Organic Chemistry: Structure, Properties, and Reactions

Editors

Salah Hassan Abhoul Al-Ziyadi
Department of Chemistry, College of Sciences, Al-Muthanna University

Zahraa Mohammad Abd _Alsada
Department of Chemistry, College of Science, University of Kufa

Mohammed Wesam Shukr Khanjar
Department of Chemical Sciences, College of Science, Diyala University

Mohammed Adel Hadi
Department of Chemistry, College of Science, University of Diyala,

Kazem Abdel Zahra Jabr Abbas
Department of Chemistry, College of Science, University of Kufa

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Editors: *Salah Hassan Abhoul Al-ziyadi, Zahraa Mohammad Abd _Alsada, Mohammed Wesam Shukr Khanjar, Mohammed Adel Hadi and Kazem Abdel Zahra Jabr Abbas*

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Abstract

Organic chemistry is an intricate and absolutely fascinating field of science that is primarily focused on the thorough and detailed study of the structure, properties, and reactions of a vast and varied array of organic compounds that are known to contain the essential element carbon. This significant branch of chemistry is deeply engaged and concerned with garnering a comprehensive and thorough understanding of the myriad of complex molecules that are prevalent within living organisms, as well as many of the diverse and useful products and materials that are sourced from these important and essential compounds. The unique and incredibly versatile characteristics of the carbon atom itself, particularly its remarkable ability to form not only strong but also stable bonds with itself, as well as with a diverse variety of other elements including hydrogen, oxygen, and nitrogen, contribute significantly to making this particular class of chemical compounds remarkably extensive and incredibly diverse, encompassing a multitude of different forms and functions. Within just the confines of a few chapters, an introductory course in organic chemistry must strive diligently to effectively convey crucial fundamental information that students need to succeed, imparting a deep awareness of the vast relevance and importance of organic chemistry to various fields of study and practical applications, introducing essential concepts that can be extrapolated and applied to structures that students have not yet encountered or learned about, and supplying a coherent organizing framework that enables the presentation of a staggering amount of new content in a way that is both digestible and manageable for students. Successfully achieving all these educational objectives within a modest page limit over the course

of just one or possibly two semesters makes the task of fully understanding organic chemistry a particularly noteworthy and impressive accomplishment for students engaged in this intricate and fascinating discipline that demands both time and intellectual investment.

Chapter - 1

Introduction to Organic Chemistry

Organic chemistry specifies the structures, properties, and reactions of organic compounds. The word organic initially applied to substances obtained from living organisms but is now known to relate to carbon compounds. Organic chemistry is the largest discipline in the field: more compounds, reagents, and solvent systems derive from carbon than from any other element. Carbon uniquely forms stable bonds to many other elements (such as hydrogen, nitrogen, oxygen, phosphorus, and sulfur) and to itself.

The curbed work offers substantial contributions to the expansive field of organic chemistry. Section 2 introduces essential fundamental concepts, providing a thorough explanation of atomic structure and bonding while also outlining various functional groups that are critical for understanding organic compounds. Section 3 carefully examines molecular structure in the intricate context of isomerism, along with a detailed exploration of three-dimensional geometry, which plays a vital role in the behavior of molecules. Section 4 comprehensively addresses the physical properties of organic compounds, placing a significant focus on boiling and melting points, along with various solubility patterns which govern how substances interact in different environments. Section 5 deals extensively with the chemical properties of these compounds, detailing various reactivity patterns and the important characteristics of acid-base behavior that influence organic reactions. Section 6 describes the major types of organic reactions in great depth, including addition reactions, elimination reactions, and substitution reactions, all fundamental to the discipline. Section 7 explains reaction mechanisms with a particular focus on pathways such as nucleophilic substitution and electrophilic addition, elucidating how these processes occur on a molecular level. Section 8 presents various approaches to synthesis, emphasizing the significance of retrosynthetic analysis and strategic considerations that chemists employ when designing synthetic routes. Section 9 introduces spectroscopic methods crucial for the study of organic compounds, including nuclear magnetic resonance, mass spectrometry, and infrared spectroscopy, outlining their applications in identifying and characterizing substances. Section 10 connects organic chemistry to biological systems by discussing the role and importance of biomolecules and enzyme catalysis, showcasing the interplay between chemistry and life itself. Section 11 devotes an exploration to environmental aspects, analyzing the impact of pollutants on ecosystems and discussing the guiding principles of green chemistry that aim to minimize harm and foster sustainability. Section 12 surveys the industrial applications of organic chemistry, with a particular focus on the critical fields of pharmaceuticals and polymers, illustrating the practical significance of this area of study. Section 13 discusses insightful future directions for organic chemistry, highlighting the importance of sustainable practices and emerging technologies that could shape the future landscape of the discipline. The final section offers a comprehensive conclusion that synthesizes the key insights gained throughout the course of the work, thus providing a solid and coherent basis for understanding the structure, properties, and complex reactions of carbon-containing compounds, ultimately reinforcing their importance in both science and industry [1, 2, 3, 4].

Chapter - 2

Fundamental Concepts

Organic chemistry has its roots in a dual focus that encompasses both the intricate understanding of structure and the practical aspects of synthesis and reactivity. The primary objective was to gain a profound understanding and accurate description of the structures inherent to organic compounds. Simultaneously, there was a significant emphasis on synthesis and reactivity—this entailed preparing compounds that held both theoretical significance and practical applications. It also involved developing a comprehensive understanding of the phenomena associated with chemical reactivity and unraveling the complex mechanisms underlying various reactions. The determination of molecular structure was greatly facilitated by advances in techniques such as X-ray crystallography and spectroscopy, which provided critical insights into the arrangement of atoms within the molecules.

In terms of synthesis, this period marked the emergence of practical design strategies that allowed chemists to construct complex molecules with precision and efficiency. Synthesis not only involved the actual creation of these molecules but also required an in-depth understanding of the pathways that could be employed to achieve desired products. Reactivity and mechanisms offered further insight into structural characteristics, thereby enriching the knowledge base of organic chemistry and significantly contributing to the advancement of retrosynthetic analysis. This analytical approach aided chemists in planning synthetic routes by working backward from target molecules.

In contemporary practice, the emphasis has shifted prominently toward synthesis. This shift can be attributed, in part, to the fact that the structures and stoichiometries of organic molecules can now be determined with remarkable accuracy using various spectroscopic methods. Consequently, a substantial body of knowledge has accrued regarding the structural and electronic features that dictate reactivity and selectivity in chemical processes.

Despite the vast expanse of current knowledge, the foremost challenge that spans the fields of chemistry, medicine, biology, and materials science remains the effective exploitation of this existing knowledge. The goal is to devise efficient catalytic and stereoselective methods that facilitate the preparation of increasingly complex molecules. These methods must rely on readily accessible and cost-effective starting materials, utilizing a meticulously defined sequence of transformations that lead to the desired outcomes in synthesis. As organic chemistry continues to evolve, the quest for innovative methodologies remains a driving force behind the discipline's advancements and its applications across various sectors [5, 6, 7, 8, 9].

2.1 Atomic Structure and Bonding

An understanding of bonding is absolutely essential for effectively learning several key chemistry topics, including but not limited to chemical reactions, molecular structure, and thermodynamics. Despite their increased education and various teaching methods employed, students still struggle significantly to fully grasp the intricate nuances of chemical bonding, with many lingering misconceptions about these concepts. These misconceptions often arise from flawed and incomplete mental models regarding the various interrelated and complex concepts that underpin the world of chemistry. Organic chemistry is explicitly defined as the study of carbon-containing compounds, along with their numerous properties and different types of reactions that they can undergo. Lewis structures provide a ubiquitous and widely accepted representation of molecules in the realm of organic chemistry, serving as a foundational tool for students. Even after receiving thorough instruction on advanced topics such as resonance and aromaticity, students are often unable to successfully apply these concepts in a new and different context that might be presented during examinations or practical applications. Misconceptions persist regarding the actual impact of resonance and other related effects on various chemical properties, leaving many students unable to coherently explain important chemical phenomena. Thus, molecular visualization-including Lewis structures in particular-becomes crucial to student success and performance in organic chemistry, allowing them to better understand and engage with the material at hand [10, 11, 12, 13].

2.2 Functional Groups

The functional-group approach serves as the essential foundation of organic chemistry. This approach enables a systematic and organized description of a wide range of chemical reactions. Trying to analyze molecules from an atom-by-atom perspective is often impractical due to the considerable size and inherent complexity of these structures. Organic compounds frequently consist of numerous atoms. For instance, vitamin B12 is notable for containing approximately 80 carbon atoms, in addition to several hundred other atoms, illustrating the intricate nature of such molecules. Most organic molecules are described in terms of a specific functional group or a unique combination of functional groups. Functional groups themselves are characteristic of well-defined portions within the overall structure of the molecule. They play a crucial role in controlling the behavior of a molecule when it is subjected to various situations. These groups dictate how the molecule interacts during chemical reactions and significantly influence various chemical properties, including polarity, solubility, and boiling point, thereby playing an indispensable role in the understanding and application of organic chemistry [14, 15, 16, 17, 18].

Chapter - 3

Molecular Structure

Molecular structure is a fundamental concept in organic chemistry. The physical properties of an organic compound are governed largely by its molecular structure, which in turn influences its chemical properties.

Organic compounds can have the same atomic connections but differ in structures. Such compounds are known as isomers, a word derived from the Greek isos, meaning "same," and meros, meaning "part." Isomerism is a major topic, worthy of detailed discussion. A comprehensive description of three-dimensional structures is key to understanding molecular structures.

Two compounds are considered structural isomers if they differ in the actual connections and arrangements among their atoms, leading to variations in their structures. Structural isomers possess unique physical and chemical properties because the specific arrangement of atoms ultimately determines these characteristics. Since they have different structures, structural isomers can exhibit different behaviors in various chemical reactions. Furthermore, structural isomers are free to rotate around their bonds, which allows them to adopt a wide array of three-dimensional conformations depending on their specific atomic connections. They can also be represented in both two-dimensional and three-dimensional forms. In the gas phase, the freedom of molecular rotation is relatively unrestricted, allowing for a diverse range of spatial orientations and interactions. Thus, understanding structural isomerism is crucial in the study of chemistry and the behavior of compounds [19, 20, 21].

3.1 Isomerism

Isomers, which share the same molecular formula but exhibit different structural or spatial arrangements, fundamentally influence the properties of organic compounds. These compounds can therefore be distinguished by their structure or the method through which they are obtained. Structural isomers have identical numbers of atoms and the same bonding arrangements but differ in the geometric positions of the atoms within the molecule. They function as model compounds for exploring structure 6property relationships and are stabilized by chemical bonds, rendering photochemical or thermochemical isomerization difficult [22]. For example, studies concerning syn- and anti-isomers of thiophene derivatives demonstrate that anti-isomers possess higher charge mobilities, promoting the performance of organic field-effect transistors. Furthermore, naphtha [1, 2-d] imidazole isomers exhibit enhanced efficiencies in organic light-emitting diodes when comparing structural variations; the naphtha [1, 2-d] imidazole configuration facilitates more efficient electron injection, enabling the device to achieve higher brightness and current efficiency.

The distinction among various types of compounds is not limited solely to simple structural differences and variations. Chiral molecules, which are unique in that they exist as non-superimposable mirror images of one another, are specifically termed enantiomers. Each pair of enantiomers that are related to each other constitutes a stereoisomeric pair within a broader category, but it is essential to understand that each individual chiral molecule, when considered on its own, is not classified as a stereoisomer. Stereoisomers inherently possess the same molecular formula, display identical bonding patterns, and undergo indistinguishable developmental processes throughout their formation. Compounds that share the same formula yet fail to meet these strict criteria are classified as structural isomers.

Furthermore, it is important to note that the products that correspond to different sets of structural formulae remain distinctly recognizable through their behavior in substitution reactions. As a consequence of these differences, the products associated with one particular set of structural formulae are structurally identical to one another; however, those that pertain to different sets and yet possess an identical empirical formula are categorized as structural isomers. An exemplary case in point is the group describing structural isomerism of cyclopropane, which fascinatingly has an order of 48. Analyzing the action orbits of this group serves to facilitate a comprehensive enumeration and better understanding of the various isomers present for this compound [23, 24, 25, 26, 27].

3.2 Three-Dimensional Structures

Morphine demonstrates that different spatial arrangements within three-dimensional structures can lead to distinctly different chemical properties and behaviors. Importantly, organic compounds inherently possess specific three-dimensional structures that define their characteristics. The spatial arrangements of atoms play a crucial role in elucidating various physical properties, which can be examined through the comparison of the boiling points of butan-1-ol and butan-2-ol, highlighting how small changes in structure can lead to significant differences in physical behavior. Furthermore, the spatial arrangements of atoms are also pivotal in influencing chemical reactions. This is exemplified by the notable differences in chemical reactivity observed between (R)- and (S)-isomers, which demonstrate how stereochemistry can impact reaction pathways and outcomes. Hence, a thorough interpretation of chemical reactions necessitates a fundamental understanding of the three-dimensional structures of molecules. Because the molecules that constitute crystals are organized and arranged in a regular manner, crystalline compounds are more likely to produce good-quality X-ray diffraction patterns, which are essential for the determination of molecular structures and the analysis of material properties [28, 29].

Chapter - 4

Physical Properties of Organic Compounds

Organic molecules fund daily life and underpin industrialized economies. They serve as fuels, dyes, polymers, paints, pharmaceuticals, flavors, and explosives. Although billions of organic molecules exist, only a few thousand appear in the literature to date. A fully referenced intermediate-level textbook covers the structures and properties of important organic compounds, reaction types and mechanisms, synthetic analysis and strategies, spectroscopic identification, biological function, environmental impact, industrial applications, and new directions in the field.

Organic compounds are defined as compounds containing carbon. This definition was initially formulated by Jons Jacob Berzelius in 1807. Currently the characterization of organic compounds is well beyond the scope of this chapter, which emphasizes the physical properties of the compounds. Carbon and its compounds are of great importance in recent human history. These compounds are the basis of living organisms; all of the majority of the food we consume and the fuels that power vehicles and engines are organic compounds. Carbon's formation of numerous, stable structures provides a basis for the diversity of organic compounds. The formation of four bonds to satisfy the octet rule allows for many atoms to bond to a central carbon atom to form a large number of stable compounds [1].

Organic compounds are those substances whose molecules contain carbon atoms forming covalent bonds mainly to hydrogen atoms and other carbon atoms [1]. Although many substances other than carbon dioxide and carbonates contain carbon atoms, the term organic compounds is conventionally restricted to the hydrocarbon group of substances – the study of which is popularly known as organic chemistry.

The various kinds of organic compounds are commonly subdivided into three main groups: those composed of open chains, chains containing a benzene ring, and compounds composed of ring structures. The classes of organic compounds skew to open-chain rather than ring-containing structure. Consequently, the largest portion of the work concerns only these open-chain-type compounds.

Aliphatic compounds include aldehydes, ketones, alcohols, ethers, carboxylic acids, esters, amines and amides, and many hydrocarbons, such as alkanes, alkenes and alkynes. They belong to the classes of open-chain structures and consist of a linear arrangement of atoms with straight, branched, or cross-linked chain. Straight-chain aliphatic compounds are called normal (n) compounds. Aliphatic cyclic compounds form a bathtub-shaped cyclic structure with atoms arranged in a ring, and are known as cycloalkanes, cycloalkenes, and cycloalkynes.

Both aliphatic and aromatic cyclic compounds are referred to as cyclic compounds. The subset of cyclic aromatic compounds includes a few special molecules considered separately in the category of heterocyclic compounds, such as pyrimidine, pyridine, and quinoline. Other organic compounds of this group are known as Ahetars or heteroaromatics. Many carbon compounds are derivatives of aliphatic structures and are part of the compounds belonging to the class of open-chain structures.

Aromatic compounds form a principal class of organic compounds distinguished by the predominance of specific ring systems within their molecular structures, exemplified by the benzene ring. A benzene molecule consists of six carbon atoms arranged in a planar ring, with one hydrogen atom bonded to each carbon. The unsaturation present in the benzene ring is not localized but is distributed evenly, giving rise to the concept of aromaticity. This delocalized electronic configuration and ring structure confer the designation 'aromatic' upon such compounds, in contrast to aliphatic classes.

Aromatic compounds are widely distributed in the natural environment and occur as natural products of considerable practical importance. Several polycyclic aromatic hydrocarbon compounds are carcinogens [2]. Aromatic compounds can be considered as derivatives of arenes and are often represented by starting from benzene and replacing hydrogen atoms with different elements or groups of elements.

Cyclic organic compounds are molecules that contain one or more rings of atoms as part of their structure. They can be subdivided into Alicyclic and Aromatic compounds. Alicyclic molecules feature atoms arranged in ring shapes but chemically resemble open-chain compounds. Aromatic compounds contain distinctive stable ring structures with delocalized electrons. Some cyclic substances, such as terpenes, naturally exhibit their rings as isolated subunits rather than continuous systems.

