are a dedicated set of different volumes covering all contemporary developments in organic synthesis. The contents of each volume are thoughtfully picked to capture the dire need of the readers and at the same time, it is rewarding to quench the thirst of researchers. The first chapter of volume 18 describes the latest syntheses and biological activities of anti-cancer Ferrocenes. Mehra and Lumb gave a brief account of the stable aromatic nature of ferrocene and bioferrocene compounds that possess reversible redox properties, and low toxicity that has also revolutionized the area of medicinal organometallic chemistry.

Masdeu *et al.* compiled a review on the synthesis of fused nitrogenated heterocycles using intramolecular Povarov Reaction. This strategy helped in synthesizing tri-, tetra-, penta-, hexa-, hepta-and octacyclic-fused heterocyclic compounds of diverse biological activities. While Singh and Kumari in their chapter 03 described the recent applications of barbituric acid as a synthetic precursor for the synthesis of various bioactive compounds. Barbituric acid can be employed in the condensation reaction as well as 5-/6- membered oxygen/nitrogen-containing heterocycles.

The use of ionic liquids (ILs) in organic syntheses has made a renaissance. It has revolutionized the entire trajectory of the synthetic pathway. In Chapter 4, Khokhar *et al.* described emerging applications of ILs as green solvents, green catalysts, and in coupling reactions. It depicts their remarkable use in environmentally benign organic synthesis which is the main focus of discussion in this chapter.

The last three chapters of these volumes are exclusively dedicated to the newly emerging field of nanotechnology. For example, chapter 05 of this volume illustrates the advanced use of Zinc oxide (ZnO) nanomaterials for biomedical applications. In this chapter, Bhuiyan *et al.* showed that ZnO nanomaterials could be developed by the organic synthesis process for excellent biocompatibility, selectivity, sensitivity, good chemical stability, non-toxicity, and fast electron transfer properties in a cost-effective manner. While Higazy *et al.*, in their chapter 06 covered the contemporary development of nanocomposite hydrophobic coatings for effective corrosion protection. Organic-inorganic nanocomposites can be employed as outstanding anti-corrosive coatings to provide longevity of steel construction service. Overall, they gave an overview of present and advanced research developments, such as graphene nanocomposite surfaces, etc. Interestingly, the last chapter of this volume by Zdiri *et al.* covers the morphologies and properties of virgin and waste polypropylene nanocomposites. The article gives information on different types of nanoparticles used for the enhancement of thermo-mechanical and physical behaviors of PP nanocomposites. Moreover, it also discusses the improvements in the properties of waste PP by nanoparticles’ incorporation and the influence of clay nanoparticles on waste PP-based nanocomposites.

I hope that the readers will enjoy reading this volume which covers contemporary developments in organic syntheses. I would like to express my sincere thanks to the editorial staff of Bentham Science Publishers, particularly Ms. Asma Ahmed and Mr. Mahmood Alam for their constant help and support.

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CHAPTER 1

Recent Synthetic and Biological Advances in Anti-cancer Ferrocene-Analogues and Hybrids

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Abstract: Cancer is among the most severe risks to the global human population. The enduring crisis of drug-resistant cancer and the limited selectivity of anticancer drugs are significant roadblocks to its control and eradication, requiring the identification of new anticancer entities. The stable aromatic nature, reversible redox properties, and low toxicity of ferrocene revolutionized medicinal organometallic chemistry, providing us with bioferrocene compounds with excellent antiproliferative potential, which has been the focus of persistent efforts in recent years. Substituting the aryl/heteroaryl core for ferrocene in an organic molecule alters its molecular characteristics, including solubility, hydro-/lipophilicity, as well as bioactivities. Ferrocifen (ferrocene analogues of hydroxytamoxifen) has shown antiproliferative potential in both hormone-dependent (MCF-7) and hormone-independent (MDA-MB-231) breast cancer cells. It is now in pre-clinical trials against malignancies. These entities operate through various targets, some of which have been revealed and activated in response to product concentrations. They also react to the cancer cells by diverse mechanisms that can work in concert or in isolation, depending on signaling pathways that promote senescence or death. The behavior of ferrocene-containing hybrids with a range of anticancer targets is explained in this chapter.

Keywords: Anti-proliferative Potential, Azide-alkyne Cycloaddition, Biological Activities, Bio-organometallic, Bioferrocene Compounds, Cancer, Cytotoxicity, Ferrocene Compounds, Ferrocifen, Ferrociphenols.

1. INTRODUCTION

Organometallic chemistry and biochemistry have recently been combined to form a new subject known as bioorganometallic chemistry. This new research topic has piqued scientists' interest because of the unusual chemical structure and biological activity of organometallic compounds. These carbon-metal linkage compounds