Examples of aromatic compounds possessing single ring structures include benzene, naphthalene, and anthracene. The presence or absence of cyclic components dictates the overall connectivity of an organic molecule, thereby impacting its physical characteristics.

Free radicals may arise when molecules or molecular fragments hold unpaired electrons. Such species frequently appear as intermediates in chemical transformations and can present hazards due to their enhanced reactivity. Radical species represent intermediates during polymer formation processes involving free radical mechanisms.

Cyclic systems feature topological indices subjected to extensive investigations. Compounds composed of single rings also undergo structural scrutiny. The Bcut descriptor quantifies the cumulated strength of all bridging bonds connecting adjacent overlapping paths within the ring. When cyclic organic molecules bear one or multiple acyclic branches, structural complexity escalates relative to branched open-chain analogues. Quantitative measures rely on alterations in the sum of topological distances (Wiener number) within respective molecular graphs. These topological principles find reflection in isoalkyl-benzene properties. Multiple methodologies assess the relationship between property values and molecular architecture; however, additive schemes encounter constraints concerning accuracy and applicability, particularly for parameters governed by intermolecular interactions. Consequently, contributions from structural fragments may exhibit intricate behavior, with certain quantities defying decomposition into summations of individual component effects. In such scenarios, variable selection techniques of an algebraic nature prove valuable, utilizing flexible structural elements coupled with computer-assisted correlation analyses to pinpoint dominant fragments influencing specific molecular attributes [3].

Organic compounds consist of carbon atoms bonded to elements such as hydrogen, oxygen, nitrogen, or sulfur. Although the majority of organic molecules contain just these three elements, a wide range of physical properties exists within this group. Organic molecules vary in length, branching, and shape, and they may contain functional groups with distinctive physical properties.

Historically, the synthesis and study of organic compounds focused predominantly on substances containing carbon and hydrogen, referred to as organic chemistry [4]. The presence of additional elements in organic molecules often leads to significant differences in reactivity and biological function. Commonly incorporated elements include oxygen, sulfur, nitrogen, and fluorine.

Organic compounds are classified into three primary categories: Aliphatic, Aromatic, and Cyclic.

Aliphatic compounds constitute the largest group, encompassing both linear and branched-chain molecules. These compounds may exist as straight chains or disconnected linear fragments (e.g., chains of 15 or more carbons without branching). An important subgroup includes the homologous series or families, which possess an identical functional group and exhibit similar chemical reactivity. The compound with the fewest carbon atoms and a given functional group is termed the parent compound; when on-going reactions alter the document structure without changing the initial hydrocarbon chain length, the resulting molecules are termed substituted derivatives.

Aromatic compounds are characterized by ring structures that include a delocalized (rather than purely localized) π-electron cloud. This delocalization enhances the molecules' stability and increases their likelihood of competing reactions.

Cyclic compounds consist of carbon atoms arranged in ring structures encompassing more than six carbons. Many of the molecules in this group are not conjugated or aromatic; thus, they do not possess the associated electronic properties. Molecular structure, the arrangement of atoms within a molecule, dictates molecule shape. The strength of the bond between atoms relates to the number of electrons shared.

The bonding of organic compounds takes place through localized bonds involving electrons well localized between adjacent atoms. Organic compounds are covalently bonded molecular substances where discrete molecules are held together by weak intermolecular forces. Characteristic chemical behavior of an organic compound depends on its functional groups, certain atoms or groups of atoms responsible for its specific chemical properties. The carbon atom in organic compounds is bonded through four single bonds to four other atoms or, sometimes, to other carbon atoms through a double or triple bond. One of the most interesting features of organic compounds is their ability to display structural isomerism-compounds with the same molecular formula but different structures. The spatial organization of the atoms within molecules is referred to as molecular geometry. All of these features influence the physical behavior of a molecule [4].

Isomers are molecules with the same molecular formula but different structures. They are commonly classified into two groups: constitutional (or structural) and stereoisomers [5]. Constitutional isomers possess the same molecular formula but differ in the connections of atoms within the molecule. They are represented by different bond-line structures and are not related as resonance forms [6].

The study of constitutional isomers offers a low-tech route toward the design of easily accessible but nevertheless effective molecular materials often suited for specific applications. Dimethyl-substituted inorganic compounds were synthesized systematically according to the number and position of the substituent. Parachloromethyltriphenylmethylbenzene-dimethyl derivative possesses the highest solubility among the isomers [7]. This effect corresponds to their crystal packing, the former is stabilized by van der Waals interactions from the biphenyl groups and the latter benefits from the introduction of methyl substituents.

No molecule exists in isolation. As described in the articles on bondings, chemical bonds hold together the atoms that comprise a molecule-intra-molecular forces. Beyond that, molecules themselves exert forces on their neighboring molecules, referred to as inter-molecular forces. These forces explain the physical properties of organic compounds.

Hydrogen bonding is a specific dipole–dipole interaction between hydrogen atoms in polar H–X bonds and lone pairs of electrons in H–Y groups (where X and Y are nitrogen, oxygen, or fluorine). Van der Waals forces occur not only between two adjacent atoms but also between two adjacent molecules that are very close to each other, allowing their electrons to be attracted to the positive nuclei of the other. Induced dipole–induced dipole forces, or London dispersion forces, arise among non-polar molecules when temporary dipoles are induced by the electrons of one molecule on those of another. Collectively, these interactions shape the range and nature of the physical properties discussed subsequently.

Hydrogen bonding determines the physical properties of many organic compounds. It also plays an important role in many organic reaction mechanisms. The stability of the eclipsed, gauche, and anti-staggered conformers of organic compounds bearing electronegative functional groups is often governed by hydrogen bonding. The laboratory identification of many organic compounds depends on the formation of crystalline adducts with known reagents that bond to the structure by hydrogen bonding.

Hydrogen bonding is defined as a two-center interaction involving a hydrogen atom situated between a pair of hetero-atoms (electronegative atoms other than carbon). The hydrogen atom is usually covalently bonded to one of the electronegative atoms and lies co-linearly on the bond connecting the two atoms. Hydrogen bonding requires three initiators: a donor site (D–H), a hydrogen bond, (H···A), and an acceptor site, (A) [8].

The donor site (D–H) involves an atom covalently bonded to a hydrogen. The atom must be more electronegative than hydrogen so that the size of the H atom is reduced and it develops a positive charge. Lower electronegativities generate larger atoms with smaller positive charge such as Si–H, that cannot form a strong hydrogen bond. The acceptor site (A) provides a lone pair of electrons. Hydrogen bonding explains why CH3OF boils at 25.2 °C, whereas CH3Cl boils at –24 °C even though the dipole moment of chloromethane is more than twice that of fluoro-methanol. It is also responsible for the structure of the tertiary structure of proteins and the double helical arrangement of DNA. The development of a positive charge on hydrogen takes place for other halogens, but the larger size of the atoms reduces penetration and the effectiveness of the interaction. Hydrogen bonding can be classified as either intermolecular or intramolecular.

Van der Waals forces arise from transient dipoles between neutral molecular entities. Even symmetrical or nonpolar atoms or molecules exhibit spontaneous, temporary polarization due to fluctuations in electron distribution. Polarizable electron clouds in neighboring atoms or molecules respond by aligning to form a coordinated fluctuating dipole system, leading to net attractive forces [9]. These dispersion forces remain operative throughout all chemical scenarios. When molecules lie in close proximity, atom-atom dispersion interactions between unscreened components frequently achieve strengths comparable to basic chemical bonds.

Three circumstances amplify the impact of dispersion forces: 1) large areas of close molecular contact produce significant, extensive atom-atom interactions; 2) high polarizabilities substantially enhance each interaction; and 3) the molecular assembly is geometrically arranged to enable multiple interactions to continue working cooperatively rather than competing. While the combined dispersion between two moderately sized molecules rarely exceeds about 50 kcal/mol, unattenuated atom-atom dispersion forces between components within a molecule can reach many hundreds of kcal mol–1. When these large intra-molecular forces maintain the geometry of a single chemical bond, their magnitudes are typically 100–250 kcal mol–1, with values closer to the higher end observed for shorter components like C–F, C–O, or C–N. The total dispersion between different parts of the same molecule can be efficiently channeled through a single bond-linking region. The control of bond stability and geometry often rests on the connection between covalent bonding and dispersion, with the overall magnitude of dispersion comparable to that of covalent bonds.

The interaction between covalent bonds and dispersion forces accounts for many structural features. Different chemical forms of the same species illustrate the influence of dispersion on chemical behaviour, particularly phenomena such as valence tautomerization and resonance stabilization. Tautomerism involves an equilibrium between two structurally and electronically distinct isomers, one stabilized primarily by strong covalent bonds and the other held together predominantly by dispersion interactions. In resonance-stabilized species such as benzene, the observed structure comprises equal bond lengths that reflect a balance or superposition of chemically distinct bonding arrangements.

A dipole-dipole interaction is an interaction between the positive end of a permanent dipole and the negative end of another permanent dipole. Dipole-dipole forces therefore only exist between polar molecules. Clearly, molecules with no dipole moment (nonpolar molecules) will not experience dipole-dipole forces. The forces between polar molecules are considerable weaker than either ionic or covalent bonding, typically about 1 kcal/mol. Dipole-dipole interactions increase the boiling and melting points of compounds relative to similar nonpolar molecules. The origin of the charge separation within a molecule is the difference in electronegativities of the atoms [10].

The solubility of a solid in a liquid is of wide interest in physics, chemistry, biology, materials science and engineering. Solubility results from the balance of intermolecular forces between the molecules of the solid and the interacting solvent molecules. In a simple system such as a solid with no solid–solid phase transitions dissolved in a solvent that is not involved in solid-state equilibria and does not form solvates, the fundamental relationship describing solubility is the temperature-dependent Weeks–Chandler–Andersen–based excess chemical potential of the solid phase. Once solid- and liquid-state properties of the solute and the solvent are known to a sufficient degree of accuracy, the solubility of a solid is therefore predicted directly from this fundamental relationship.

The activity coefficient of the solute is also a measure of the solute–solvent interactions, determined from measured solubility and solid-state properties: solid phase composition, solid sub-cooled liquid properties and the pure solvent, Svap, the normal boiling point, critical temperature and pressure, liquid density, molar volume, surface tension and Henry's law constant. The activity coefficient can be related to a number of widely used thermodynamic models for excess Gibbs free energy, which describe the molecular interactions with their surroundings. Chemistry or physical properties are reflected in the model parameters, establishing a molecular picture of the interactions experienced in different mixtures. Compounds with activity coefficients less than 1 show negative interaction parameters with the different pure fluoroethers as the solvent, which implies that the interactions in the pure solute and pure solvent molecules are similar to the interactions when they are mixed [11].

Solubility quantifies the maximum amount of a compound that can dissolve in a solvent to form a homogeneous system at specified conditions of temperature and pressure. The effectiveness of various solvents in dissolving particular compounds is crucial for purification and extraction processes. Many complex organic substances exhibit low solubility in water, making the choice of an appropriate solvent essential [11].

Two important measures related to solubility are the activity coefficient of the solute in the saturated solution and the thermodynamic solubility. The value of the activity coefficient reflects the extent of solute–solvent interactions and can be derived directly from solubility and solid-state data. For instance, the ortho isomers 2HBA and PIC have higher activity coefficients than the corresponding meta and para isomers, indicating behavior closer to ideality and explaining their higher solubility in non-polar solvents. Thermodynamic models based on excess Gibbs free energy provide valuable insight into the molecular interactions between dissolved species and their environment; variations in the interaction energies of these components strongly affect both local and overall concentrations. Compounds with an activity coefficient less than unity exhibit a negative interaction parameter, signifying roughly equivalent interactions with either the neighbors in the pure solute or the surrounding molecules of dioxane, toluene, or other components. Temperature-dependent solubility serves as a critical design parameter in operations such as crystallization, but current approaches aimed at estimating composition often yield poor results due to limited or inaccurate solid-state data, which in turn adversely affects the direct determination of activity coefficients and the prediction of appropriate crystal structures. The temperature-dependent solubility of 18 APIs and intermediates was measured in 1,4-dioxane, toluene, and cyclopentyl methyl ether over a wide interval from 0 to 70 °C. The data were correlated with the Van’t Hoff, Apelblat, and kh equations, with Van’t Hoff providing the best performance. Liquid-phase thermodynamic models such as Margules, Van Laar, Wilson, and NRTL were used to describe activity coefficients and solubility as a function of the excess Gibbs energy.

Solvents can be singled out from among the physical properties of a compound because they influence its solubility and are almost exclusively molecular in origin. The solvent properties primarily emphasize the capacity of the solvent to combine with the solute and thus change its rate of dissolution. A solvent's ability to dissolve a variety of organic compounds depends very much on its own molecular structure and whether its molecules are polar or non-polar in nature.

The ability of a solvent to dissolve an organic compound depends largely on four intermolecular interactions: the dispersion force, the induced-dipole force, the dipole force, and the hydrogen-bonding force. The first two of these forces occur in all molecules, and the polar molecules of the last two provide extra dissolution power for polar organic compounds. Solubility usually decreases sharply if the solvent is incapable of producing a given force.

Solvent properties of a liquid can be related to ultraviolet and infrared absorption spectra. These curves are changed by dissolution in the liquid, so that the lines provide a molecular fingerprint of the liquid. However, quantitative correlations require a description of the solvent properties in the ultraviolet region, where absorption occurs in the 200–300 nm range.

The solvent properties of THF, acetone, chlorobenzene, and aniline are well represented by two linear functions of spectral parameters (the π, α, and β parameters, where π provides a measure of solvent dipolarity-polarizability and α and β are respectively the solvent H-bond donor acidity and H-bond acceptor basicity, related to the Gutmann donor number) [12].

Organic compounds exhibit a broad range of melting and boiling points that demonstrate systematic trends related to molecular structure. The boiling-point range for organic compounds is remarkably broad, extending from 20 to 900 degrees Celsius. Many organic compounds undergo thermal decomposition before reaching their boiling points; consequently, it is often more practical to measure sweating points, which represent the temperatures at which a solid begins to liquefy, rather than the true melting points. For alkanes, the difference between melting and sweating points is typically less than 10 degrees Celsius. Certain classes of organic compounds do not liquefy upon heating; instead, they sublimate, transitioning directly from the solid to the gas phase without passing through a liquid state.

The melting point constitutes a fundamental physical parameter of organic compounds. This temperature marks the transition from a solid to a liquid state under atmospheric pressure and is one of the principal properties listed in chemical dictionaries and reference texts. Knowledge of a compound’s melting point is also essential for selecting suitable refrigeration technologies and furnaces, with implications for safety management [13]. Within the solid state, the crystal features conform to the external shape of the compound’s molecules. The lattice parameters, and consequently the melting point, depend on molecular shape and the amplitude of intermolecular interactions. These influence both polymeric and associate molecular crystals and have a bearing on polymorphic transitions.

The boiling points of organic compounds exhibit a progressive increase with the addition of carbon atoms; an increase by approximately one carbon atom corresponds to a 20 to 30°C rise in the boiling point within the same homologous series, with the chain length accounting for 75 to 90% of the variation. This trend serves as a predictable guide for interpolations and extrapolations within each series. Branching generally lowers the boiling point since branched molecules, having smaller surface areas, experience weaker van der Waals forces-boiling points of branched isomers are typically 10 to 30 °C below those of their normal-chain counterparts [14].

Positions of functional groups in the carbon chain further influence boiling points f e. o. alcohols, the polarity of the hydroxyl group exerts the greatest effect. The polarization effect index (PEIOH) accounts for contributions from both the alkyl skeleton and the OH group's position. For normal alcohols, the difference in PEIOH between branched and normal structures is zero. Accompanying equations enable effective prediction of boiling points for a wide range of alcohols. The NPOH equation extends versatility to linear and branched organic compounds with functional groups situated along the alkyl chain.

Density is the ratio of mass of an object to its volume, which changes with temperature in solids and liquids because of expansion or contraction. It is expressed in grams per cm^3 or kg per m^3. Substances with densities less than that of water are more buoyant. Specific gravity or relative density is the ratio of the mass of a substance to the mass of an equal volume of water; therefore, specific gravity is a dimensionless quantity. Bomb calorimeters estimate the heat of combustion of a solid or liquid by determining the temperature rise in water. For example, the specific gravity of an oil lubricant is important because it determines the cooling effect of the oil on the parts lubricated. In the case of aircraft fuels, specific gravity is used to check the extent of contamination by water or other settled material.

The specific gravity of an organic liquid also provides a means of identifying it or assessing its degree of purity. The physical basis underlying almost every application of specific gravity lies in the relationship between the mass or weight of a body and its size or volume. The composition of the liquid being examined determines its specific gravity; the more carbon and hydrogen atoms it contains, the closer its specific gravity is to unity. Nonpolar compounds that have an oxygen, nitrogen, or chlorine atom generally behave as heavy molecules. Because of the low atomic mass of fluorine, an increase in fluorine content causes the specific gravity to decrease, unlike that produced by the other atoms.