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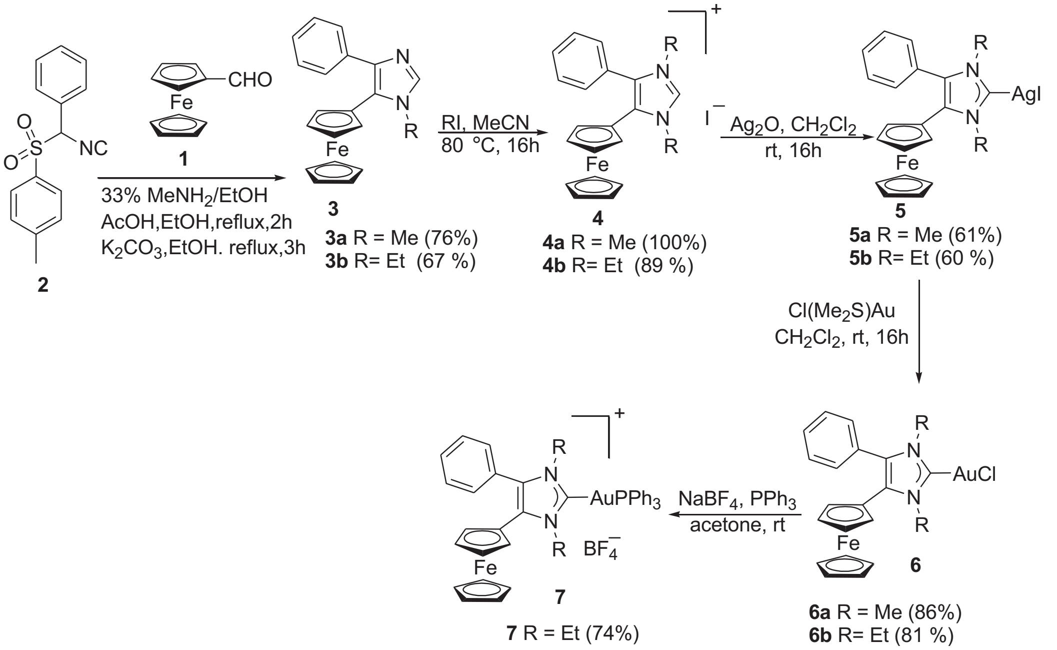
offer a potentially rich sector for the discovery of new pharmacological medicines with novel mechanisms of action, and the field is rapidly increasing. In recent years, there has been an increased interest in developing organometallic compounds as structural variants of existing drugs for treating drug resistance cancer [1]. Among the various organometallics, ferrocene [2], the archetypal organometallic compound, serves as a useful platform in bio-organometallic chemistry because of its important role in various fields, including stereoselective, stereospecific, and asymmetric transformations, electrochemistry, polymer chemistry, material science, biochemistry, crystal engineering, and drug design and development [3]. Ferrocene compounds are particularly appealing candidates for biological applications because of their durability in aqueous and aerobic settings, as well as the availability of a wide range of derivatives and outstanding electrochemical characteristics [4]. Ferrocene [5, 6] is a compelling target in fields like drug design mediators of protein redox processes, internal standards in electrochemistry, and organic synthesis, such as functionalization of cyclopentadienyl ligands, due to its sandwich-like structure and chemical representation $(\eta^5\text{-}C_5H_5)_2Fe$. In many ways, ferrocene is similar to benzene in that it behaves like an aromatic ring and conducts electrophilic reactions, including Friedel-alkylation, Craft's acylation, Vilsmeyer formulation, and mercuration reactions, which are all phenyl ring properties. Ferrocene derivatives with asymmetric substituents are extensively used as asymmetric hydrogenation catalysts [7]. Among organometallic compounds, ferrocene has a remarkable range of chemistry. Numerous studies have demonstrated ferrocene's efficacy *in vivo* and *in vitro*, as well as its potential as an anticancer, antimalarial, and antifungal agent [8 - 11]. The anticancer action of ferrocene-based compounds is linked to the oxidation state of the central iron atom. Only the ferrocenium salts with the central iron atom in the oxidation state of +3 have been found to exhibit anticancer activity. Incorporating ferrocene into bioactive compounds is a common technique in this field, with the most successful example being its incorporation into tamoxifen, resulting in the potential therapeutic candidate ferrocifen, which has the unique property of being antiproliferative against both the MCF-7 (hormone-dependent) and MDA-MB-231 (hormone-independent) breast cancer cell lines [12]. Many studies have also shown that ferrocene analogues have the potential to treat a wide range of illnesses, including fungal/bacterial infections, malaria, HIV, and cancer. This chapter aims to keep researchers informed about recent advances in the synthesis and evaluation of ferrocene-containing bioactive pharmacophores, focusing on the structure-activity relationship (2015-2020).

FERROCENE-BASED CONJUGATES HAVE ANTIPROLIFERATIVE POTENTIAL

Schobert and co-workers synthesized and analyzed the antiproliferative potential of ferrocene-derived *N*-heterocyclic carbene complexes of Gold (I) [13]. Ferrocene-carboxaldehyde **1** was initially treated with toluene sulfonyl methyl isocyanide **2** and methylamine, resulting in imidazoles **3.** Alkylation reaction of **3** with iodomethane or iodoethane provided the corresponding imidazolium salts **4,** which upon subsequent reaction with silver (I) oxide yielded the complexes **5**. Complex **5** was transmetallated with chloro (dimethyl sulfide)gold (I), resulting in the derivative **6**. The subsequent reaction of **6** with triphenylphosphine and sodium tetrafluoroborate afforded the target complex *viz.* cationic phosphano gold complex **7** (Scheme **1**).



Scheme (1). Synthetic route to ferrocenyl substituted *N*-heterocyclic carbene complexes of Gold (I) **7**.

Ferrocene-substituted biscarbene complex **8** was prepared by substituting BF_4 for the counter anion in imidazolium iodide **4b**. The desired silver carbene complex **9** was synthesized by transmetallation of the complex **8** with chloro (dimethyl sulfide)gold (I) (0.5 equivalents) (Scheme **2**).

CHAPTER 2

Synthesis of Fused Nitrogenated Heterocycles: Intramolecular Povarov Reaction

Carme Masdeu[1], **Jesús M. de los Santos**[1], **Francisco Palacios**[1] and **Concepcion Alonso**[1,*]

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Abstract: Nitrogenated heterocycles take part in the structure of many natural products and agents with important biological activity, such as antiviral, antibiotic and antitumor drugs. For this reason, heterocyclic compounds are one of the most desired synthetic targets nowadays. In this review work, the literature related to the preparation of polyheterocyclic compounds by using the intramolecular Povarov reaction will be collected. The Povarov reaction is a process in which aromatic amines, carbonyl compounds and olefins or acetylenes participate to give rise to the formation of the nitrogenated compounds. Then, intramolecular Povarov reactions to carry out these syntheses are described according to the key processes involved; catalytic reactions with transition metals will be included discussing the reaction mechanisms and examining the effect of catalysts and solvents in the preparation of the products, thus reflecting the synthetic potential of this strategy. Moreover, applications of prepared compounds will also be considered.

Keywords: Aldimines, Aza-Diels-Alder Reaction, Brönsted and Lewis Acid Catalysis, Cycloaddition, Intramolecular Povarov Reaction, Nitrogen-containing Fuse Heterocycles.

1. INTRODUCTION

Heterocyclic systems play an important biological role and are essential in various aspects of life and material science. The vast majority of naturally occurring compounds, as well as a significant number of compounds synthesized in the laboratory, have a nitrogenated heterocyclic structure, which has led to various applications in different fields [1 - 4].

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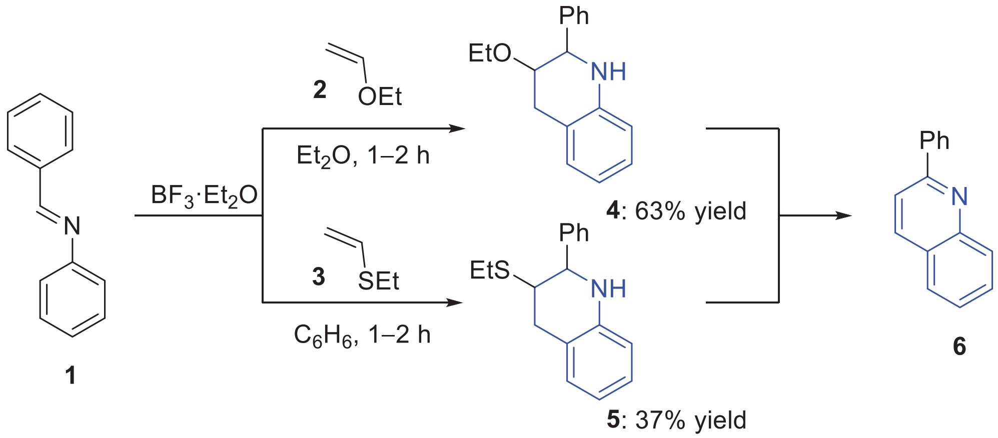
In other words, many of the pharmacologically significant compounds and agrochemicals are nitrogenated heterocyclic compounds.