The refractive index characterizes the optical properties of a compound by measuring the ratio of light speed in a vacuum to the velocity in a given medium [15]. Because the difference in thermal expansion coefficient between solid and liquid can introduce systematic errors [16], refractive indices are typically recorded at room temperature (20–25 °C) for organic liquids. Various methods are applied in pharmaceutical solids and optical materials, including near-infrared measurements, ellipsometry, and light scattering techniques. Tomographic and digital holographic microscopy provide detailed cell and material analysis. Measuring refractive indices of polymers and microspheres helps in understanding their optical properties. Dispersions across different wavelengths are also studied, aiding in the development of optical devices. Industrial applications include index matching in formulation chemistry to make materials transparent by matching the refractive indices of particles and the matrix. Moreover, the refractive index yields information on the mean molecular polarizability through the Lorentz-Lorenz relationship. London established that induced dipole interactions are closely linked to polarizability, even in neutral atoms and molecules.

With the speed of light in vacuum as c and its velocity in the medium as v, the refractive index (n) is defined as: $n = c/v$. The refractive index of a compound varies with wavelength due to dispersion.

Organic liquids exhibit a resistance to flow that is a manifestation of intermolecular forces, described mechanistically through the interactions, collisions, and repulsions between molecules [17]. Since inorganic liquids also show this behavior, the property is not unique to organic substances; nonetheless, viscosity remains an important physical characteristic of organic liquids.

The dynamic viscosity, η, is the force (per unit area) required to move a plane of liquid parallel to another plane at a unit velocity, separated by 1 cm. The units of η in the CGS system are poise (P), where 1 P = 0.1 Pa·s in the MKS system. The kinematic viscosity (ν) is the dynamic viscosity divided by the density (ρ) and is expressed in stokes (St), where 1 St = 10 m^2/s.

Heat capacity and thermal conductivity are also significant thermal properties of organic compounds. Heat capacity, expressed in units such as J·K- 1·mol- 1, indicates the amount of heat that a material can absorb without undergoing a substantial temperature increase. Thermal conductivity measures the material's ability to transmit heat. Table 10.1 summarizes the heat capacities and thermal conductivities of selected organic liquids [18].

Heat capacity transcends the framework of traditional physical properties by providing deep insight into an organic compound’s internal dynamics through a thermodynamic lens. It depends sensitively on the relief of steric constraints upon heating and serves as a sensitive indicator of intermolecular forces and molecular flexibility. These features significantly influence or can even supersede the effects of molecular weight and symmetry on physical and thermodynamic characteristics such as boiling points, vapor pressures, and phase equilibria. For certain compound families, heat capacity serves as the single most reliable predictor of thermodynamic properties and phase equilibria.

Material heat capacity determines the consequent temperature change following a known net heat transfer. Within engineering and synthesis, it governs transient temperature profiles arising from stepwise heat inputs and allows for temperature-time predictions in adiabatic systems. Industrially, it is crucial for the calculation of energy demands during conductive or convective cooling or heating processes. The temporal evolution of system pressure and temperature is particularly sensitive to the accuracy of heat capacity data, especially when equilibrium constants are strongly temperature dependent.

Extensive research over the past five decades has addressed the thermodynamic properties of organic compounds. The heat capacities of pure substances are intrinsically connected to phase equilibrium and vapor-pressure prediction models [19]. Heat capacity data can indirectly reveal the internal degrees of freedom and constituent interactions of a substance. Understanding these properties also facilitates the determination of unknown parameters for molecular structures that have yet to be synthesized or isolated [2].

Organic compounds exhibit a broad range of physical and chemical properties. Molecular and electronic structures, with principal participation of covalent bonding, are well understood and can be exploited in many applications. More challenging to predict are the changes in physical properties that accompany the transition from one class of organic compounds to another. Moreover, relatively little is known about the physical properties of organic compounds in the liquid, mixed liquid, solid, and, especially, supercritical states even though these states provide an interesting platform to associate molecular and electronic structures with both chemical reactivities and measurable physical properties, such as densities, dielectric constants, distribution coefficients, and solubilities.

Thermal conductivity of nano-structured polymer films is investigated experimentally, theoretically and numerically. The polymer films possess a complex structure consisting of aligned, interconnected, cylindrical-shaped nanofibers with different size distribution and length. The measured thermal conductivity of polymer films exceeds the reported value for individual nanofibers of a comparable diameter by an order of magnitude [20].

Several thermo-mechanical parameters such as thermal conductivity, thermal diffusivity, specific heat and heat capacity are integral to the characterization of materials. They have a wide spectrum of engineering applications such as thermal insulation, cryogenics, microelectronics, heat pipes, automobile industries and electronic industries. Most insulators used in the thermal industry are or have been organic-based materials due to the low thermal conductivity of long hydrocarbon chain polymers. The physics of thermal transport in macromolecular materials deserves attention for the exploitation of efficient applications [21].

The thermal conductivity of some orientational glasses of protonated and deuterated ethanol, cyclic substances, and freon 112 has been analyzed in the temperature range 2–130 K. The investigated substances demonstrate new effects related to the physics of disordered systems. Universal temperature dependences of the thermal conductivity of molecular orientational glasses have been revealed. At low temperatures, the thermal conductivity exhibits a universal behavior described by the soft potential model. At higher temperatures, the thermal conductivity shows a smeared maximum then decreases with increasing temperature, similar to behavior in crystalline structures [22].

Thermal-and thermo-mechanical-property measurement methodologies employed for characterizing materials with an emphasis on thermal energy storage materials are reviewed. The techniques discussed include axial heat flow (steady state), transient hot wire, transient plane source and laser flash systems. These methods have been widely used for studying the thermal properties of a range of polymeric composites systems containing highly thermally conductive fillers, such as boron nitride nanotubes and microflakes, graphene nanoplatelets and crystalline nanocellulose, metallic and ceramic hollow micro-spheres, cellular metals, metallic foams, micro-encapsulated phase-change materials, carbon-based nano-fibres, micro-fibres and shaped fibres, and hybrids of different fillers. Thermal transport in polymeric materials and across polymer-filler interfaces governs the development of efficient, thermally conductive, electrically insulating composites. Characterization methodologies of thermally conductive thermal-management materials are discussed.

Electrical conductivity and dielectric constant are important consideration for organic compounds. Pure water is a very bad conductor of electricity because it has very few ions. The conductivity of a solvent increases with addition of a solute that can ionize in solution to produce ions. Acetic acid (VC=72.5 ohm-1 cm-1 mol-1) has greater conductivity than chloroform (VC=2.3 ohm-1 cm-1 mol-1) because acetic acid ionizes in solution.

The dielectric constant (J9) is the important property in relation to the optical behavior of organic liquids and solids. It provides information about dipole moment and the nature of molecules. Electrical conductivity and dielectric constant are useful for predicting the properties of materials used in communication devices. The dielectric constant of alcohols is more than that for normal paraffins because of hydrogen-bonding present in the former.

Electrical conductivity is the physical property that electrically charged particles of a substance can move through the material in an electric field [23]. Electrical conductivity determines the ability of organic compounds to conduct an electric current. While conductivity of organic crystals for applications in electronic devices is limited, light-emitting diodes, field-effect transistors, and solar cells prepared from organic materials have become promising alternatives to those made from inorganic materials [21]. Dielectric constant defines the ability of a substance to insulate charges from each other and is measured as a ratio of the capacitance of a capacitor with the substance between the plates to the capacitance of the same capacitor with a vacuum between the plates. It is one of the most used physical parameters to study structural, compositional, and microstructural properties of materials. A mono-atomic carbon chain has the highest mechanical stiffness, the smallest width, and a tunable band gap. These chains can be obtained by unraveling carbon atoms from graphene ribbons. The formation of the chains is accompanied by a characteristic drop in the electrical conductivity. The conductivity of carbon chains is much lower than the one of ideal chains. Strain in the chains determines the conductivity in a decisive way. Carbon chains are always under a varying non-zero strain, which induces a band gap. Strain converts a chain from a cumulene to a polyyne atomic configuration, implying that both cumulenic and polyyne systems could coexist under appropriate conditions.

The dielectric constants of organic compounds determine their behaviour in electric fields, and are of particular interest because of the use of these compounds in electrical equipment. For instance, materials with high dielectric constants find wide application in electronic devices such as capacitors, wave guides, and electromagnetic reflectors. According to the mechanisms outlined in Section 11.5, the dielectric constants of dyes can reach exceptionally large values, as demonstrated by perylene dyes. Contrary to the expectation of a simple decrease with increasing molecular weight, these systems exhibit high dielectric constants due to the high polarizability of electrically neutral dyes with large conjugated systems, which render them suitable as dielectrics.

Organic compounds are ubiquitous in the materials that surround us. Understanding the physical properties of organic compounds is paramount in fields such as pharmaceuticals, materials science, and environmental science. Physical properties also facilitate the characterization and identification of materials. Intermolecular forces including dipole-dipole, hydrogen bonding, and van der Waals interactions govern many phenomena such as solubility, melting and boiling points, vapor pressure, viscosity, and surface tension. Measurement of these physical properties imposes constraints on theoretical models. Spectroscopic methods such as infrared and nuclear magnetic resonance spectroscopy provide means to directly probe molecular structure. Analytical methods including mass spectrometry, inductively coupled plasma emission spectroscopy, ultraviolet and visible spectroscopy, X-ray diffraction, and chromatography complement these techniques. Additional topics of concern encompass electrical conductivity and various chromatographic techniques. Three main classes of organic compounds inspired by historical use and organometallic chemistry include aliphatic, aromatic, and cyclic compounds. Bonding and geometry play central roles in determining the properties of organic compounds. Isomerism, which arises when molecular formulae do not uniquely specify molecules, is common given the diversity of molecular structures. Infrared (IR) spectroscopy employs infrared light irradiation to analyze compounds. The IR spectrum functions as a fingerprint to identify the presence or absence of specific bonds within a compound. Nuclear magnetic resonance (NMR) spectroscopy involves the absorption of radio waves by nuclei placed in a magnetic field. The NMR technique distinguishes isomeric compounds that proton NMR cannot, such as certain isomers of C8H10 and quinones. Different groups of carbons exhibit characteristic signals, enabling detailed structural analysis. Relevant functional groups appear in specific regions; for example, the methyl carbon typically resonates near 20 ppm, while aromatic carbons occur above 100 ppm. The presence of enol-keto tautomerism in compounds such as ethyl acetoacetate manifests in identifiable spectral features, enhancing the understanding of enolate chemistry. Multiplet structures in the 1H NMR spectrum of ethyl crotonate allow deduction of coupling constants and geometrical isomerism of the alkene moiety. Mass determination and elemental analysis are often the initial steps in elucidating chemical composition and formula. Electricity and electrical circuit frameworks provide analogs for understanding organic molecules far from equilibrium. Atomic and molecular properties, including ionization potential, electron affinity, and chemical hardness, govern the direction of chemical reactions. The corresponding states principle facilitates prediction of thermodynamic properties of gases using experimentally determined properties of a single gas and a universal compressibility factor table. Torsional potential energy barriers dictate rotational isomer populations. Collective descriptions of molecular states smell of selective entropy, wherein reduced entropy drives molecular self-organization. Group contribution methods can calculate thermodynamic properties such as Gibbs energy, enthalpy, and entropy. Distributed Machine Learning and evolutionary algorithms have been applied to the inverse design of organic molecules based on properties such as refractive index and dielectric constant. Density functional theory calculations, combined with machine learning, expedite prediction of melting points, heat capacities, and vaporization properties. Organ-on-chips demonstrate the potential to benefit from technologies centered on the physical properties of organic compounds. Drag and heat transfer in rarefied hypersonic flows with chemical reactions have been investigated using direct simulation Monte Carlo analyses coupled to reaction mechanisms for air and fuels [24, 25].

Infrared (IR) absorption occurs when the energy of incident radiation matches the energy required to excite a molecular vibrational mode. The frequencies at which such changes occur reflect the type of vibration and are characteristic of particular atoms and their environment, permitting deduction of molecular framework and complementing techniques such as nuclear magnetic resonance (NMR) and mass spectroscopy [26, 27].

Nuclear magnetic resonance (NMR) has become the primary technique for determining the structure of organic compounds, with the ability to analyze spectra for complete interpretation. NMR is non-destructive and effective from small sample sizes. The nuclei of many isotopes, particularly 1H, 13C, 19F, and 31P, have spin states of I=1/2, which are crucial for NMR analysis. The phenomenon relies on spinning charges generating magnetic fields, creating a magnetic moment. In an external magnetic field, two spin states (+1/2 and −1/2) exist, with energy differences dependent on the field strength. Modern NMR spectrometers use strong magnetic fields (1 to 20 T), since the energy difference is minimal, typically expressed as a frequency in MHz. These small energy differences are much less than those involved in infrared and electronic transitions [25].

Mass spectrometry (MS) is a fundamental technique to determine the mass of molecules and perform quantitative analysis of chemical species. All mass spectrometers comprise three basic components: an ion source where neutral molecules are ionized; a mass analyzer where ions are separated by their mass-to-charge (m/z) ratios; and a detector that measures the relative abundances of ions to produce a mass spectrum [28]. In the ion source, neutral molecules are ionized under vacuum and transferred to the mass analyzer as molecular or fragment ions, along with nuclei or electrons.

Mass spectrometers generally fall into two groups: scanning instruments and ion trapping mass spectrometers. Scanning instruments, such as magnetic sectors and quadrupoles, manipulate ions while they pass through the analyzer. Ion trapping analyzers, including quadrupole ion traps and Fourier-transform ion cyclotron resonance (FT-ICR) instruments, confine ions within the same spatial region, using electric fields for storage and manipulation [29]. All types of mass spectrometers can perform single-stage MS to determine molecular weights and elemental compositions. When coupled with suitable dissociation methods, tandem mass spectrometry (MSn) enables structural analysis through the isolation of ions and subsequent collision-induced dissociation. Collision-activated dissociation (CAD) is widely employed to induce bond cleavage and extract structural information.

In practice, mass spectrometric analysis involves three main phases: sample evaporation and ionization; separation of ions according to their m/z values; and detection of the separated ions. Trapping mass analyzers like linear quadrupole ion traps (LQIT) and FT-ICR systems offer high sensitivity and resolution by confining ions to a specific region. Scanning analyzers direct selected ions along distinct paths for m/z separation prior to detection. The availability of diverse geometries and methods for generating ion motion enables instruments to tailor experimental conditions to a wide range of analytical objectives.

The physical properties of organic compounds are widely used in pharmaceuticals (e.g., sensing the concentration of an active pharmaceutical ingredient in solution), materials science (e.g., measuring specific gravity to determine additives or contamination in a liquid), environmental science (e.g., quantifying volatile organic compound emissions), and many other areas. The vast majority of these applications rely on the connection of polyatomic structure to physical property; consequently, one property cannot be employed for the wide variety of applications that physical properties generally span.

Thermodynamics is concerned with the relations between heat and mechanical energy or work, and the conversion of one into the other. Investigation of vaporization enthalpy and vapor pressure is important to disciplines such as chemical engineering, manufacturing, pharmaceuticals, environmental science, and technology development. Vaporization enthalpy corresponds to the energy required to transform a liquid into a gas, and vapor pressure is the pressure exerted by a vapour in thermodynamic equilibrium with its condensed phases at a given temperature [2].

An important application of organic compounds lies in the pharmaceutical industry. Active pharmaceutical ingredients (APIs) and excipients often contain extensive organic portions, forming the basis for tablets and injections and for additional formulation into suspensions and medicated liquids.

In pursuance of APIs with suitable biopharmaceutical properties, an understanding of physical properties can assist in the design of appropriate molecules and help identify adequate syntheses of chosen compounds. Often, selection among a number of serious candidate molecules follows miniaturized protocols of solubility screening, thermal resistance, and re-crystallisation in various solvents. A variety of tablets and formulations has been tested extensively in head-to-head comparisons of physical properties. Correlations of the physical properties of molecules and designed generally as quantitative structure–property relationships (QSPRs) have appeared. Although adoption has not been widespread, QSPRs do offer a means of preliminary comparison and ranking of molecules. Physical properties deliver valuable, often unique, information on a molecule, which spread across many fields of interest [30].

By adjusting pressure loading and rotation speed, catalyst material can undergo phase transformations that significantly impact catalytic activity without permanent structural changes. This principle is exemplified in supported Pt nanoparticles for ammonia oxidation; small Pt particles (<2 nm) achieve equilibrium between metallic and surface-oxide phases, with the metallic phase being catalytically active. Pressure variation alters the cycle between kinetic regimes because the transformation conditions differ between high- and low-activity states. Consequently, fluctuations in catalytic activity persist over a broad pressure range, a phenomenon expected to extend to other catalytic systems undergoing pressure-induced phase transformations of metal catalysts or supported catalytic materials. Recognizing these mechanisms yields insights into catalytic-activity oscillations across sectors such as materials science, heterogeneous catalysis, and geochemistry [2].

Volatile organic compounds (VOCs) emitted by plants during summer—terpenes and sesquiterpenes, for example—interact with sunlight and atmospheric species to produce smog [2]. An important class of VOCs is semi-volatile organic compounds (SVOCs), typically pesticides and plasticizers such as phthalates from building materials and polybrominated diphenyl ethers (PBDEs) from furniture. Although these SVOCs have low vapor pressures and tend to reside mostly in the gas phase at outdoor temperatures, many are distributed between the gas phase, airborne particles and surface materials in indoor environments, where they contaminate indoor air and house dust. Numerous studies indicate that indoor dust contains SVOCs at concentrations several orders of magnitude above those in outdoor air.

The study of the physical properties of organic compounds relies on an understanding of the classification of organic compounds, molecular structure, and the forces active within and between molecules. Organic compounds are classified as aliphatic, aromatic, or cyclic. The molecular structure is discussed in terms of geometry and the types and effects of different types of isomerism. The consequently arising intermolecular forces, including hydrogen bonding, van der Waals and dipole–dipole forces, are treated in detail, along with their influence on the physical properties of organic compounds. The solubility of organic compounds is largely determined by the strength of the intermolecular forces that can be formed between the constituent molecules and the molecules of the solvent. The melting and boiling points of organic compounds are related to the magnitude of these forces and various trends are highlighted. Density and specific gravity tend to increase as the molecular weight of the compound increases. The principles of refractive index are described, as is the manner in which it varies with molecular structure. Viscosity is another property related to the magnitude and extent of intermolecular forces, and it tends to increase as the number of intermolecular bonds possible increases. The physical properties of heat capacity and thermal conductivity are discussed. Electrical conductivity and the dielectric constant depend on molecular structure and symmetry and both can be correlated with those large-scale properties from which they were derived. The spectroscopic methods most frequently used to correlate the physical properties of organic compounds with their molecular structure are considered. These include infrared spectroscopy, nuclear magnetic resonance and mass spectrometry. The physical properties of organic compounds find application in fields as diverse as pharmaceuticals, materials science and environmental science.

The physical properties of organic compounds are significantly influenced by their molecular structure. Consequently, the arrangement of atoms and the types of bonds within a molecule play a crucial role in determining its reactivity. As summarized in the following sections, these intricate relationships have been systematically exploited to enhance both the efficiency of synthesis processes and the selectivity of the resulting compounds. This evidence underscores the paramount importance of thoroughly understanding the intimate connection that exists between molecular structure, the various properties exhibited by organic compounds, and the reactions they undergo. Such comprehension is vital for advancing the field of organic chemistry and improving synthetic methods [3, 30, 31, 32].

4.1 Boiling and Melting Points

The physical properties of organic compounds are closely related to their molecular structure. A notable example is the trend in boiling points demonstrated by two series of hydrocarbons: paraffins and alkylbenzenes. Within each family, boiling points rise with increasing molecular weight due to augmented surface area and enhanced van der Waals forces. For a given hydrocarbon weight, alkylbenzene boiling points surpass those of the paraffins because the polarizable benzene ring exerts stronger van der Waals forces than methyl groups. Furthermore, a molecule’s shape influences its boiling point; symmetrical molecules occupy less surface area, weakening van der Waals forces and thereby reducing boiling points.

Melting points are influenced by several factors, including molar mass, symmetry, and polarity. It is observed that an ascending molecular weight correlates with higher melting points, particularly noted in n-alkanes. As the molecular weight increases, the melting points tend to rise accordingly. Increased polarity further contributes to elevated melting points by enhancing dipole–dipole interactions between molecules. Additionally, symmetry plays a crucial role in governing the trends associated with melting points; highly symmetrical molecules tend to exhibit significantly elevated melting points as their geometric configurations allow for more efficient packing when transitioning into solid states. A prime example of this principle can be seen with benzene, which serves as an illustrative case within the realm of hydrocarbons. Although benzene has a comparatively low boiling point among the C_6 hydrocarbons, it possesses a surprisingly high melting point primarily due to its remarkable symmetry, which favors dense solid formation [33, 34, 35].

4.2 Solubility

Solubility describes the process by which a solid, liquid, or gas forms a solution in a liquid solvent and is frequently considered a fundamental property of matter. The dissolution process is governed by the balance between intermolecular forces that hold the solute molecules or ions together and the solvation forces that develop between the solute and solvent. Substances with similar intermolecular forces tend to form solutions together, a general rule often expressed as "like dissolves like" [29]. Organic compounds are usually more soluble in organic solvents than inorganic ones; nevertheless, exceptions exist. For example, even though alcohols exhibit dipole–dipole interactions, their solubility curves common with hydrocarbons rather than with simple oxygen-containing molecules [36]. Carbon tetrachloride (CCl4) ranks among the prime organic solvents for nonpolar solutes, yet its molecules possess a large dipole moment generated from the polar carbon–chlorine bonds.

A preliminary approach to the solubility of a substance in a solvent assumes that both are solids at the temperature of interest. The interatomic or intermolecular forces that affect the energy of melting or vaporization, formation of a solution, and solubility at a given temperature can be correlated quantitatively with thermodynamic considerations.

The solubility of a substance in a particular solvent depends on the magnitude of the intermolecular forces in both the pure components and the solution; the stronger the attractive forces, the larger the energy required to separate the molecules, and the lower the solubility. In general, relatively large molecules tend to have smaller solubilities than smaller analogues; this difference arises, at least in part, from a much larger ratio of surface area to molecular volume for the smaller molecules. A large surface-to-volume ratio introduces a higher adsorption energy per gram of adsorbent, and hence stronger interaction between adsorbed molecule and solvent molecules.

The solubility of amides in alkaline sodium borohydride solutions is notably influenced by the complex interplay between the relative strength of the chromophoric group and the specific characteristics of the solvent being used. In environments where a suitable solvent is present, amides engage in reactive processes with sodium borohydride, leading to the formation of hydrogen gas, a urea-NaBH4 complex, which ultimately yields urea upon hydrolysis, along with lesser quantities of ammonia as byproducts. For instance, when benzamide interacts with sodium borohydride, the reaction produces not only hydrogen gas, but also benzonitrile, and a small amount of the compound known as 2,4,6-triphenyl-s-triazine. This demonstrates the interesting chemistry of amides and their reactions in alkaline conditions, emphasizing the importance of the solvent and the chromophoric groups in determining the pathways and products of these reactions.

Chapter - 5

Chemical Properties of Organic Compounds

The chemical properties of organic compounds describe their reactivity toward other chemical compounds and the way these compounds react. Many organic compounds do not dissolve in water because their molecules possess similar intermolecular forces to those possessed by the sample molecule. For a molecule carrying dipole–dipole moments, the molecule or sample also exhibits dipole–dipole moment. Thus, in order to dissolve in water, which is polar in nature, the molecule must be polar or possess dipole–dipole moments. However, for molecules that possess induced dipole moments, such as alkanes, they only dissolve in solvents that also possess induced dipole moments (nonpolar in nature). When an organic compound can be classed as either an acid or a base, the tendency towards either behavior is commonly defined by the pKa of the conjugate acid. Such compounds are generally polar and interact with water via dipole–dipole moments and hydrogen bonding.

Certain groups of organic compounds exhibit distinct and specific reactivities, which greatly facilitates the prediction of the products formed in various chemical reactions. These specific groups of compounds are referred to as functional groups. For instance, organic compounds that contain these functional groups undergo well-defined and characteristic types of reactions, such as nucleophilic substitution reactions, acid-base reactions, or even additions to double bonds. Similarly, the elements and participants involved in reaction mechanisms are also defined by the presence of these functional groups, which include key players such as nucleophiles, electrophiles, leaving groups, free radicals, carbocations, carbanions, and carbenes. Numerous common reactions that are frequently encountered in most organic chemistry textbooks include processes such as the transformation of alcohols into alkyl halides, the attacks on electrophilic alkenes, and the substitution reactions of aromatic compounds. When the aforementioned types of reactions occur, products are always formed as a result of the reactions taking place. Consequently, the careful selection of particular reagents will ultimately result in the formation of the desired final product in the reaction. Furthermore, reactions can be broadly classified into several categories, which include addition reactions, elimination reactions, and substitution reactions. This classification is crucial for understanding how different types of reactions can yield various products that are fundamental to organic chemistry [31, 3, 37, 38].

5.1 Reactivity Patterns

The reactivity of organic compounds can be rationalized in terms of just a few reaction types. Alkene and alkyne π bonds are reactive because the π electrons lie outside the axis between the two C atoms and are therefore relatively loosely held. Further, they can easily be shared with another atom (a Lewis acid) because of the presence of loosely held electrons.

A few general principles can be used to predict the products of homogeneous and cross-coupling reactions. Metal-containing species (such as transition metals in relatively low oxidation states; Pd(0) and Ni(0) are the most common) able to do oxidative-addition reactions are excellent candidates to insert selectively into a C–X bond under mild conditions. The net result is the formation of a discrete metal-containing reagent via oxidative addition, a reaction that can be used to generate a variety of organic-metallic species from simple organic halides or triflates (e.g., R–X).

Many of the organic-metallic reagents that have served as crucial coupling components in various chemical reactions are notably sensitive to the presence of water and air, which significantly limits their overall utility in practical applications. This sensitivity poses challenges when researchers and chemists seek stable reaction conditions. Generally speaking, the more reactive the reagents are, the less stable they tend to be, which has historically been a particular and significant problem for the initially generated organomagnesium (Grignard), alkyllithium (RLi), alkyltin (R3Sn–X), and alkylzirconium (ZrR4) reagents utilized in organic synthesis. When carbonyl addition occurs, it yields a functionalized metal alkoxide, emerging at the carbon atom that is directly attached to the metal center in a distinctly anti-Markovnikov orientation. Furthermore, certain reactions in this realm, which include nucleophilic substitutions, nitrations, Bamberger rearrangements, and Diels–Alder or ene transformations, frequently produce tertiary carbon stereogenic centers that can be pivotal in determining the outcome of synthetic pathways. It's important to note that, although Eu(fod)3 induced shifts represent a fascinating area of study, they are not entirely equivalent to the behavior of a traditional catalytic shift reagent; rather, the proton signals observed are not selectively shifted in a manner that closely reflects steric accessibility. Consequently, this technique does not provide clear or unequivocal evidence of conformational homogeneity among the compounds studied, thus posing an obstacle in thoroughly understanding the potential complexities of these reactions [6, 39, 40, 41, 42].

5.2 Acid-Base Properties

Although acid-base interactions play an important role in all facets of chemistry-organic chemistry included-particularly in the behavior of amino acids and many enzyme-catalysed reactions, this section is, for the most part, brief. It simply presents the terms broadly employed to describe electron-transfer reactions and discusses the behavior of organic compounds as either acids or bases. The importance of hydride transfer in many organic reactions is a notable exception.

The involvement of various organic compounds in different electron-transfer processes is covered in much greater detail in the extensive Mechanisms of Organic Reactions section. In this section, acid-base reactions are analyzed and viewed from both the definitions that arise from such involvement, and also in terms of practical considerations that can significantly affect the most common species typically encountered in the majority of organic syntheses conducted in the laboratory. It is important to understand how these processes interrelate with one another to gain a clearer picture of organic chemistry overall [43, 44, 45, 46].

Chapter - 6

Types of Organic Reactions

Organic reactions are classified into types according to the overall result of the reaction, and each type contains many specific named reactions. Common classes include addition reactions, elimination reactions and substitution reactions. Although these categories are often taught as separate classes, a single reaction can belong to multiple types. Addition, elimination and substitution reactions represent the main categories that are covered when the term 'organic reaction' is used.

Addition reactions across double or triple bonds 67e caused by the breaking of bonds in unsaturated molecules and the formation of two new single bonds 67can be explained by the losses in energy that often accompany the strengthening of bonds during such reactions. Molecular rearrangements involve changes to the covalent structure of a molecule without changing its molecular formula [5]. Isomerization involves the conversion between isomers. Rearrangements can be classified by the number of atoms that move within a molecule, the size of a ring that opens or forms, or the origin (ring or open-chain) of the compound [6]. Rearrangements have also been classified based on whether they involve carbocationic rearrangements, alterations in electron systems or simultaneous migration (if more than one substituent moves on one main structure). In addition, organic reactions are divided into functional group transformations and carbon-carbon bond-forming reactions [36].

6.1 Addition Reactions

Addition reactions occur between alkenes and either electrophiles or reagents that can be converted to electrophilic species. The reaction can proceed spontaneously when the alkene is electron-rich or when the additional reagent is particularly reactive. However, if the alkene lacks electron density or the reagent is relatively unreactive, the reaction will not proceed without the help of a catalyst. Addition reactions can proceed through either free-radical or ionic mechanisms [6].

In a typical free-radical mechanism, the initial step involves the homolytic cleavage of a bond in the reagent. This step often requires activation by heat, light, or a radical initiator, generating radicals that subsequently react with the alkene. One example is the reaction of HBr with alkenes in the presence of peroxides, which leads to the formation of alkyl bromides through a radical chain process, a notable exception to the general rule of addition reactions.

6.2 Elimination Reactions

Elimination reactions, commonly encountered in organic chemistry, involve the removal of two substituents along with the formation of a multiple bond. Consider, for example, the reaction of 2-bromopropane with hydroxide ion. A bromide and a β-proton are replaced by a new π bond, yielding propene. The net change in the reaction is loss of two substituents accompanied by the generation of a double or a triple bond.

Whereas addition reactions always increase the number of substituents on a double bond, elimination reactions subtract substituents and generate multiple bonds. Elimination reactions are therefore the microscopic opposite of addition reactions.

The Hofmann rule states that amines or quaternary ammonium salts usually give the less substituted alkene product.

Thus, when an amine is treated with nitrous acid, the Hofmann elimination provides an alkene with the double bond located next to the amine group.

Halides usually produce more substituted alkenes, leading to a predominance of alkyl halides according to the Zaitsev rule. Hence, the hydrohalogenation of alkynes generally furnishes cis- and/or trans-substituted alkenyl halides. The hydrolysis of alkoxyl groups on oxiranes generates halohydrins under SN1-like conditions [47].

6.3 Substitution Reactions

Substitution reactions represent a crucial and significant class within the realm of organic reactions. This particular class involves the replacement of an atom or a group of atoms, referred to as the functional group, by another atom or group of atoms in various molecular contexts. Substitution reactions not only stand out as a major category in organic chemistry but also play a pivotal role in numerous other types of reactions, which often incorporate substitution steps throughout their mechanisms. Thus, having a thorough and clear understanding of this class of reactions is beneficial and essential for anyone studying organic chemistry.

To better comprehend substitution reactions and their significance, it helps to organize them by outlining the two broad categories that encompass all organic reactions. The first class is composed of reactions where two separate molecules come together to form a larger, more complex molecule. This often involves the addition of a new functional group to an existing double or triple bond within one of the reacting molecules. These kinds of reactions are classified under the umbrella of addition reactions.

On the other hand, there exists a second class of organic reactions where the focus shifts towards the removal of an atom or a functional group from a molecule. In these reactions, the breaking of a double or triple bond occurs, leading ultimately to the formation of two smaller, distinct molecules. These reactions are known as elimination reactions.

Importantly, a broader category encompasses many types of organic reactions, where one particular functional group is substituted with another, leading to a diverse range of chemical transformations. This area captures the essence of substitution reactions, which are integral not only in synthetic organic chemistry but also in a variety of biochemical processes. Moreover, it is noteworthy that many additional reaction mechanisms utilize substitution reaction steps, highlighting their versatility and widespread application.

Furthermore, a specific mechanistic feature of conjugate substitution reactions is particularly interesting and significant. In these reactions, the methyl substituent exhibits a unique behavior by leaving the molecule simultaneously while a nucleophile is added to the allylic position. This process allows for the recovery of extended conjugation, which is a key aspect of the overall chemical transformation. By understanding these intricate details, one can gain deeper insights into the dynamics of substitution reactions and their importance within the broader context of organic chemistry [23, 48, 3, 49, 50].

Chapter - 7

Mechanisms of Organic Reactions

Understanding the mechanisms by which organic reactions occur is an important aspect of organic chemistry. A reaction mechanism describes, at the electron level, how an organic reaction occurs and how bonds are broken and formed during the overall reaction.

Organic reactions often occur at sites where molecules are electron-rich or where they are electron-poor. Understanding how reactions take place can therefore be assisted by categorizing them according to the electron density changes that occur. For instance, nucleophiles are electron-rich molecules or sites within molecules, while electrophiles are electron-poor, electron-deficient molecules or sites within molecules. Organic reactants or sites within reactants are nucleophilic when synthesis involves donation of electrons from the reactant to the product. In contrast, the reactant or site is electrophilic when the product is formed by donation of electrons from the other reactant to the reactant or reactive site.