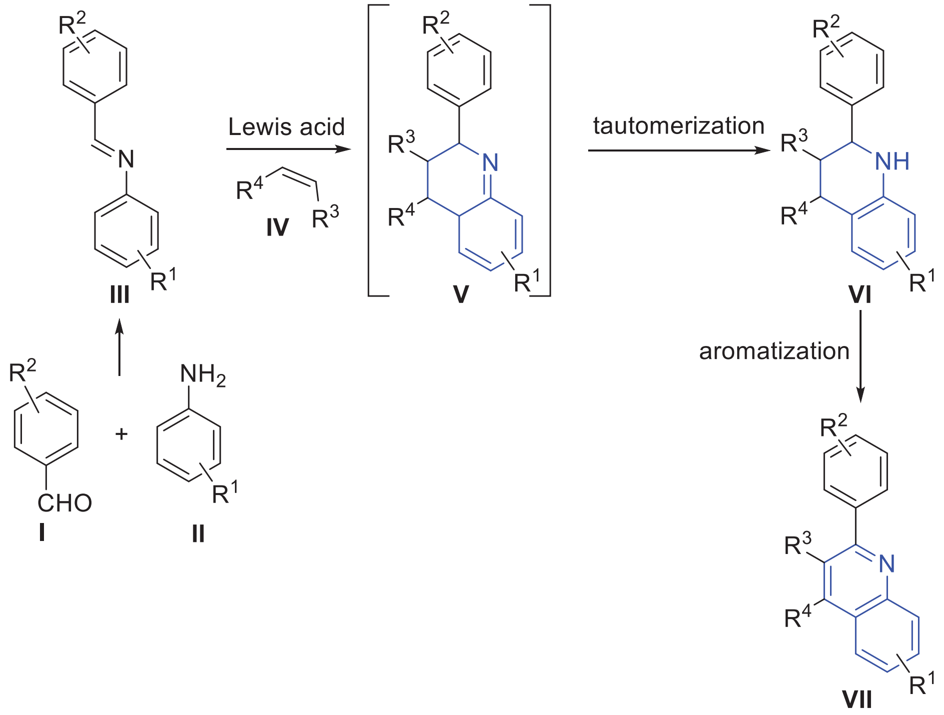
Therefore, the development of new methodologies for the construction of nitrogenated heterocyclic compounds has been a central issue in the synthesis of organic and natural products, pushed especially by the increasing demand for these compounds in the last decades. In particular, among the different strategies developed for the synthesis of heterocyclic compounds, the Povarov reaction has been described as a very versatile tool for the construction of nitrogenated heterocycles [5 - 9].

In the middle of the 20th century, Povarov and co-workers [10] described the preparation of tetrahydroquinolines by the reaction between aromatic Schiff bases (aromatic aldimines) and electron-rich alkenes. The early works of Povarov described reactions of ethyl vinyl ether **2** or ethyl vinyl sulfide **3** and *N*-aryl aldimine **1** under acid catalysis ($BF_3 \cdot OEt_2$) to give 2,4-substituted tetrahydroquinolines **4**, **5**, which were converted after oxidation to the corresponding quinoline **6** Scheme (**1**).



Scheme (1). Reaction described by Povarov for the first time.

In general terms, the formation of tetrahydroquinoline derivatives **VI** by Povarov's reaction could therefore be explained by a formal [4+2] cycloaddition between aldimines **III**, obtained by condensation between aromatic aldehydes **I** and aromatic amines **II**, and olefins **IV** to give adducts **V** whose subsequent tautomerization would give the tetrahydroquinoline **VI**. Aromatization of these tetrahydroquinolines **VI** would generate the corresponding quinolines **VII** Scheme (**2**). This strategy represents a very powerful tool for the preparation of quinoline derivatives by generating three stereocenters in a single step. In general, the reaction shows a high regio- and diastereoselectivity with the isolation in most cases of a major isomer. In those cases where mixtures of diastereoisomers are observed, the ratio of the *endo*/*exo* diastereisomers formed is modulated and determined by the catalyst and solvent used in the process.



Scheme (2). General scheme of the Povarov reaction.

Regarding the mechanistic aspects of this reaction, Kobayashi *et al.* suggested a stepwise reaction mechanism for the imino-Diels-Alder reaction of aniline-derived imines with alkenes [11]. On the other hand, experimental results pointed toward a concerted asynchronous cycloaddition process [12]. Moreover, a combined theoretical and experimental study of Povarov-type cycloaddition reactions between *N*-(3-pyridyl) imines and ethylene, or substituted ethylenes (styrene, cyclopentadiene or indene) catalyzed by $BF_3 \cdot Et_2O$ was carried out in our research group [13]. These computational studies gave light to understand the mechanism of the Povarov reaction between aldimines **VIII** Scheme (**3**) derived from 3-aminopyridine and benzaldehyde with different olefins. In this case, we studied the most favorable orientation of the pyridine ring in the cycloaddition reaction, the influence of the $BF_3 \cdot Et_2O$ and if this Lewis acid preferentially coordinates to the pyridinic nitrogen or to the iminic nitrogen. In addition, we

CHAPTER 3

Use of Barbituric Acid as a Precursor for the Synthesis of Bioactive Compound

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Abstract: Barbituric acid is an organic compound containing a pyrimidine heterocyclic skeleton. It is a water-soluble and odorless compound. Barbituric acid served as a starting material for many barbiturate drugs. The variable properties of the products achieved from barbituric acid motivate organic chemists to investigate its chemistry and current developments have suggested it by multicomponent reactions (MCR). Barbituric acid and its derivatives, commonly known as barbiturates, are important in pharmaceutical chemistry because they are fascinating building blocks for synthesizing biologically active compounds. The first barbiturate to be prepared was Barbital (5, 5-diethyl barbituric acid), and it is hypnotic and sedative and was used as an anxiolytic and sleeping aid. Barbituric acid derivatives act on the central nervous system and are used as sedatives, anxiolytics, anticonvulsants, and hypnotics. Recent investigations show that barbituric acid derivatives may have applications in matrix metalloproteinases, inhibiting collagen-ase-3 (MMP-3), anti-invasive, recombinant cytochrome P450 enzymes, fungicides, methionine aminopeptidase-1 (MetAP-1), herbicides, antibacterial, anti-tumor antiangiogenic, antioxidant, antiviral, and HIV-1 integrase inhibitors. Furthermore, recent literature accounts have shown that barbituric acid derivatives may also perform as immune modulators. Barbituric acid has been exploited in designing and preparing various types of carbocyclic and heterocyclic compounds. An extensive range of multicomponent reactions utilize barbituric acid as a starting material. By using the Knoevenagel condensation reaction, a wide range of barbiturate drugs, that act as central nervous system depressants can be synthesized using barbituric acid. Barbituric acid is a precursor in the laboratory production of riboflavin (vitamin B_2).

Keywords: Barbituric acid, Chromeno[2,3-*d*]pyrimidine-triones, Condensation Product, Heterocyclic Compounds, Knoevenagel Condensation, N-acylation, N-alkylation, O-methylation, Spirofuropyrimidines, Spirooxindoles, Thiobarbituric acid, Trisheterocyclic System.

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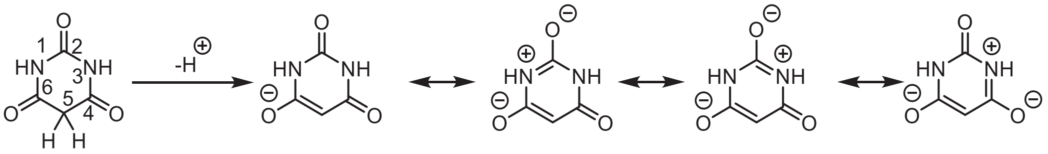
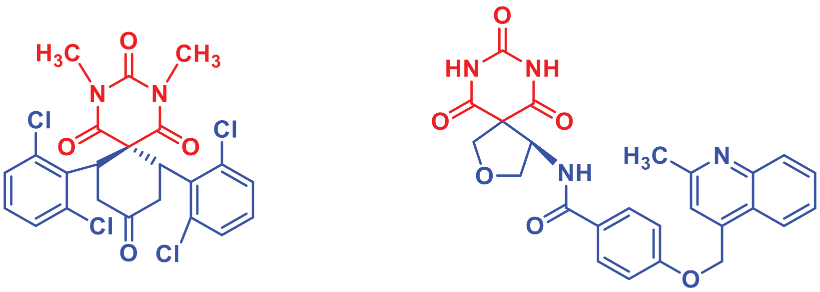
INTRODUCTION

Barbituric acid (pyrimidine 2,4,6(1*H*,3*H*,5*H*)-trione, H_3BA) is an organic compound containing pyrimidine heterocyclic skeleton (Scheme **1**). It is a water-soluble and odorless compound. The chemistry of barbituric acid derivatives, commonly recognized as barbiturates (BAs), has got considerable attention owing to their importance in medicine and biology, and they have appeared in a large number of biologically active compounds (Fig. **1**) [1-11b]. Barbituric acid itself has no bioactivity of its own, but its derivatives exhibit good pharmacological activities [12 - 19]. After invention, barbiturates first came into medical treatment in 1904, modifying access to psychiatric and neurological disorders [20 - 22]. In 1912, a significant barbituric acid derivative, Phenobarbital (Fig. **2**), was discovered and utilized as an antiepileptic drug [23, 24].

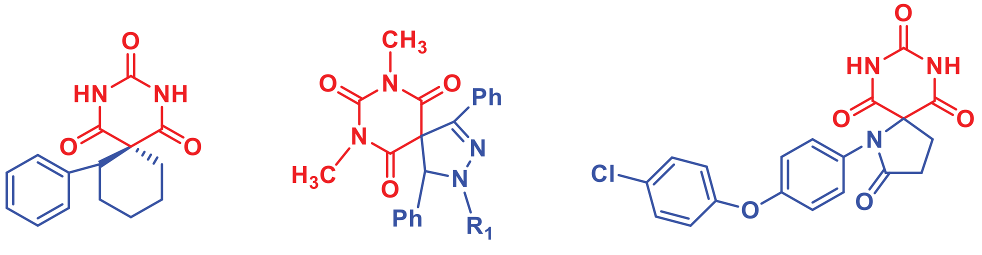


Scheme (1). Molecular structure of barbituric acid (H_3BA) and resonance structures of its deprotonated form.



α-glucosidase inhibitor

TNF-α converting enzyme inhibitors



anticonvulsant agent

Hypotonic agents

R_1=2,4-$Cl_2C_6H_3$

MMP-13 inhibitor

Fig. (1). Biologically active compounds containing barbituric acid moieties.

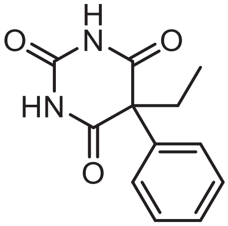


Fig. (2). Phenobarbital: an antiepileptic drug.

Barbituric acids have been generally categorized as compounds that affect the central nervous system and utilized for therapeutic uses such as sedatives [25], anticonvulsants [26, 27], and hypnotics [28, 29]. Current investigations have provided the information that barbituric acids have significant applications in anti-inflammatory [30], antifungal [31], antioxidant [32a-33], antibacterial [34-36c], antitumor [11a], antimalarial [36d], antimicrobial[36e,f], anticancer [36 g-i] as well as anti-viral [37] treatments (Fig. **3**).