7.1 Nucleophilic Substitution

In nucleophilic substitution, a nucleophilic species forms a bond with a carbon atom while concurrently replacing a leaving group that was previously attached to that carbon atom. Because this substitution process replaces one functional group with another, chemists often refer to these types of reactions as "exchange" reactions. The central task in any nucleophilic substitution mechanism is to effectively break the bond that exists between the carbon atom and the leaving group, subsequently forming a new bond between the carbon atom and the nucleophile. There are two primary mechanisms that accomplish this important task. The first mechanism is known as unimolecular nucleophilic substitution, abbreviated as SN1; the second mechanism is called bimolecular nucleophilic substitution, commonly referred to as SN2. Unimolecular nucleophilic substitution proceeds in a sequence of two distinct steps (as illustrated in Figure 7.1). In the initial step, the bond between the carbon and the leaving group is broken, leading to the formation of a reactive species known as a carbocation. This unstable intermediate possesses only six electrons within its outer shell, rendering it electron deficient and planar in shape. In the second step of the process, the carbocation, which is quite reactive, is then attacked by the nucleophile to ultimately form the desired organic product. This reaction pathway is essential for many chemical transformations and plays a significant role in synthetic organic chemistry [51, 52, 53, 54].

7.2 Electrophilic Addition

Electrophilic addition contributes to many reactions of compounds that contain π bonds. In these reactions, an electrophilic reagent adds to the π bond to make a carbocation intermediate. The carbocation then loses a proton to generate a product with an additional substituent on each of the carbons formerly involved in the π bond [55]. The limited stability of the carbocation intermediate governs many of the characteristics of such additions.

Molecules that contain multiple double bonds tend to exhibit a variety of complex reactivity patterns that can be quite interesting. In certain molecules, multiple double bonds adopt specific positions in which they are linked exclusively through a single σ bond, which are commonly referred to as conjugated dienes. The unique resulting electronic structure of these molecules makes them especially reactive when exposed to electrophilic reagents. Most electrophilic addition reactions typically involve the addition of the "H" portion of an electrophilic reagent to the doubly bonded carbon that initially has fewer attached hydrogens. This mode of addition is specifically known as Markovnikov selectivity, highlighting the preference for adding to the less hindered carbon. Additionally, a limited number of reagents, which includes hydroboration as will be described later, add negatively charged portions to the carbon that initially had fewer hydrogens, demonstrating another layer of reactivity in such molecular systems [56].

Chapter - 8

Synthesis in Organic Chemistry

Synthesis constitutes a fundamental facet of organic chemistry, representing the construction of organic compounds from simpler organic or inorganic precursors. The synthetic challenge resides in achieving the desired product in a timely, selective, and cost-effective manner. Practical approaches incorporate retrosynthetic analysis, wherein the target molecule is recursively deconstructed into simpler precursors that are either commercially viable or readily synthesizable from other compounds [5].

Large molecules pose a considerable synthetic conundrum that researchers frequently encounter in the chemistry field. The presence of multiple functional groups, each potentially capable of engaging in a variety of chemical reactions during each synthetic step, compels the use of protecting groups to avoid unintended reactions. These protecting groups strategically render a specific functional moiety inert to the intended reaction, thereby facilitating the transformation of other functional groups that are present in the molecule. In many cases, alternative strategies that effectively obviate the need for the deployment of protecting groups are favored if they prove to be feasible and efficient in the synthetic process [28].

8.1 Retrosynthetic Analysis

Retrosynthetic analysis, a significant procedural technique first introduced by the renowned chemist E. J. Corey in 1967, serves as an invaluable problem-solving approach employed in the intricate design of organic syntheses. The essence of this technique lies in its ability to facilitate the transformation process, wherein the complex structure of a target molecule is dissected into progressively simpler precursor structures. This iterative transformation continues until the chemist can identify starting materials that are either simple to procure or already available commercially, thus streamlining the synthetic pathway.

Each precursor structure identified in this method represents a crucial potential synthetic operation, providing various routes to the final target molecule. To achieve an accurate retrosynthetic analysis, an intelligent algorithm capable of effectively solving the subgraph isomorphism problem is essential. This requirement arises because numerous reactions can belong to the same overarching type; these types are specifically concerned with the intricate transformations involving functional groups. In the field of organic chemistry, the different types of reactions are frequently represented through a shorthand notation system, wherein molecular segments that do not actively participate in the reaction processes are conveniently replaced by "R" groups. Distinctions between varying non-essential segments of these reactions are often indicated through the use of tick marks.

For instance, in reactions like Claisen condensation, the ester groups involved prominently dominate the reactant structure, while the accompanying R groups serve to denote the non-crucial or ancillary parts of the functional group under consideration. In the contemporary landscape of organic chemistry, methods for predicting various organic reactions are predominantly reliant on rules derived from experimental data. These experimentally determined rules are meticulously stored within extensive reaction databases, which not only serve as a repository of information but also constitute the foundational basis necessary for understanding the requisite steps and specific needs associated with diverse chemical reactions. Through this process, chemists are equipped to navigate the complexities of organic synthesis with greater efficiency and insight [14, 57, 58, 59, 60].

8.2 Synthetic Strategies

Synthesis, which involves constructing target molecules from simpler precursors, plays a vital and significant role within the expansive discipline of organic chemistry. The thoughtful design of an efficient synthesis is crucial as it addresses how to effectively assemble a particular molecule from readily available organic compounds. This process also involves careful consideration of several factors, including the precursor materials that will be used, the specific steps that are required to reach the desired target structure, and practical constraints that include reaction compatibility, reagent compatibility, energy requirements, yield, safety, and cost. The overall strategic approach for building complex target molecules significantly depends on the type of product being synthesized and the specific synthetic goals that are to be achieved. For instance, when considering the synthetic strategies employed for fine chemicals—such as those that are utilized as catalysts, cosmetic ingredients, or pharmaceuticals—there is often a strong emphasis on maximizing product yield and selectivity. Additionally, these strategies prioritize the minimization of by-products, materials, and the number of synthetic operations required throughout the process. In contrast, the synthesis of polymers may concentrate more heavily on effectively controlling the distribution of molecular weight within the resulting products. Although the field of organic chemistry encompasses a diverse multitude of different reaction types, it is noteworthy that the number of fundamental transformations that remain viable for final synthetic planning is relatively limited. Though the total synthesis of complex structures often demands exceptionally challenging strategies and innovative methodologies, it particularly excels in important areas such as structural elucidation, drug development, and scalability. These domains highlight the profound impact that well-planned synthetic approaches can have on advancing both scientific knowledge and practical applications in chemistry and related fields [14, 61, 62, 63, 64, 65].

Chapter - 9

Spectroscopic Methods

Chemists use spectroscopic methods to analyze organic compounds [66]. Nuclear magnetic resonance (NMR) spectroscopy allows researchers to study molecular structure and demonstrates the abundance and arrangement of atoms within a compound [67]. Mass spectrometry (MS) provides information on the molecular mass of a compound and analyzes its fragments.

Organic compounds with polar bonds absorb electromagnetic radiation at particular frequencies. The pattern of absorbance, called the spectrum, can identify functional groups and other structural features.

9.1 Nuclear magnetic resonance spectroscopy

Nuclei with an odd number of protons (and neutrons) possess a spin that generates a magnetic field. When placed in an external magnetic field, these nuclei resonate at a specific frequency dependent on the chemical environment surrounding the nucleus. This principle underpins nuclear magnetic resonance (NMR) spectroscopy. Because both the wavelength and the materials used for the coil determine the frequency at which the coil resonates, different coils are required for work in different frequency ranges. The way that protons with different chemical environments interact with each other provides detailed structural information. Heteronuclear NMR uses nuclei such as 13C, 19F, or 31P, which have nuclear spins and a reasonable natural abundance. A 1H NMR spectrum can provide extensive information about the structure of an organic compound.

Elements such as nitrogen, sulfur, and oxygen, which lack magnetic nuclei, can still influence the spectrum.

Deuterium at low levels within a deuterium-locked instrument remains undetectable and therefore invisible; this phenomenon makes it necessary for NMR solvents to incorporate this specific isotope of hydrogen. By doing so, it effectively prevents the solvent peaks from overwhelming and dominating the 1H NMR spectrum, allowing for clearer analysis. All commonly used NMR solvents are at risk of oxidation when exposed to oxygen. This exposure leads to the formation of peroxides, which can be potentially explosive and pose significant safety hazards. To mitigate this risk, it is crucial to remove oxygen from the system as thoroughly as possible, thereby minimizing the chances of dangerous reactions. In addition, modern NMR software packages have advanced features that enable them to automatically apply a baseline correction. This correction helps to minimize signal distortion that can arise from off-frequency signals or inaccurate phase adjustments that could skew the results. Furthermore, performing shimming before commencing a run can greatly enhance the uniformity of the magnetic field and improve the overall quality of the spectral data obtained. Importantly, no Doppler broadening is present in NMR spectra due to the fact that the sample remains stationary within the magnetic field throughout the duration of the analysis. In contrast to other techniques, the resolution in NMR spectroscopy primarily depends on the precision associated with the magnetic-field setting itself [68, 69, 70, 71].

NMR spectroscopy can be valuable in identifying the hydrogen positions in alkenes; for instance, a triplet resonance at around 1.4 ppm corresponds to a methyl group, while a triplet at about 5.4 ppm indicates a vinyl proton.

9.1 NMR Spectroscopy

NMR spectroscopy is widely regarded as the technique of choice through which precise molecular connectivity is determined in both organic and biological systems. The primary aim of this powerful technique is to elucidate the intricate structure of a compound based on a one-dimensional frequency plot that can be analyzed. This plot translates into an intensity mode, wherein detailed spectra are generated through the application of a Fourier transform to the experimental data collected. The very first report of nuclear magnetic resonance (NMR) for the specific purpose of structure elucidation was given by the physicist Isidor Rabi back in 1939. The expansive field of study surrounding NMR, which was originally known under the name of molecular beams, continues to be published and discussed under that same relevant heading by the American Chemical Society as well as various other academic journals. The majority of the foundational early development of NMR spectroscopy was undertaken during the transformative time periods of the 1940s and 1950s. Therefore, the identification and understanding of molecular structure remains the central purpose of spectroscopic analysis today. Such choices and techniques have been readily available to organic chemists for over 150 years through a variety of other techniques, such as mass spectrometry, infra-red (IR) spectrometry, and ultraviolet–visible spectroscopies. Furthermore, the ability to work backward from the final products to the initial precursors through a systematic set of straightforward and reproducible steps is a critical skill that needs to be developed through comprehensive practical organic chemistry training and education [67, 66, 72, 73].

9.2 Mass Spectrometry

Mass spectrometry (MS) has undergone significant evolution since its initial discovery in 1913, transforming into a widely recognized and extensively utilized analytical technique, particularly suited for organic compounds. All mass spectrometers are fundamentally composed of three principal components: an ion source, a mass analyzer, and a detector. Within the ion source, neutral molecules are subjected to ionization; the resulting ions are then meticulously separated in the mass analyzer based on their mass-to-charge ratios. The relative abundances of these individual ions are subsequently measured by the detector and converted into a mass spectrum, which provides critical information. Mass spectrometers can be categorized into two main types: scanning instruments, such as magnetic sectors and quadrupoles, which have the ability to manipulate ions of different mass-to-charge ratios concurrently, and ion-trapping instruments, like quadrupole ion traps and Fourier-transform ion cyclotron resonance, where ions of varying mass-to-charge ratios are stored and manipulated within the same physical space but at different times. All of these instruments are capable of performing single-stage analyses to accurately determine molecular weights and elemental compositions. Furthermore, they can conduct tandem mass spectrometry (MSn), wherein ions of preselected mass-to-charge ratios are isolated and then subjected to a diverse array of reactions. One particularly important example of such reactions is collision-activated dissociation (CAD). This process generates fragment ions that often contain invaluable structural information essential for further analysis. Consequently, tandem mass spectrometry has emerged as the most versatile and widely applicable variant of mass spectrometry for the purpose of organic structural analysis, offering immense potential for researchers and scientists in the field [74, 75, 76, 77, 78, 79].

9.3 Infrared Spectroscopy

Infrared spectroscopy serves as a crucial analytical technique widely utilized in the realm of chemical research, providing deep insights into molecular structure and dynamics through both vibrational and rotational transitions. Upon exposure to infrared radiation, molecules interact with the energy in a manner that leads to frequency-specific absorption. This phenomenon results in intensities that are intricately related to the specifics of vibrational displacement as well as variations in molecular changes occurring within the sample. The characteristic frequency of absorption is inherently dependent on the unique structure of the molecule in question. As such, a careful and thorough analysis of these absorption frequencies can reveal the precise and intricate nature of an unknown compound.

At the core of infrared spectroscopy lies the fundamental principle that there is a direct correlation between the variations in molecular dipole moments and the absorption phenomenon of infrared radiation. In essence, any vibrations or rotations that lead to alterations in the dipole moment of a molecule will allow that molecule to effectively interact with the infrared light being used in the analysis. One of the significant advantages of employing infrared spectroscopy as an analytical method is rooted in its fundamentally non-destructive nature. This means that the amount of material required for analysis is exceedingly small—typically only a few milligrams—thus enabling the technique to study even very small quantities of material successfully. Importantly, the samples analyzed can often be subjected to additional types of analysis afterward, without experiencing any significant loss, due to the fact that they are only minimally destroyed in the process [80, 81, 82, 83, 8, 84].

Chapter - 10

Organic Chemistry in Biological Systems

Organic chemistry studies the structure, properties, and reactions of carbon-containing compounds. All biological molecules are organic compounds, encompassing biomolecules such as polysaccharides, lipids, nucleic acids, and amino acids. Enzymes facilitate the synthesis and breakdown of these biomolecules via catalysis.

Organic chemistry encompasses the detailed investigation of the structure, properties and reactions of organic chemicals. Phenols can be identified from their esters of 3,5 dinitrobenzoic, pnitrobenzoic, benzoic and acetic acids. The new compounds prepared during the investigation included p-phenylphenyl 3,5-dinitrobenzoate, p-benzylphenyl 3,5dinitrobenzoate, and 2,4-dinitrophenyl 3,5dinitrobenzoate, together with p-phenylphenyl p-nitrobenzoate, p-benzylphenyl p-nitrobenzoate, and 2,4-dinitronaphthyl p-nitrobenzoate [85]. Dihalobenzenes undergo reaction with salts of various organic acids.

10.1 Biomolecules

Life fundamentally revolves around the intricate chemistry of carbon compounds, which are essential to the formation and function of living organisms. The study of organic chemistry specifically pertains to the bonding, reactivity, and unique properties of molecules that are constructed around carbon frameworks. Within this fascinating field, a few of the more common types of biomolecules are presented and analyzed, and their critical roles within various biological systems are discussed in some detail. Additionally, the modeling of enzymatic catalysis, which is grounded in well-established organic chemistry principles, is briefly described, showcasing how these concepts apply in biochemical processes essential for life. Understanding these elements provides insight into the complex interplay of molecular interactions that sustain living systems [85].

10.2 Enzyme Catalysis

Enzyme catalysis represents an exceptionally vibrant and active research area within the field of organic chemistry, largely due to the fact that bio-catalysts are not only compatible with a wide array of reaction conditions but also possess the remarkable ability to be adjusted or optimized for numerous types of substrates. The seamless integration of these catalysts into multicomponent reactions (MCRs) facilitates the implementation of simple yet effective protocols that can be utilized in the diversity-oriented synthesis of intricate and complex molecules. This approach allows for chemo-, regio-, and stereoselective synthesis, as well as specific modes of reaction, without requiring the often cumbersome and time-consuming protection and deprotection of functional groups. The application and utilization of bio-catalysis in MCRs is a highly welcome and significant advancement. It is increasingly emerging as a vital tool in various domains, including drug development, discovery, and combinatorial chemistry. Recent breakthroughs and technological advances have led to innovative strategies involving MCRs, where three or more components react together in a single reaction vessel, or "one pot," to generate complex molecular architectures that would be challenging to produce through traditional methods. In comparison to conventional synthesis techniques, MCRs offer the significant advantage of enabling rapid construction of diverse molecular structures under mild reaction conditions. Remarkably, these reactions often result in the formation of heterocyclic compounds with impressive atom efficiency, selectivity, and minimized toxicity. As a result, MCRs have experienced exponential growth and popularity due to their wide-ranging applications in pharmaceuticals, fine chemical production, drug discovery, and further optimization processes. Historically, the Strecker reaction holds the distinction of being the first documented MCR, a pivotal reaction that produces α-amino acids through the reaction of aldehyde or ketone, ammonia, and hydrogen cyanide. Since then, numerous additional MCRs have been discovered, including but not limited to the Asinger, Biginelli, Hantzsch pyridine synthesis, Mannich, Strecker, and Ugi reactions. Importantly, most of these diverse MCRs are typically mediated by a variety of innovative catalysts, showcasing the versatility and significance of this area of research in modern chemistry [86, 87, 88, 89, 90].