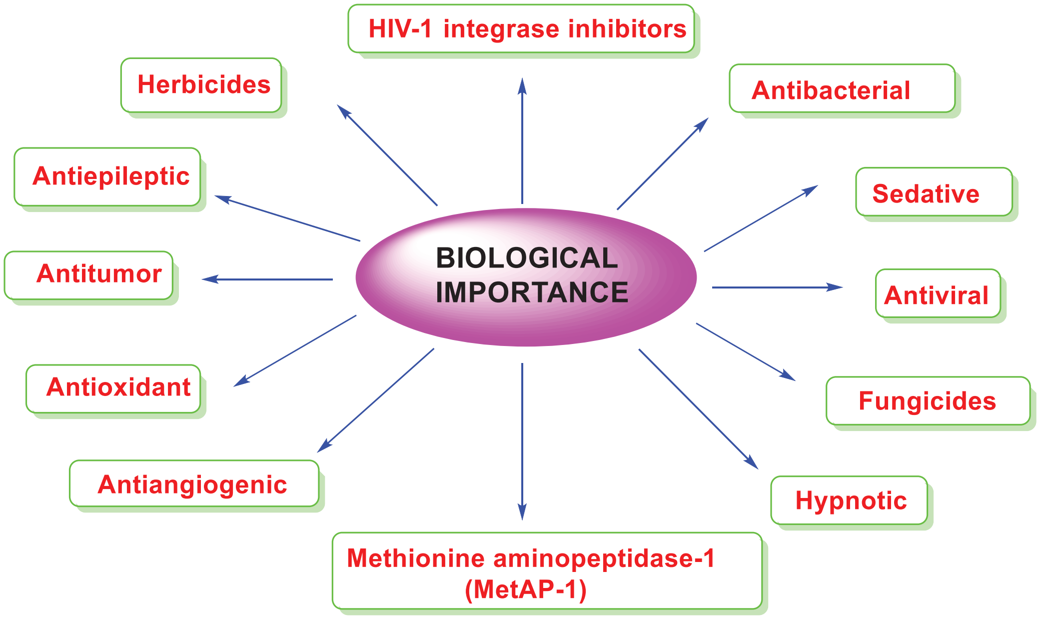


Fig. (3). Biological importance of barbituric acid derivatives.

The existence of the pyrimidine-trione ring and the type of the substituent on the C-5 position regulate the nature of the biological property of the barbiturate derivative [38]. The modifications of barbiturates produce many compounds with varying biological activities, enabling the transformation of barbiturates into a

CHAPTER 4

Ionic Liquids as Solvents and/or Catalysts for Organic Synthesis

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Abstract: Ionic liquids (ILs) are receiving increased enticement from synthetic organic chemists; world-wide due to their extraordinary physicochemical properties. The wide-ranging applications of ionic liquids as solvents and catalysts in organic synthesis are mainly due to their non-volatile nature which arises from very low vapor pressures. Since the past few decades, researchers have explored the efficacy of these designer solvents as green substitutes of toxic and volatile organic solvents for a variety of value added synthetic organic reactions. Furthermore, the tremendous potential of ILs as catalysts is also worth mentioning. Unlike organic solvents of comparable polarity, they often act as catalysts in various organic reactions. Thus, the present chapter aims at observing and exploring the application of ionic liquids as solvents and catalysts in various synthetic organic reactions. The green chemistry aspects of the solvent as well as the catalytic use of ionic liquids in order to develop environmentally benign organic synthesis is also the focus of discussion in this chapter.

Keywords: Catalyst, Diels-Alder reactions, Epoxidation, Friedel-Crafts Reaction, Green Solvent, Hydrogenation, Isomerization Reactions, Oxidation.

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1. INTRODUCTION

Ionic liquid is a topic of immense importance due to their unusual physicochemical properties and wide-spread application potential. In the past two decades, ionic liquids (ILs) have shown burgeoning interest in various fields of science and technology due to their several striking properties, such as, low melting point, negligible vapour pressure, wide electrochemical window, high thermal stability and high ionic conductivity. More importantly, these unique materials are termed as designer solvents as their physicochemical properties can be effectively tuned just by tuning the structure of the cation and/or anion. Owing to several benefits of ILs over conventional molecular solvents, these find numerous applications in the field of organic synthesis. They have become attractive and alternative reaction media for various useful and important organic reactions. A series of reactions that can be performed in ILs has grown tremendously in the mid-1990s with the advancement of water stable neutral ILs. However, the reaction chemistry in ILs was initially restricted to the use of chloroaluminate(III) ionic liquids. Currently, ILs have shown tremendous application potential as designer solvents for variety of organic reactions [1 - 8]. The distinct characteristics and unique features of ILs have prompted researchers to use them as a reaction media in a variety of chemical transformations.

Further, ILs have shown vast applications as solvents or co-solvent, for the catalysis of various organic and inorganic reactions along with their self-catalysis activity. Catalysis is integral in the greater part of both the industrial sector and academic research [1 - 8]. A catalyst accelerates a chemical reaction and is not consumed during the reaction, thus allowing the catalysts to be employed in multiple cycles. However, the recyclability of a catalyst depends on the whole reaction system including the solvent, co-solvents, reactants and the reaction conditions as well. It is a primary requisite to design system with not only efficient catalyst but good recyclability and reusability. The use of catalysts also helps in minimalizing the side products, cutting the energy requirements, and increasing the selectivity. Consequently, catalysts render the various chemical reaction sustainable and environment-friendly. However, the use of certain organic solvents lessens the credibility of the process. In this regard, ILs have come up as a fascinating alternative solvent for biphasic catalysis and in IL thin film catalysis. From early 2000, there was a striking boost in publications for catalysis in ionic liquids. Ionic liquids are good solvents for a wide range of organic and inorganic materials, and their temperature-dependent miscibility with water, non-volatility and thermal stability brand them as favorable media for numerous chemical processes [1 - 8]. The liquid-liquid biphasic catalysis using ILs has found application in a variety of catalysis processes; organic reactions, such as Friedel-craft alkylation, Diels-alder reaction, and transition metal-catalyzed reactions, and many more [9 - 12]. The phase separation enables the easy removal of the products and catalyst for re-use. Apart from the biphasic system, the Supported Ionic Liquid Phase Catalysis (SILPC) and Solid Catalyst with Ionic Liquid Layer (SCILL) have also garnered much-deserved attention [13 - 15]. There are two ways to immobilize IL on support, (a) IL is fixed onto the support *via* physisorption (b) the IL phase is impregnated onto the support by chemical bonds. In SILPC, a thin film of ILs containing dissolved catalysts is dispersed on the support, *i.e.*, a porous material surface (alumina, silica, or active carbon) characterizing supported homogeneous catalysis. Since the dissolved catalysts are near the reaction interface and the diffusion rate is reduced, these systems often result in a high reaction rate. The SLIPC material is synthesized using the following possible methods: (a) the physical confinement/or encapsulation method; (b) the immersion method; (c) the covalent anchoring method. SCILL material is characterized by a solid support catalytic surface, or a catalyst deposited on a solid support, coated with a thin IL film, resulting in a modified heterogeneous catalyst system.

These different possible approaches of incorporating ILs in catalysis has opened a wide door of opportunities for ILs as solvents or as catalyst/co-catalyst in a varied array of reactions. Several task-specific ILs (TSILs) of mostly imidazolium salts have been designed and synthesized by incorporating acidic or basic functional groups into cation/anion of IL which can serve as both the reaction media and catalyst [16, 17]. Acidic ILs have been generated in which carboxylate groups or alkane sulfonic have been covalently bonded to the cation of different ILs such as imidazolium, ammonium, and pyridinium or by the addition of Bronsted acid to the halide based ILs. In basic type ILs, usually organic amine bases are tethered to the IL cations. A class of modified ILs, polyoxometalates-based acidic ILs (POM-ILs) were reported to behave like a co-catalyst and reactant activator in coupling reactions and biomass conversion [18, 19]. Thermoregulated ILs have shown great potential in catalysis. The conversion of a homogeneous to a heterogeneous system with a change in temperature allows easy separation of the reaction system. The assimilation of these ILs and catalysis have found numerous applications. This review presents a brief discussion on the diverse classes of chemical reactions including transition metal-catalyzed hydrogen transfer reactions, coupling reactions, ring-closing reactions, oxidation/reduction reactions, and various organic reactions. The present book chapter highlights the importance of ILs as a solvent and/or as a catalyst in organic synthesis. In Chart **1**, structure of some commonly used cations in combination of different anions are depicted.

CHAPTER 5

Zinc Oxide Nanomaterials for Biomedical Applications

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Abstract: Semiconducting metal oxide nanomaterials are the future potential materials for biomedical applications. Zinc oxide (ZnO) nanomaterials are developed by using the organic synthesis process for excellent biocompatibility, selectivity, sensitivity, good chemical stability, non-toxicity, and fast electron transfer properties. They have a high surface-to-volume ratio that performs proper contouring on the human body to feel comfortable. Recent advanced studies on these nanomaterials show that they are promising materials for effective antibacterial and antifungal agents against a variety of microbes. They also promise to provide advanced technology for biomedical applications that can be used to destroy several types of malignant cells in the human body. Moreover, they can be used as antibacterial agents in the human body. This chapter briefly discusses the cost-effective approach to organically synthesizing ZnO nanomaterials. Moreover, these ideas can be developed to characterize these materials as biomaterials to perform easily upscaled in biomedical applications.

Keywords: Antibacterial and Antifungal Agent, Band-gap Energy, Biomaterial, Biomedical Applications, Cost-effective, Nanoparticles, Nanostructure, Organic Synthesis, Semiconductor, ZnO Nanomaterial.

INTRODUCTION

Zinc oxide (ZnO) is the II–VI metal oxide semiconductor material with outsized exciting-binding energy of 60 meV. It has a high dielectric constant, broad band-gap energy of 3.37 eV at 300 K, and a small Bohr exciting radius of 2.34 nm. It can exhibit nanostructures in forms that possess significant optical, electrical, and semiconducting performance. The ZnO nanoparticles can be studied for extensive utilization. In the synthesis process to develop ZnO nanoparticles, these processes

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are generally classified into three categories: first the physical, second the chemical, and third, the green synthesis process. The physical and chemical synthesis processes generally are involved in laser/vapor deposition, spray-pyrolysis, epitaxy, thermal evaporation, sol-gel, sonochemical, electro-deposition, solvothermal, and hydrothermal [1 - 10]. The other synthesis process is a green synthesis that involves plants and herbal extracts [11 - 15]. Among the various metal oxides, ZnO nanoparticles have been accepted by researchers because of their exceptional electrical and optical characteristics. ZnO is a low-cost specimen in electrical appliances, such as an excellent sensor and a more acceptable agent for targeted drug delivery purposes. It has revolutionized industrial sectors like agriculture, drug delivery, and the food industry [16]. It is also widely used in ethanol gas sensors, UV light-emitting devices, pharmaceuticals, photo-catalysts, and cosmetic industries. These nanoparticles are also used in sunscreen because they absorb ultraviolet light effectively. Compared to other metal oxide nanoparticles, it has inexpensive and relatively low toxic properties that can exhibit excellent application in biomedical sectors, such as bioimaging, antibacterial, antimicrobial, anticancer, and drug delivery purposes.

According to our previous work, some of the materials are silver gallium di-selenide ($AgGaSe_2$) thin films [17 - 21], bismuth telluride (Bi_2Te_3) nanostructure materials [22 - 26] that are more acceptable for device manufacturing purposes, unlike thin films. Recently, ZnO nanoparticles have attracted more attention from scientists for their remarkable biological properties and biomedical uses. It shows the prospect and promise of a biomedical application field by developing the perfect size of nanomaterials. Zinc is an important trace element that extensively exists in human body tissues, along with the muscle, brain, skin, and bone marrow. It plays a crucial role in the nucleic acid synthesis, protein, neurogenesis, and hematopoiesis as a prominent part of different enzyme systems. It also takes part in the body's metabolism [27 - 30]. Low-dimensional ZnO nanoparticles can make zinc more easily absorbed by the human body. ZnO nanoparticles are a proficient platform for biomedical applications [31 - 35]. Nanoparticles exhibit improved characteristics that are supported by particle size, distribution, and morphology. They consist of particles that have nano-scale dimensions. These nanosized elements can enhance the reactivity of catalytic processes and thermal and non-linear optical activity [36 - 38]. These nanoparticles have received more consideration in biomedical applications for these characteristics. The ZnO nanoparticles can perform excellent biomedical applications compared to other metal oxide nanoparticles. Recently, in medical science, ZnO nanoparticles have started to be thought of in order to be used as nano-antibiotics for their antimicrobial activities. One of the reasons behind acute consent is nanoparticles consisting of a particle size less than 100 nm. The typical diameter of many human cells is around 7 µm, so the nanoparticles are comparable to naturally occurring proteins and bio-molecules of the cell. The contraction of particle size to the nano-scale formation can frequently change their structural, morphological, electrical, optical, magnetic, and chemical characteristics. The nano-scale particles have been making them for physical transport into the internal structures of cells and interacting with cell bio-molecules in unique ways. The particles typically possess a large atomic percentage on the main exterior of an element, which can easily lead to enhanced surface reactivity. It can also enhance their capability to be loaded with therapeutic agents to deliver them to target bimolecular cells. By using proper mixing dilation, these particles can acquire the ability to target selectively. It has emerged as a promising candidate for antibacterial fields [39 - 43]. It has a very effective way of destroying the cancer cells in the human body [44 - 48]. Strain is the most important parameter in the biomedical sensing arena. Flexibility and incompatibility in the biomedical field are two major issues with the use of biosensors [49 - 53]. ZnO nonmaterial may be used for biosensor manufacturing purposes. Recently, many researchers have shown that ZnO nanostructures are suitable materials for manufacturing biosensors. There is ongoing research to investigate the bio-imaging sensing function. It has shown positive results only in mice so far. The requirements of this sensor are non-allergenic, non-carcinogenic, high sensitivity, good reproducibility, and non-toxic characteristics. It can help in diagnosing the early stages of cancer germs. Moreover, sensing is important for monitoring and tracking the disease of a patient.