Chapter - 11

Environmental Organic Chemistry

Many organic compounds are present in the environment. Some, such as phenols and polycyclic hydrocarbons, arise from human activities. Others, such as natural phytotoxins, also affect the environment. Circulation of organic chemicals in the environment depends on their physical properties, especially solubility. However, physical removal processes such as volatilization and sorption to particles arc often rapid enough to prevent significant organic chemical build-up in a given environmental compartment. Consequently, concentrations of organic chemicals in the environment often are controlled more by reaction than by physical removal processes. Reactions of organic chemicals in the environment are additionally important for their regulatory role and are relatively well understood. Although many reactions have been studied on a laboratory scale, only a few have been demonstrated to be significant environmentally. These include hydrolysis, chemical and biochemical oxidation, reduction, and photolysis. Photolysis has received the greatest attention because of its direct influence on the fate of certain pesticides and organic chromophores.

The broad view of environmental studies emphasizes their similarity to the concept of chemistry being studied within living systems. The extension of this view to include ecological systems and human influences on those systems provides a more complete approach for understanding environmental phenomena. The solution to many environmental problems caused by organic compounds maybe found in principles established in the major areas of organic chemistry. The motivation for such a solution lies in the concept of green chemistry that all potential environmental problems can be dealt with in an environmentally acceptable way consistent with economic growth [85, 36, 5].

11.1 Pollutants and Their Reactions

Over 80 million metric tons of organic pollutants enter the atmosphere annually from industrial and vehicular sources. Gas-phase pollutants undergo complex transformation reactions that change the chemical and physical properties of the molecules.

11.2 Green Chemistry Principles

The practice of chemistry is guided by a set of twelve principles that define green chemistry. The first six focus on the molecular design of chemical products and processes, a predominant theme throughout the present topics. The last six shift the perspective to the operational and organizational conduct of laboratories, emphasizing the broader context of chemical practice. In the following, the molecular approach is taken, aligning with the notion of a chemical approach to chemistry.

1. Prevention. It is preferable to prevent waste than to treat or clean up waste after it is formed. The preferred strategy is to begin with the most benign materials, allowing a large safety margin for unexpected processes and serving to protect the environment if a synthetic transformation is uncontrolled. Synthetic routes that produce particularly hazardous substances are thus best avoided. For methods that are widely distributed, developing alternative approaches that generate less waste should take priority, exemplified by the Debus method of imidazole synthesis [5].
2. Atom Efficiency. Synthetic methods should be designed to maximize the incorporation of materials used in the

process into the final product. The imperative of atom economy dictates the conscientious design of new synthetic processes and the critical appraisal of existing ones. Priority is given to reactions in which the final structure already contains the maximum number of sets of reactive groups; the introduction of an apparently unnecessary third substituent is thus undesirable. Carbonyl to alkene conversions (6.1) tend to be preferred over alkene to carbonyl conversions (6.2). For addition and elimination reactions, the relative efficiencies are reversed.

3. Less Hazardous Syntheses. Wherever practicable, synthetic methods are designed to use and generate substances that posses little or no toxicity to human health and the environment. Formaldehyde (H2CO) and polyphosphoric acid are less desirable substitutes for phosphorus oxychloride (POCl3) and phosphorus pentachloride (PCl5). Generalizing, corrosive reagents are to be avoided to the greatest extent possible.
4. Designing Safer Chemicals. Chemical products are designed to effect their desired function while minimizing their toxicity. Designing derivatives of the classical physical-organic tools to enhance their biological activity is a specific example. Optimizing the pharmacophore leads to enhanced efficiency and reduced toxicity.
5. Safer Solvents and Auxiliaries. The use of auxiliary substances (e.g., solvents, separation agents, etc.) should be made unnecessary wherever possible and innocuous when used. Examples of computational methods employed so far include group additivity (UA0) and semi-empirical quantum chemistry calculations (ZINDO). Analysis of relative energies aids in optimizing

kinetic solvation effects on transition states, guiding the selection of solvents in terms of solvatochromic parameters.

Chapter - 12

Industrial Applications of Organic Chemistry

The pharmaceutical industry is heavily reliant on a wide variety of organic compounds to effectively produce pharmaceutical treatments through meticulous processes that include design, synthesis, and large-scale manufacture. A significant number of medicines available in the market today are either organic compounds themselves or are derived from organic compounds through various structural modifications that are thoughtfully guided by established structure–activity relationships. It is essential to recognize that both medicines and the numerous organic compounds from which they are derived can exhibit a remarkable range of complexity. Additionally, these organic compounds can vary significantly in size, with some encompassing only a small number of atoms, while others can comprise several thousand atoms, creating vast structural diversity. The industrial-scale manufacture of pharmaceutical products presents a multitude of challenges that must be navigated effectively. As a result, organic chemistry emerges as a critical discipline playing significant roles in many key activities accentuated within the field, including research initiatives, product development streams, process research undertakings, and the vital manufacturing processes that follow. In parallel, polymers, which are substances produced through the polymerization of various monomers, exhibit diverse properties that have opened the door to a broad range of applications across numerous industries.

Organic chemistry, the study of carbon-containing compounds and their transformations, straddles the divide between science and technology. Historically a scientific endeavor, industrial demands have propelled organic chemistry into wider realms. Its rigors and rationales underpin all economic sectors: petroleum, food, polymers, fine chemicals, fragrances, dyes, agrochemicals, and pharmaceuticals. To supply consumers with affordable commodities, enormous quantities of organic chemicals must be manufactured with economies of scale. Research establishments respond by devising novel synthetic strategies and optimizing existing routes. Continual advances in bulk and fine chemicals enable new products and improved performance.

While specific sectors exhibit distinctive organic-chemical characteristics, the industrialist's perspective overwhelmingly features commodity chemicals. They fulfill every conceivable function, from flavouring chocolates to powering spacecraft. Products, applications, and technologies often span sectoral boundaries, thereby encouraging cross-fertilization of ideas and techniques. Nonetheless, some customers possess highly specialized requirements: they desire features a commodity cannot provide, be it inexpandability of a binder during space missions or rapid color change in chronic wound dressings. Synthesis is usually the straightforward component in the evolutionary sequence: development, scale-up, plant design, manufacturing, formulation, packaging, distribution, and usage. Although synthetic chemistry constitutes the bedrock of a supplier's activities, it represents only a fraction of business concerns. Nevertheless, it assumes crucial dimensions when attempting product innovation or process improvement.

Organic chemistry plays an essential role in pharmaceutical applications, encompassing drug discovery, development, industrial synthesis, and formulation processes. The development of pharmaceutical agents typically begins with the identification of a compound that interacts with a specific biological target associated with a pathological condition. Modern synthetic organic chemistry facilitates the large-scale preparation of such compounds, enabling the supply material necessary for biological screening and advancing promising candidates toward commercial production [1]. Industrial organic synthesis depends on a multitude of chemical transformations and methodologies, frequently integrated through synthetic design, achieving molecules that conform to stereochemical and functional group specifications within a market-driven financial framework [2].

Formulation chemistry defines the physical characteristics and delivery methods of pharmacologically active compounds, often involving additional synthetic organic steps to impart desired properties. The manifestation of oral drugs in tablet form exemplifies extensive design and development efforts within formulation chemistry. Consequently, pharmaceutical applications provide industrial organic chemistry with a comprehensive backdrop and a compelling challenge to devise new, improved, environmentally responsible, operationally safe, and cost-effective synthetic procedures capable of addressing the global demand for pharmaceutical agents.

The discovery and development of new therapeutic agents often involve a multifaceted combination of computational, experimental, and clinical models [3]. Although modern methods have increased efficiency, the process remains lengthy, costly, and complex. It begins with the design of compounds that interact specifically with a molecular target, frequently guided by computer modeling and bioinformatics tools. Synthetic strategies must take into account environmental impact, safety, and principles of green chemistry. The goal is to identify compounds that combine high affinity and selectivity for the target with optimal efficacy, metabolic stability, and oral bioavailability.

Until the early twentieth century, drug discovery proceeded empirically, relying on trial-and-error testing of natural products against infectious organisms [4]. Advances in extraction, analytical technologies, and structural elucidation transformed natural-product and synthetic chemistry, enabling the derivatization of natural products; at the time, 75% of antibacterials were natural products or their derivatives. Subsequently, the pharmaceutical industry expanded programs for drugs and vaccines addressing infectious diseases, transforming healthcare worldwide. During the 1960s, however, complacency led to reduced support for antiparasite research as priorities shifted toward chronic conditions such as cancer and diabetes. Genomics and molecular biology then established target identification as the paradigm for therapy development. Combinatorial chemistry and high-throughput screening initiatives sought novel compounds, yet only one clinically applied drug from these approaches emerged over 25 years. Many libraries contained similar molecules favored for synthetic accessibility rather than relevance. Current guidelines for drug-like compounds emphasize small, lipophilic molecules with appropriate stereochemistry, hydrogen-bonding capacity, and polarity—although notable exceptions exist, including covalent inhibitors exemplified by aspirin. Enhanced resolution and automated structural determination by x-ray diffraction and NMR facilitated rapid three-dimensional modeling of therapeutic targets, a critical advancement in early-stage drug discovery.

Synthesis of active pharmaceutical ingredients (APIs) is a central task of industrial organic chemistry and still a major challenge. Contemporary pharmaceuticals involve molecules of increasing complexity, and required functionalization frequently is at sites far removed from readily available functional groups. In its 70-year history of industry, organic chemistry has undergone continuous transformation to supply the needed synthetic methodology, the necessary building blocks, and access to any functionalization pattern. Generations of chemists and engineers have collaborated successfully to supply the existing demand, and open-access databases exist that list synthetic routes to a considerable proportion of known drugs. Biocatalysis extends the synthetic options because the potential of enzymes lies outside the scope of classical synthetic methodology. Enzymes distinguish themselves through superior regio-, stereo- and enantioselectivities, allow shorter multi-step routes, and exhibit enhanced substrate scope at mild reaction conditions that result in considerably reduced quantities of side products, waste and byproducts. Protein engineering enables sophisticated design of biocatalysts and adaptation of existing enzymes to novel substrates or to novel types of reaction. Biocatalysis is now established throughout the pharmaceutical and fine chemical industry and is applied for numerous reactions, e. g., chiral-alcohol synthesis or the production of atorvastatin precursors. Several examples from pharmaceutical production are well known, including the biocatalytic manufacture of sitagliptin on a scale of tons per year. Industrial enzyme applications are based not only on known and well investigated wild-type enzymes but also rely on innovative methods that enable the exploitation of the full potential of biocatalysis. Enzymes of interest are supplied through recruitment from novel environmental sources, transferred to new substrates by adaptation of substrate specificity, or integrated into enzyme cascades that convert readily available starting compounds into the targeted products [5].

Drugs are usually formulated as tablets, capsules, or liquid suspensions rather than pure chemical compounds, to enable ease of ingestion and promote desirable patterns of bodily delivery. To achieve these properties, formulation chemistry uses a thorough understanding of the interactions between active ingredients, excipients, and the body [1].

Pesticides comprise a variety of substances intended to repel, destroy, or control any pest. Herbicides, a subclass of pesticides, are chemicals used to kill or inhibit the growth of plants, such as weeds [6]. Fertilizers contain essential nutrients that promote the growth of certain plant species and serve as their food source. Organic chemistry governs all processes within the agricultural industry, ensuring the protection and growth of crops [7]. One particularly engaging branch of green chemistry focuses on the development of biopesticides to provide a more environmentally friendly way to safeguard plants. For example, numerous drugs that have been utilized in pharmaceutical research can be adapted for use as pesticides [8].

Pesticides and herbicides have become indispensible tools in the global management of agricultural pests and weeds. They are based on chemical substances designated for preventing, destroying, repelling, or mitigating pests of all pedigree. The synthesis of pharmaceutical products and active ingredients of veterinary pharmaceuticals follows similar strategies. The introduction of pesticides in agriculture helped establish a reasonable balance with pathogens produced and hence contributed to attaining food quality on a regular basis. The fertilizer industry offers the required nutrients for the balanced growth of plants and contributes to increased crop productivity. Biopesticides, defined as microbial pesticides.

Nitrogen, phosphorus, and potassium are the most important elements for plants, constituting the main components of fertilizers. Fertilization also influences quantity and quality indicators, chlorophyll assimilation, and mineral nutrition [9]. Influencing the growth and development processes as well as biochemical processes, organic substances with a bio-stimulation role affect these functions, with the relative efficacy of a fertilizer depending on the rate and size of nutrient transport in the plant. A fertilizer can increase the amount of the harvest as well as the content of vitamin C in the fruit and, at the same time, can maintain the acidity within the optimum range, but a difference appears when the fertilizer is of organic or chemical origin.

Biopesticides are naturally derived agents designed to control plant diseases, pests, and other harmful organisms. They have emerged to replace or supplement synthetic pesticides that pollute the environment and disturb ecosystems. Being biodegradable, biopesticides are compatible with integrated pest management (IPM) programs and cause less harm to natural enemies of target pests.

The major biopesticides include: (i) microbial pesticides (such as fungi, bacteria, or viruses), (ii) biochemical pesticides (natural substances that control pests by non-toxic mechanisms), and (iii) plant-incorporated protectants or genetically modified plants. The advantages are low toxicity, less environmental risk, and lower poison risks to resident people.

A new generation of polymers with improved durability, reduced toxicity and enhanced performance continues to emerge in diverse industrial sectors. Durable water-repellent, antimicrobial and ultraviolet-absorbent treatments applied to fabrics, paper and foods have made radical changes in everyday well-being and safety. Construction of vast bridges has become possible with the advent of high-performance composites. Aircraft and spacecraft have been made lighter and more efficient using organic composite materials. Polymers are widely used in the electronics industry, for example, as insulators in the extremely harsh conditions experienced by computers. Innovations in organic coatings, lubricants, paints and polymers have also provided a vast arsenal of specialised paints and coatings that protect a wide variety of surfaces and have been invaluable in reducing corrosion-related damage in industrial processes [7].

The industrial applications of organic chemistry have utilised many of the processes and synthetic strategies originally developed within academia; for example, the preparation of active pharmaceutical ingredients on multi-tonne scales, the synthesis of crop protection agents and the manufacture of polymers used for a plethora of everyday applications. In each case, clear chemical links that a trained chemist would recognise exist between the respective industrial processes. Numerous opportunities for cross fertilisation have therefore arisen during the course of the last century, and continue to do so. For instance, advantageous features arising in one sector of the chemical industry have often been transferred to another: developments in the multi-step syntheses of complex molecules, initiated more than a century ago in pharmaceutical production, have been adopted and developed further in the fields of agrochemicals and polymers [6]. Similarly, catalysts and blocking groups initially designed to simplify synthetic operations in the pharmaceutical sector have found beneficial application in other areas of industrial chemistry [8].

The use of organic chemistry as a means to produce and modify polymers remains one of the most important industrial endeavours to date. A polymer consists of a vast chain of organic molecules whose properties differ significantly from the small molecules used to produce them. Polymers have found applications in myriad areas key to the global economy, including coatings, paints, adhesives and elastomers, as well as in everyday items such as packaging and hygiene products [10].

The organic chemistry of polymers is especially important to the development of copolymers as well as polymer composites and blends. In the former, the properties of two types of monomer are combined into a single polymer chain, which can provide significant enhancements in performance. The latter can be similarly tuned by the incorporation of a polymer of different physical properties or a polymer composite in which an inorganic filler becomes uniformly dispersed within the polymer phase [11]. Coatings also represent an important industrial application of polymers and an avenue through which organic chemistry is used for enhanced functionality. Rather than to supply the bulk properties of the coating, the chemical functionality of the polymer directly dictates the adhesive or protective function of the material [12].

Nanomaterials have gained considerable attention due to their widespread commercial applications in sectors such as electronics, packaging, energy storage, automotive exhaust treatment, fuel cells, biomaterials, sensors, and health and fitness. Advanced materials manufacturing technology has become a key ingredient of many national economies; chemical production accounts for nearly 4% of the global gross domestic product. Polymer matrix composites offer numerous advantages, including small size, light weight, low fuel consumption, low manufacture and operating cost, and high mechanical properties.

Organic-inorganic composites serve as an important class of hybrid materials, comprising multi-component substances that contain organic and inorganic constituents. Polymeric nanocomposites combine polymer matrices with nano-sized inorganic fillers and are emerging as a promising new class of materials. Magnetic polymer composites can exhibit multifunctional properties such as a large surface area and light weight, with extensive applications ranging from environmental protection to electromagnetic shielding, microwave absorption, sensing, and biomedical uses. Nanostructures significantly alter material properties compared to their bulk counterparts, as exemplified by the remarkable strength of carbon nanotubes and the more efficient light transmittance of extremely thin films. Thermosetting epoxy-based composites are widely utilized in coatings, adhesives, laminates, printed circuit boards, and automotive materials.