There are various synthesis processes that have been employed to develop ZnO nanostructures due to their vast areas of applications. It has drawn researchers' interest because of its various applications in the fields of electrical, optical, and biomedical sectors. The ZnO nanoparticles can be prepared easily, inexpensively, safely, and securely. Generally, ZnO is a safe metal oxide material recognized and enlisted by the US FDA. At ambient conditions, crystalline ZnO has a wurtzite crystal structure. It has two lattice constants, a & c, with a hexagonal structure. It belongs to the C^4_{6V} or $P6_3mc$ space group. Fig. (**1**) shows the hexagonal wurtzite ZnO crystal structure. The structure of ZnO wurtzite occurs along the c-axis within energy polar exteriors that exist as O^{2-} terminated, or Zn^{2+} is relatively high.

CHAPTER 6

Superhydrophobic Polymeric Nanocomposites Coatings for Effective Corrosion Protection

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Abstract: The contemporary era of studying superhydrophobic surfaces began in 1997, when Neinhuis and Barthlott discovered the self-cleaning qualities of the lotus effect. Corrosion of steel represents an important industrial issue with well-known negative economic and environmental consequences. The protection of steel objects during service operations is inexhaustible research subject because of the steel's high demand in the industry. Anticorrosive coatings have aided in extending the life of the material without impairing its bulk qualities. The microporous structure of polymers allows corrosive ions to pass at the coating–metal interface, resulting in poor serviceability. Advanced structural modifications, such as polymeric nanocomposites, have been used to solve these disadvantages. Organic-inorganic nanocomposites are employed as outstanding anti-corrosive coatings to provide steel constructions' service longevity. Superhydrophobic nanocomposite coatings tend to be one of the most promising methods for avoiding corrosion in steel. Various nanostructured fillers have the ability to significantly improve the corrosion-barrier efficiency of polymeric coatings. Superhydrophobicity in nature will be briefly addressed to provide a comprehensive study. This chapter focuses on introducing the anticorrosive properties of superhydrophobic coatings. It gives an overview of present and advanced research developments, such as graphene nanocomposite surfaces.

Keywords: Anticorrosive Coatings, Corrosion of Steel, Graphene, Lotus Effect, Nanomaterials, Nanofillers, Organic-inorganic, Polymeric Nanocomposites, Superhydrophobic Surfaces, Self-cleaning.

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1. INTRODUCTION

Nanomaterials sciences play an important role in every aspect of technology, helping to solve issues and improve our lives [1]. Developing advanced nanomaterials is necessary to satisfy the demand for betterment [2]. The negative environmental and economic consequences of metallic corrosion have prompted the development of anti-corrosion materials. Corrosion is predicted to cost the world economy $2.5 trillion annually [3]. The significant corrosion impact on different aspects of contemporary life is depicted in Fig. (**1**). Superhydrophobic surfaces have emerged as viable alternatives for a variety of engineering applications, including self-cleaning, biofouling resistance, and corrosion resistance [4]. Many natural surfaces, such as butterflies' wings as well as plants' leaves (including the Indian cress), represent superhydrophobic and self-cleaning surfaces [5]. Lotus plant leaves (Nelumbo nucifera) are the most famous hydrophobic self-cleaning example from which *"Lotus Effect"* was derived [6]. Electron microscopy revealed projecting nubs 20–40 µm apart on the lotus leaf surface coated with a nanorough waxy crystalloids [7]. The contact angle quantifies the wettability of a solid surface by a liquid *via* the Young equation. It is conventionally measured through the liquid, where a liquid–vaporinterface meets a solid surface. Water contact angles (WCA) measurement is a qualitative way to evaluate whether the surface has a hydrophobic (>90°) or hydrophilic (<90°) characteristic.

Fig. (1). Corrosion's impact on various facets of recent life.

On the other hand, the sliding angle is a measure of the mobility of a drop on the surface [8]. It is the tilt angle at which the movement of the drop across the surface begins [9]. It provides information about the adhesion conditions of a droplet on a surface [10].

Superhydrophobic surfaces exhibited (WCAs) ≥150°, reduced sliding angles, and self-cleaning properties. Such processes can be facilitated by micro/nano binary roughness and low surface free energy (SFE) [11]. Superhydrophobicity is a strategy to protect sensitive surface properties [12, 13]. Controlling both oxidation and reduction reactions is necessary to prevent metal corrosion. As a physical barrier, organic coatings are often used to separate steel from its surroundings [13]. Nanoparticles (NPs) cover the spaces between large particles utilizing nanocomposite organic coatings, preventing corrosive solutions from diffusing through these rapid routes. Fabrication of superhydrophobicity surfaces entails the creation of a hierarchical rough morphology with low-energy molecules [14]. To make superhydrophobic nano-surfaces, researchers used etching, lithography, biomimetic, and stamping processes. Also, simple methods of dispersing NPs and graphene-based materials in a hydrophobic polymer matrix can develop water-repellent nanocomposite surfaces [15]. Controlled NP structures aid in the creation of a rough morphology and the generation of extra capabilities for a superhydrophobic surface [16]. Surface roughness and hydrophobicity can be increased by trapping air between the roughness and the liquid drops [17].

As air is a superhydrophobic substance (WCA of 180°) [18], the trapped air can increase the surface self-cleaning property. Superhydrophobicity is thus caused by a hierarchical micro-nano structured surface and a low SFE [19 - 24]. Superhydrophobic surfaces have a near-perfect non-wetting state with minimized contact angle hysteresis (CAH), which are widely used for corrosion-protection applications. CAH is a reflection of the activation energy required for the movement of a droplet from one metastable state to another on a surface [25]. It expresses the difference between advancing contact angle and receding contact angle and is essential to investigate the surface non-wettability and chemical heterogeneity. This chapter looks at recent developments in anticorrosion superhydrophobic surfaces for the steel coating industry, as well as their development methods. Furthermore, it covers the manufacturing approach of stable superhydrophobic coatings for corrosion-resistant coatings. It can present long-term superhydrophobic materials for steel surfaces. It is divided into five sections; the first two of them are devoted to illustrate the coatings' superhydrophobic self-cleaning notion as well as superhydrophobicity in nature. The third section discusses superhydrophobic surface manufacturing and anticorrosion coatings. The importance of polymeric nanocomposite structures for developing anticorrosion superhydrophobic surfaces is discussed in these sections.