Besides materials science, coatings and adhesives represent another important industrial domain where organic chemistry is essential. Protective and decorative coatings are widely applied to surfaces for corrosion protection, preservation, gloss, paintability, wetting, and dirt repellency. Sprayable nanocomposite coatings can be cured at lower temperatures than conventional PTFE coatings and provide excellent anti-adhesive properties essential in food production, where they also require high chemical stability to withstand cleaning treatments [13]. Acrylic coatings are used extensively due to their balance of performance and cost, and silicone coatings provide high-temperature protection.

Adhesives-liquids, pastes, or films that bond two substrates—are versatile systems of variable composition. Their industrial applications span aerospace, pharmaceutical, food, semiconductor, packaging, and furniture industries. Poly(hydroxyurethane) (PHU) adhesives and coatings have attracted attention as alternatives to isocyanate-based products. Isocyanate-free PHUs are particularly interesting due to the toxicity and regulatory pressure associated with isocyanates. Current technologies include solvent-free 1K silane-terminated prepolymers deployed in automotive applications, 2K systems offering rapid curing for structural bonding in building and flooring, hot-melt reactive systems with low free isocyanate used in wood and footwear, solvent-based prepolymers with excess NCO groups in several sectors, water-borne formulations suitable for shoes, bookbinding, furniture, and textiles, and radiation-curable acrylate prepolymers enabling rapid curing on flexible, heat-sensitive substrates. PU coatings employ viscous reactive formulations applied to substrates; in coatings, chemical resistance, flexibility, and appearance are prioritized, whereas bond strength is more critical for adhesives [14].

Organic chemistry plays a pivotal role in petrochemicals, particularly in refining crude oil for fuels and lubricants and in producing feedstocks for chemicals and polymers [6]. Secondary refining processes further upgrade base fuels to optimal performance standards for internal combustion engines. Lubricants, essential for reducing friction and wear, comprise high boiling point materials selected for appropriate viscosity at operating temperatures. Modern high-quality lubricants blend refined base stocks with additives to meet performance specifications. Petrochemical feedstocks serve as critical inputs for polymers, synthetic fibers, pharmaceuticals, and agrichemicals, demonstrating organic chemistry's broad industrial relevance.

Refining processes enable the conversion of feed materials into fuels that meet stringent molecular specifications and market demands. Indirect liquefaction products must match the molecular profiles of petroleum-derived fuels, with constraints on density, vapor pressure, sulfur content, and benzene concentration. Feed materials cannot be upgraded before sorting along typical boiling fractions, which form the basis for organizing refining operations.

Methanol synthesis yields predominantly methanol with high selectivity. Fischer–Tropsch synthesis produces a broad spectrum of compounds categorized as gaseous hydrocarbons, light oxygenates, and naphtha.

Gaseous hydrocarbons comprise alkanes and alkenes; C3−C4 hydrocarbons extracted from Fischer–Tropsch synthesis undergo refining after separation. Due to their low boiling points, similar hydrocarbons are typically removed from crude oil before transportation. Consequently, petroleum refineries generally handle little straight-run gaseous hydrocarbons.

Light oxygenates, including methanol and ethanol, are water soluble and characteristic of indirect liquefaction routes. They dissolve in water during the condensation of synthesis gases and are absent from conventional petroleum streams. Nevertheless, oxygenates are occasionally imported into refineries for blending and etherification processes.

Naphtha fractions boiling within 30−175°C primarily contain C5−C10 hydrocarbons such as alkanes, alkenes, and alcohols. Additional components may include aromatics, ketones, and acids. Refining strategies for each category must address the molecular composition constraints dictated by fuel specifications [15].

Petroleum refining is a complex process in which a large number of individual operations, chemical and physical, are combined to produce a variety of petroleum products and petrochemical feedstocks in required quantities and qualities at a reasonable cost. A broad knowledge of crude supply, chemistry of petroleum in both the raw and refined states, the demand for these processed products, an understanding of unit operation and engineering principles, and project economics are required in order to manufacture petroleum products competitively and economically. Refining involves two major components: separation and conversion. The separation methods are distillation, absorption, adsorption, stripping, and membrane techniques. Conversion operations generally are catalytic chemical processes: catalytic reforming, cracking, hydrocracking, isomerization, alkylation, polymerization, and hydrotreating [16]. Fuels and lubricating oils are among the many products obtained from liquid petroleum by means of the refining process mentioned above. A fuel is any substance that can be burned, or oxidized, in air to produce heat or power. These fuels generally are carbonaceous materials such as wood, peat, coal, coke, petroleum, and natural gas. Fuels that are used to power internal-combustion engines, jet engines, steam engines, and many other thermal machines all have different physical and chemical properties, yet they all require a source of pure hydrocarbons. Single hydrocarbons are not suitable fuels, but rather mixtures of hydrocarbons make the best practical fuels. With proper formulation, internal-combustion engine fuels can be custom-made to fit almost any requirement. Gasoline, diesel fuel, kerosene (jet fuel), turbine fuel, and heating oil are all examples of mixtures of hydrocarbons that are designed to fit the particular needs of an engine or heating appliance. Although petroleum is the world's main source of fuel and the hydrocarbon structure and composition of the feedstock have a strong influence on the number and type of products formed, the refiner can manipulate the processing of the petroleum by catalytic cracking, reforming, isomerization, and other methods to obtain the products required by the markets and at qualities needed to provide proper combustion patterns, reduce emissions, and perform to the expectation of the customer. Lubricating oils play an important role in today's machines, with applications ranging from the internal combustion engine, to bearings and turbines, to all kinds of industrial processes and even brakes and clutches. Any machine that has moving parts has to be lubricated to reduce friction and wear. Otherwise, it will fail prematurely. Since lubrication is so important, much effort has been spent in the development of lubricating oils that will meet specific needs and operate under adverse conditions.

Organic synthesis of chemical feedstocks constitutes a pivotal sector of the petrochemical industry. Refinery streams obtained by distillation at atmospheric and at reduced pressure constitute the basic raw materials, which upon further transformation yield an enormous variety of chemical products. After blending and sometimes the addition of appropriate additives, refined fractions find direct applications as petrol (motor spirit), aviation fuel, diesel oil, furnace oil, and fuel oil.

Synthetic strategies, such as thermal or catalytic cracking, hydrocracking, and visbreaking, increase the proportions (low-molecular fractions) of petrol and middle distillates. Catalytic reforming converts low-octane naphtha into high-octane fuel that is universally used in modern combustion engines. Special applications include reactions for the production of elastomers and commodity polymers, as well as those for obtaining the desirable elements for the design of detergents and other additives.

Among the essential reactions involving feedstocks, the following processes are noteworthy: • Alkylation: This acid-catalysed reaction introduces alkyl groups (methyl, ethyl, propyl, isopropyl, butyl, and isobutyl) and is chiefly used for the production of high-octane components of motor fuel (alkylate) and additives. Alkylation steps in the synthesis of many important drugs and materials are well documented.

Hydrotreatment: Hydrogenation processes control quality parameters, eliminate undesired components, and produce intermediates used in chemical, material, and pharmaceutical manufacture. Heavy naphtha and kerosene are extensively treated by such means. Hydrotreatment also leads to processed feedstocks for the production of special lubricating materials.

Catalytic reforming: Irrespective of the feedstock, this widely practiced process produces premium gasoline, high-quality aromatics, intermediate feedstocks (cyclohexane and methanol), hydrogen, and light hydrocarbons. Reforming is, therefore, of great commercial importance.

Steam cracking: This incorporates the fractionation of crude oil or imported hydrocarbons into lighter paraffins and olefins (ethene, propene, butenes, etc.), aromatic hydrocarbons, and diolefins. It is a crucial stage in the generation of chemical feedstocks.

Increasing environmental concerns motivate the development of new methodologies that reduce the human footprint on Nature. The application of green chemistry as well as waste management and recycling addresses alternatives for cleaner processes and the use of less harmful products and materials. Bioremediation is also pertinent to the efficient removal of organic contaminants. Many of these applications meet the expectations of a global agenda and demand the constant adaptation of organic-based materials [8, 6, 17].

The "twelve principles of green chemistry" aim essentially to provide a set of guidelines by which more sustainable ways of performing chemistry can be created. The methods and processes employed should be efficient, safe, and generate as little waste and pollution as possible. One of the most common measures of efficiency is ''atom economy'', which indicates how many of the atoms from the starting chemicals can be incorporated into the final product [18]. For example, if all of the reactant atoms are transferred to the product it is said to be 100% atom economical.

Atom economy describes efficiency in terms of mass, but does not take parameters like materials cost and environmental impact into account, which can be as important in industrial processes. These latter effects can be reflected somewhat by using the ''E-factor'', which relates the amount of waste generated per kilogram of product [19]. Catalysis is also a major concept used to prevent waste generation, increase atom economy, and reduce the number of derivatives required. These types of kinetic accelerators can be separated into two categories: heterogeneous and homogeneous. While both have advantages and disadvantages, it has recently been recognised that organic molecules may be also able to act as catalysts. This field has grown very rapidly in the last fifteen years with a large number of examples being reported since 2000.

Bioremediation exploits microbial metabolism to degrade organic contaminants associated with industrial activity, thereby reducing their adverse effects on health and the environment. The economic implementation of these methods may be facilitated by strategies such as phytoremediation. This involves the use of plants in the bioremediation process, achieved either by in situ biodegradation of organic compounds within the rhizosphere during plant growth or by hybrid methods. These hybrid methods include established remediation techniques applied to soil enhancements, followed by phytoremediation of persistent residues. Improvements in biomass production are also considered.

Industrial activities have generated large quantities of wastes, often rich in organic matters and other constituents. Their disposal presents environmental and public health problems, demanding effective treatment methods. In addition to preventing contamination, treating these wastes is a practical way to protect air, water, soil, and biodiversity, and to conserve natural resources. Organic compounds have been identified as major pollutants. Among advanced oxidation methods, Fenton oxidation stands out for degrading a wide spectrum of contaminants in industrial effluents, particularly those containing recalcitrant organic compounds. Other alternatives include chemical-physical treatments like adsorption, ozonization, photolysis, or a combination thereof, as well as biological treatments using activated sludge, biofilters, and membrane bioreactors.

Organic chemistry offers a palette of novel methods for more effective remediation using both traditional chemistry and bio-inspired approaches [20]. The use of green solvents and environmentally benign chemicals is integrated into a waste-to-wealth strategy in which waste streams are converted by means of chemical principles into reusable raw materials. Composite materials may be used for example as adsorbents, photocatalysts, and antimicrobial agents to promote depollution, while biosurfactants may be employed in the removal of heavy metal ions and have potential for oil spill recovery. Chemical doses may also be applied to stabilize waste and pollutants.

Process wastewater often represents a significant challenge for industrial remediation, as it contains a diverse range of residual products and synthetic reagents that vary in chemical composition and concentration, usually at elevated temperatures. It is found among others in the pharmaceutical industry, where treatment is confounded by the complexity of the effluent and the disparity of physical properties among its constituents [21]. Conventional technologies frequently fail to adequately remove all contaminants, and physicochemical methods may be required as pre- or post-treatment, also with recycling of solvents and original materials. Due to legislation limiting discharge of even residual concentrations, solvent transfer and exchange among industrial sites is uncommon. Contamination of surface waters results in altered flow conditions, thermal pollution and reduction of oxygen levels that damages aerobic organisms, often causing biologically imbalanced aquatic activity.

Food additives are substances added to food to enhance quality or processing efficiency. They span a broad range of organic compounds, including preservatives, antioxidants, flavorings, texturants, and sweeteners. Each additive is designed for specific purposes to make food safer, more colorful, appealing, flavorful, or longer-lasting [6]. Many such molecules consist mainly of carbon, hydrogen, and oxygen, sometimes with nitrogen or sulfur; they are often carbohydrates, lipids, or amino acid derivatives. Flavoring agents, important organic chemicals in the food industry, constitute a multibillion-dollar business.

Food often requires processing and preservation to keep it viable. Chemicals that influence food quality or the ease of preparation or processing are vital. Many preservatives prevent the growth of molds, bacteria, and yeasts, thus maintaining safety and appearance during distribution and storage. Nitrites and nitrates serve as preservatives for meat products and contribute to their flavor and color. Antioxidants prevent oxidation and the development of off-flavors in fatty foods.

Food additives and food preservatives are economic and strategic food components. Their purity is essential to guarantee safety and efficiency. Spike-responses of 19 compounds, belonging to food additives and preservatives, were evaluated using an untargeted approach on high-resolution Orbitrap mass spectrometry without any chromatographic method. A critical comparison between different chemical ionization sources and atmospheric pressure interfaces was performed. When detectable, the fragmentation of the ionized molecule (if any) was useful to obtain information about the molecular formula and the possible elemental composition of the internal standard. The obtained data can be exploited to implement selective analytical methods for the quantification of the analytes under investigation. For the development of colorants and preservatives with better performance, the modification of natural molecules may be a viable alternative [22].

The flavor is the focal point in the flavor industry, which follows social tendencies and behaviors. The research and development of new flavoring agents and molecules are essential in this field. The development of natural flavors plays a critical role in modern society. The present work proposes a novel framework based on Scientific Machine Learning to design new natural flavor molecules. From an anatomy point of view, the sensation of flavor is distinguished by taste buds that identify chemicals in food and beverages, translating them into nerve signals. Society's increasing consumption of processed and fast-food products has led to a higher demand for food additives and flavoring agents. There is a rising interest in foods labeled with natural flavoring agents due to health awareness, promoting growth in flavor R&D activities and investments. Although synthetic flavors are profitable and widely used, the market share is increasingly dominated by natural flavors owing to health concerns. The main industries utilizing flavors include beverages, bakery, savory and snacks, dairy and frozen foods, confectionery, and pet food, with growth driven by expanding applications and the development of new natural flavor products [23].

Flavors and fragrances are composed of volatile and non-volatile compounds with pleasant odors, used in perfumes, foods, and beverages. The ability of microorganisms to produce flavors and fragrances has been recognized for a long time, with recent efforts focusing on analyzing and optimizing food fermentations to harness microbial capacity for de novo synthesis or biotransformation. Most flavor compounds are obtained through extraction from natural sources or chemical synthesis, but extraction has disadvantages like low yields and seasonal variation. Chemical synthesis is often cheaper but may involve harsh conditions and produce mixtures of products, with artificially labeled compounds reducing their value. There is increasing interest in biotechnological production of flavors using microorganisms, as products derived this way can be labeled as natural. Examples of biotech-produced natural flavors include ethyl butanoate, 2-heptanone, β-ionone, nootkatone, 1-octen-3-ol, 4-undecalactone, and vanillin [24].

Production of natural flavors is increasingly important due to consumer preferences. Natural flavors are traditionally extracted from plants, but this is costly and time-consuming. Biotechnological methods use enzymes and microorganisms to convert natural precursors into flavors, offering a cost-effective alternative. Vanillin, a widely used flavor compound, is primarily produced synthetically, but research focuses on producing it naturally from precursors like ferulic acid or vanillic acid using fungi, and from eugenol via bacterial strains. Other flavor compounds such as γ-decalactone, responsible for peach-like flavor, can be produced through microbial conversions [25].

The global functional foods and nutraceuticals market has enjoyed steady growth over recent years due to heightened interest in nutrition, wellness, and preventive healthcare. Rising consumer awareness of health issues and a growing ageing population that requires enhanced nutrient uptake have also contributed to demand [26]. Since the 19th century, nutrition science has sought to understand the role of food in health and disease, revealing the significance of micronutrients, proteins/amino acids, fatty acids, carbohydrates, non-nutrient phytochemicals (e.g., antioxidants, flavonoids, phytoestrogens), and fibre [27]. Nutraceuticals may be defined as pharma-foods, food-pharma, or pharma-medicines, and are intended to provide health benefits as well as basic nutrition. 'Functional food' is an analogous term for ordinary food products fortified with additional components that either increase the contribution of existing ones (e.g., calcium-enriched orange juice) or introduce new ones [28].

Nutraceuticals and functional foods are often formulated to deliver compounds with functional properties. Isolated bioactive compounds, such as antioxidants, have been shown to protect humans from cardiovascular and inflammatory diseases, cancer, and cellular ageing. Lipids such as omega-3 and omega-6 fatty acids, conjugated linoleic acid (CLA), and phytosterols (plant sterols and stanols) may help reduce the risk of cardiovascular disease, enhance immune function, and promote brain development. Probiotics are micro-organisms introduced into the diet to promote gut health through the synthesis of metabolites such as vitamins and anti-carcinogenic compounds, and by competitive exclusion of potentially pathogenic organisms.

Prebiotics are non-digestible food ingredients (mainly oligosaccharides) that stimulate the growth of potentially health-promoting bacteria in the intestine. Synbiotics comprise a mixture of pro- and prebiotics that beneficially affect the host by improving the survival and implantation of probiotics in the gut.