CHAPTER 7

Morphologies and Properties of Virgin and Waste PP Nanocomposites

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Abstract: Polypropylene is a semicrystalline thermoplastic addition polymer used in several applications, such as plastic parts for many industries, consumer product packaging, special devices like living hinges, and textiles. Thanks to its excellent properties, it could be used only or in a nanocomposite system.

This article presents the different types of nanoparticles used for the enhancement of thermo-mechanical and physical behaviors of PP nanocomposites. The analysis of morphologies and thermo-mechanical behaviors of virgin PP nanocomposites are described. Moreover, this paper also discusses the improvements of properties of waste PP by nanoparticle incorporation. Finally, the last section of the paper covers a case study about influence of clay nanoparticles on waste PP based nanocomposites.

Keywords: Morphology, Nanocomposites, Polypropylene, Virgin, Waste.

1. INTRODUCTION

Production and consumption of plastic materials have augmented rapidly over the past decades, due to their excellent properties such as versatile, lightweight, relatively inexpensive and moisture resistant. They can be easily used to replace traditional materials, such as wood, paper, glass and metals [1]. Polypropylene (PP) is considered an essential polymer in the modern society. Indeed, it is very

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durable and commonly used in harsh environments such as fuel containers, automotive battery cases, *etc* [2].

Each year, large quantities of plastic materials like PP are thrown in nature causing environmental threats. In order to address this problem, considerable efforts have been achieved to re-use the waste PP in the manufacture of useful products [3, 4].

The recycling and reuse of waste PP not only reduces the environmental impacts, but also decreases the costs of the production. Therefore, it is more economic and ecologic to recycle PP [5]. Nevertheless, waste PP tends to have an inferior performance during the manufacturing process when compared with virgin materials. The reinforcement of waste polymers by inorganic and organic fillers is one of the techniques to modify used polymers for technological utilizations.

In this article, a comprehensive study on the incorporation of nanoparticles in virgin and waste polypropylene is investigated, which can help industrials and researchers in their future work.

2. POLYPROPYLENE

Polypropylene is one of the most common semi-crystalline thermoplastics used in industry. Roughly, 30 million tons of PP were consumed in the world during 2015. As we can see on Fig (**1**), it occupied the second range regarding mondial consumption of polymers after polyethylene (PE).

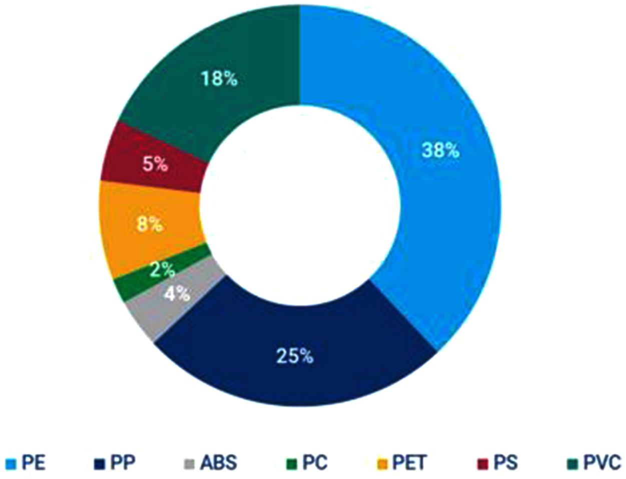


Fig. (1). Thermoplastic polymers consumption in 2015 year [6].

PP has very interesting thermo-mechanical and physical properties for use at room temperature. In fact, PP has high melting point, low density (0.9 to 0.91 g/cm^3), high stiffness and impact resistance. All these characteristic properties permit its use in the manufacture of several industrial materials. The areas of application are numerous and include textile fibers, geotextile, packaging, aerospace and automobile applications.

PP is obtained by metallocene catalysis or by Ziegler-Natta polymerization of propylene monomers. PP is a vinyl polymer with a chemical structure similar to that of PE [7]. Compared to the synthesis of PE, the particular characteristic of PP polymerization is the symmetry of monomer addition in the growing polymer chains due to the existence of -CH3 in the PP monomer (Fig. **2**) [8].

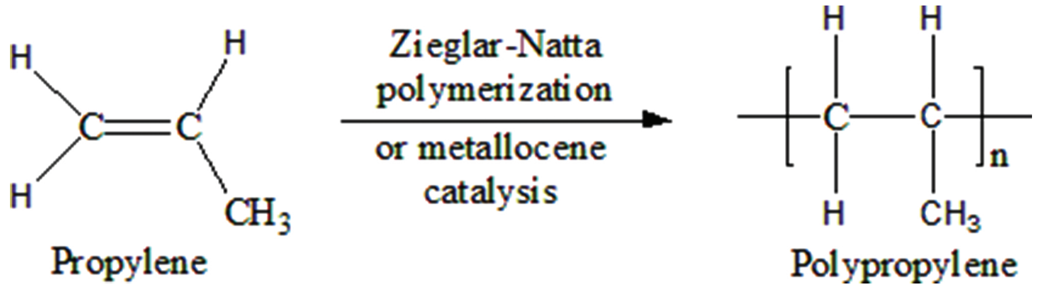


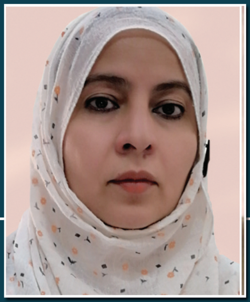
Fig. (2). Polypropylene PP Polymerization.

This polymer has a glass transition temperature (T_g) of about -18°C and a melting temperature (T_f) of about 165°C. Another important feature of polypropylene is its viscosity which has an important effect on molten state processing by extrusion or injection. Its hardness and mechanical strength are relatively interesting and its crystallinity is between 65 and 75%. The elongation limit, yield strength, tensile strength and elasticity modulus of PP are 100-600%, 31-37.2 MPa, 31-41.4 MPa and 1.14-1.55 GPa, respectively [9]. The main characteristics of PP (homopolymers, block and static copolymers) are summarized on the next table (Table **1**).

Table 1. Main characteristics of polypropylene [10].

Properties	Homo-polymers	Block Copolymers	Statistical Copolymers
Density (kg / m^3)	900-910	890-905	890-905
MFI (g / 10 min)	1-55	0.8-100	1.7-40
Water Absorption (%)	<0.05	<0.05	<0.05

SUBJECT INDEX



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As recognition of her contributions to science, she has been awarded with 03 International awards like Fellowship from Islamic World Academy of Sciences, Postdoctoral fellowship from Ministry of Culture and Education, Spain and a Young Chemist Award from Third World Academy of Sciences, Italy. She also has several national awards on her credit.