Previous sections have illustrated the relevance of organic chemistry by examining its role in the large-scale synthesis of pharmaceutically active compounds, agrochemicals, polymeric coatings and additives, fuels and lubricants, and in the use of raw materials and organic residues within the framework of green technology. The present section offers examples of contemporary industrial applications of chemistry from the pharmaceutical industry, the agricultural field, and materials chemistry.

Experience gained in the synthesis of active biomolecules is applied to the preparation of new biopesticides, herbicides, insecticides, and biodegradable-bioactive substances. The consideration of pesticides, herbicides, insecticides, and fungicides with low toxicity is regarded as a step towards controlling harmful life forms without creating additional problems for the environment or the food web. Symbiotic nitrogen fixation, which supplies the nitrogen demands of plants in the biosphere, is supported by the use of specific species of rhizobacteria and mycorrhizal fungi, capable of establishing associations in both nonlegumes and legumes. These biofertilizers promote the growth and production of plant species in a natural way−. Moreover, the use of vitamins and hormones can augment the activity of biofertilizers when they are employed as growth regulators.

Drug discovery is a highly expensive and prolonged effort, with estimates that the typical timeline for introducing new drugs into clinics is about 15 years and the associated investment exceeds $800 million per candidate [29]. A critical factor contributing to the slow pace of drug exhaustiveness is rooted in the labour-intensive and inefficient nature of chemical synthesis. Despite many advances in science and technology, the methodology organic chemists employ remains fundamentally unchanged from that of a century ago. An additional manufacturing challenge emerges once reactions are implemented on a large scale, as for safety reasons several processes cannot always be performed in large industrial batch reactors. Consequently, process redevelopment and optimisation have to be repeated several times.

Organic chemistry underpins the formulation and use of agrochemical products that ensure the global supply of raw materials for the manufacturing of food, pharmaceuticals, and other high-value products. A diversity of products exists for controlling pests and diseases, improving the quality of stored crops, and enhancing overall growth. New trends focus on the integration of bioactive molecules, such as plant steroids, which offer high efficiency with reduced toxicity and support soil fertility and nutrition. These biodegradable biopesticides are compatible with integrated pest management approaches and sustainable agriculture [30].

Long-chain molecules manifest a wide array of biological activities and function as fungicides, insecticides, herbicides, and plant growth regulators [31]. Their mechanisms differ among classes: fungicides inhibit the respiratory chain, demethylation, or DNA/RNA synthesis; insecticides act as respiratory chain inhibitors, acetylcholinesterase inhibitors, or sodium channel inhibitors; acetanilide herbicides block fatty acid biosynthesis, while others inhibit 4-hydroxyphenylpyruvate dioxygenase (4-HPPD), provoking albinism and plant death. Several natural products and derivatives exhibit pesticide activity by multiple modes of action against various pests. Ametoctradin, a triazolopyrimidine fungicide, selectively inhibits oomycetes and is applied across a suite of crops.

Organic materials serve as the foundational elements for effective electronic devices.

Proper design enables fine-tuning of structural, optical, and electronic properties, which can be integrated into daily-use devices such as organic light-emitting diodes (OLEDs), organic photovoltaics (OPVs), and organic field-effect transistors (OFETs). Emerging cases include organic thermoelectric generators that convert heat into electricity via the Seebeck effect, and energy storage systems where organic materials act as electrodes in batteries and supercapacitors.

In the context of organic electronics, the relevant materials fall into the categories of small molecules, oligomers, and polymers-each producing similar device performances.

The fundamental concepts that have advanced organic electronic materials can be distilled into three major arenas: molecular design and synthesis, electronic structure calculations, and processing and device fabrication.

Global trends in population growth, urbanization, income rise, and education continue producing an expanding global population with ever-increasing demands for food, energy, and materials. The development of new technologies is vital for the sustainable growth of these markets and for creating more sustainable and safer consumer products. Industrial developments during the 20th century have been typically focused on the domain of consumer products (e.g., pharmaceuticals and large tonnages of food, feed, and fibres). In contrast, the primary focus for the 21st century is likely to be based more on sustainability within the context of a circular economy that takes account of diminishing supplies and high prices of fossil-based hydrocarbons, a growing concern for the environment and the quality of food and consumer products, and the pronounced growth of the Asian markets. The markets for fuels, lubricants, and chemicals are likely to remain relatively stable and stable in size, reflecting both changes in technology and surpluses in production.

The 21st century and Industry 4.0 will be an exciting period for the applied sciences, both in terms of their contribution to human progress and development and in terms of a more sustainable coexistence with nature. The agricultural and materials sectors will probably experience the most significant growth in chemical consumption. The pharmaceutical sector is unlikely to see significant growth in terms of tonnages because of the current global overcapacity for drug manufacture, but it will remain the most electrifying and essential sector. The petrochemical markets are expected to shift gradually from fuels toward materials, while the food and beverage market continues to require improvements in quality and protection for the increasing global demographic.

Contemporary organic chemistry is subject to multiple emerging technologies. Digital presence and the shift to virtual chemistry have accelerated in the last decade. Automation and robotics create increasingly efficient processes, with higher reproducibility [32]. The growth of affordable robots, microfluidic reactors, and the integration of digital sensors and computational methods have transformed organic synthesis. Artificial intelligence (AI) complements this automation, reducing the time consumed by recurrent and routine manual work. Chemical processes have achieved a high degree of automation, with AI algorithms assisting optimization and synthetic route prediction.

Data-mining techniques create models incorporated as expert systems, taking advantage of stored information on chemical reactants and products. Developing advanced AI techniques requires adequate digital representation of chemical information. Since the 1980s, attempts to create chemical-structure storage and file formats were made, leading to discrete 2D and 3D chemical pattern recognition and retrieval methodologies. Recent advances in chemical representation have initiated innovative approaches to dataset analysis and comparison. Various descriptors allowing for consistent, compact molecular-expression standards have appeared; SMILES, InChI, and MOL formats are widely employed.

Beyond 2D, several 3D descriptors exist. Combining shape descriptors with reactivity and quantum-chemical calculations, enhanced by machine-learning tools, promises major methodological changes. Pattern-matching methodologies accelerate the search for chemical analogs of reference molecules. Advanced machine-learning techniques can extract critical information, detect and sort outliers, and unveil patterns and unsuspected property relationships, constituting a turning point in data-processing methods.

Screening methods enhanced by representation and informatics provide a strong basis for accelerated creation of specific candidate molecule pools or clusters with desired properties. Ultra-high-throughput virtual screening and property-prediction methodologies can accelerate modeling. Patented molecule libraries, offline, and online experimental databases constitute data sources into which the above procedures can be profitably implemented. These examples exemplify the surge in new digital technologies that confer enormous advantages and newfound importance to organic chemistry.

A Circular Economy is based on reuse-models that minimize resource extraction and avoid the waste of materials. In chemical manufacturing such solutions can only be achieved by companies collaborating with each other and/or their customers and suppliers. Information must be shared widely across value/supply chains, but the resource flows should be constrained locally so that the circular model is practical.

Covering every aspect of society and aspects of industrial manufacturing, the drive to a sustainable Chemicals and Allied Products Industry, particularly throughout Europe, is at the forefront of many businesses. Products and materials must be manufactured more sustainably and on an economically viable basis.

Increasing demand for chemicals worldwide, depleting resources, consumer pressure, stricter legislation, and rising waste disposal cost place increasing pressure on chemical and related industries. Sustainable manufacturing enables economic growth combined with environmental and social sustainability. Collaboration among chemists, biologists, engineers, environmental scientists, economists, management experts, and policymakers is essential. Workers need new skills, knowledge, and experience to support these demands. Workshops that incorporate systems thinking promote sustainability in industry. Society is evolving and pushing many areas of industry, including chemicals and product design, towards sustainability. Sustainability using a circular economy philosophy is a crucial feature [33].

The manufacture of chemicals and materials is crucial to the global economy and human development through the creation of fundamental industrial and consumer products. To maintain, and enhance, this development, it will be necessary to use chemistry and chemical engineering even more effectively. It is clearly advantageous to have a good understanding of the likely future development and to consider how this might influence the different elements that contribute to UK research. Internal drivers, external forces (such as rising energy costs and societal pressures), economic and financial factors, regulation and legislation as well as the broader global context, are influencing the development of the chemical industry.

Circuits, sensors and smart materials are widely used in everyday life. Some novel applications, particularly those involving biochemical or physiological detection that are closely coupled to digital control, are leading to many innovative ‘smart’ technologies. Materials that possess functional or switchable properties that respond to stimuli can be synthesized relatively easily, for example, photo-, electro- and magnetochromics, or thermo- and hallo-responsive m“Gated-” materials. These have applications that span electronics, detergents, optics, inks and paints, textiles and healthcare.

The World Chemistry Population is defined as the number of chemists per million inhabitants, distributed by country. It reflects the prospective demand for chemical products and the market size for supplying goods and services related to chemistry. As of the current data, the World Chemistry Population amounts to 6.46 million, with the United States, China, and the European Union accounting for 66.4%. These statistics highlight the uneven distribution of chemical professionals and the corresponding influence of these regions on the chemical market.

Future Trends

Chemistry is a pervasive science that plays a vital role in the development of new products and services. Several predictions for future trends in chemistry are available in literature. The concept of green chemistry has been developed to promote cleaner processes, the use of renewable feeds, and the generation of less pollution and waste. Bioremediation, another emerging area, uses enzymes and living organisms to degrade contaminants present in soil, water, and air. A chemicals market structured in accordance with the principles of the circular economy—including the use of renewable carbon feeds and the reuse and recycling of products—can be envisioned. The COVID-19 pandemic induced an unprecedented surge in demand for pharmaceuticals and hygiene products, demonstrating that the chemical industry possesses the necessary resources to promptly respond to fluctuations in global markets.

Organic chemistry provides knowledge and tools necessary to manufacture products such as pharmaceuticals, plastics, food additives, and many other products. Its contributions are substantial and growing, thanks to Western industrial-industrialization, Western industrial growth, and the remarkable progress seen in chemical science, which have significantly shaped the development of organic chemistry. Available methodologies allow industrial organic chemists to design new materials, new synthetic routes, and innovative technologies. Another approach to innovation is the chemical modification of known molecules, aiming to achieve improved or additional properties that enable the required new function.

Expertise in large-scale synthesis is the starting point for any discussion. Industrial chemists usually define success by the availability of high-quality, low-cost products. It is crucial to be able to convert academic routes into processes that meet these requirements, to develop performance metrics for evaluating the overall sustainability of the products or processes being studied, and to put systems in place to deliver new molecules on the timescales dictated by the marketplace

These industries include but are not limited to building and construction-where plastics like pipe and pipe fittings are essential-packaging sectors utilizing polyethylene sacks and films, transportation industries through applications such as automotive parts, clothing sectors incorporating synthetic fibers including nylon and polyester, electronics fields producing printed circuit boards, leisure and sport applications such as tennis rackets, as well as health care industries relying on items like disposable syringes and sutures for patient care. The chemistry of polymers represents an important and specialized sub-field within the broader area of organic chemistry. The application of principles and methodologies drawn from both physics and physical chemistry has given rise to yet another important sub-discipline known as polymer science. The insights and innovations brought forth by both of these intertwined disciplines substantially contribute to the ongoing development and production of novel polymeric materials that can be utilized across various applications and industries, driving forward advancements and improving everyday products that people rely on [28, 85, 29, 91, 92, 93].

12.1 Pharmaceuticals

Organic chemistry plays a significant role in the pharmaceutical industry, demonstrating its importance and versatility. A notable example of this is the production of aspirin along with other similar drugs. This process often involves the innovative use of the Michaelis-Arbuzov rearrangement, showcasing how chemical reactions are harnessed for creating essential medications [5].

12.2 Polymer Chemistry

Polymers are fascinating organic compounds characterized by a remarkably large average molecular mass, typically involving more than 1000 atoms within their structures. Their intricate molecules are composed of an extensive number of repeating elementary units known as monomers. These monomers are chemically bonded together, forming a long chain that often features numerous branches, all connected to an atomic core that constitutes the nucleus of a substantial giant molecule. Polymer chemistry, in essence, is defined as a distinct branch of chemistry that specifically focuses on the detailed study of the structure, synthesis, properties, and various reactions of polymers. The array of innovative technologies that have emerged from notable advancements in the field of polymer chemistry has exerted a significant and transformative influence on the vast range of materials and chemicals that are now accessible for human use in various applications and industries [94, 95, 96, 97].

The first synthetic polymers appeared about 70 years ago [5, 6]. This period witnessed an accelerated growth in the range of polymeric materials available. Most advances at the present time are not based on the discovery of new polymers but rather on the modification and refinement of polymerization procedures which make it possible to obtain polymers with a variety of properties. Both the commercial and technological importance of polymer chemistry are therefore enormous.

Chapter - 13

Future Directions in Organic Chemistry

Green chemistry has transitioned remarkably from being merely a reactive compliance tool to becoming a core driver of innovation, effectively securing industrial competitiveness by replacing hazardous substances with environmentally benign technologies that are more sustainable. The emergence of innovative synthetic techniques has made significant inroads into the field, utilizing advanced methods such as microwaves, sonochemistry, photochemistry, and flow processes to reduce energy consumption while simultaneously increasing selectivity in various chemical reactions. However, despite these advancements, comprehensive studies assessing their overall sustainability footprint are still lacking in depth and breadth. Furthermore, the significant advancements made in the field of biocatalysis, which include cutting-edge approaches such as enzyme design, microengineering, and cascade reactions, are aimed at achieving greater selectivity and drastically reducing waste. Nevertheless, it is important to note that the combined impact of these enabling technologies, while promising, remains largely unexamined. The current practice of merely swapping reagents-without a thorough reconsideration of foundational synthetic strategies-ultimately hinders the potential for a substantial redesign of sustainable production processes. Therefore, future work dedicated to refining, combining, and analyzing these emerging methodologies will play a crucial role in guiding a strategic transition toward a global model of sustainable pharmaceutical manufacturing that prioritizes ecological safety and efficiency [5, 98, 99, 100, 101].

13.1 Sustainable Practices

Sustainable practices in industrial organic chemistry encompass the chemistry of resources, energy, agents, regeneration, and products. Occupational safety and health receive specific attention.

Chemical resources originate primarily from fossil fuels and biomass, with fossil fuels as the dominant source. Shifting resource use from fossil fuels to other materials constitutes a major process change necessitating development efforts. Achieving large changes in chemical processes requires broad changes in overall chemical system design; thus, simply following conventional practices with substituted resources or tactics typically cannot meet sustainable-practice criteria.

Energy use in sustainable practice generally aims at reductions. Motivations include feedstock, from which energy use is a partial surrogate, and carbon dioxide emissions. Burning fossil fuels to produce energy generates large amounts of CO2. Sustainable practices minimize fossil feedstock and energy use. Sustainable-practice resource considerations always pertain to the entire resource life cycle from acquisition or harvesting through the actual practice to disposal and remediation or to reuse or recycling. Practices such as extraction, reclamation, and maintenance are all part of sustainable-practice consideration.

Processes pursued for chemical synthesis, separation, utilization, or remediation ideally should arise from starting materials rich in the desired component and proceed via techniques that separate, analyze, or maintain that component in high proportion at the conclusion of the approach. In practice, it is generally difficult to achieve these standards completely. Large numbers of fundamental-process components follow the sequencing, and in many instances, separation is difficult and multiple operations are required using large amounts of solvents and energy. Process informatics and systems analyses represent important aspects in electronics, chemical, and mechanical approaches to sustainable process components in chemical engineering.

The agent (reagent, catalyst, or solvent) plays a significant sustainable-practice role toward net resource considerations, and a regenerative approach minimizes cumulative-resource requirements. The identical agent is used repeatedly, but frequently available procedures in heterogeneous and especially homogeneous system studies have gas-flow-rate and back-pressure constraints limiting application for large-scale sustained use. Viscosity, composition, composition variation, and accumulation of impurities become critical factors governing whether sustained application is possible [85, 28, 5].

13.2 Emerging Technologies

Research and patent activities associated with organic chemistry and the field of materials innovation remain highly active and exceptionally diverse during this period, as evidenced by a growing number of studies and filings that emerge regularly. A recent and comprehensive examination of mass spectral data and reaction mechanisms confirms the involvement of radical intermediates in various chemical processes. Meanwhile, ongoing investigations into rearrangement processes continue to elucidate specific transformations and intricacies within this complex domain of chemistry. These findings highlight the dynamic nature of research in organic chemistry, emphasizing not only the breadth of innovation but also the depth of knowledge being developed in understanding these crucial chemical phenomena [5, 6].

Conclusion

Organic chemistry has a rich set of methods for assessing atomic and molecular structure, including melting point, boiling point, density, refractive index, and optical rotation, and more sophisticated electronic, vibrational, and magnetic resonance techniques. Organic chemistry also provides an extensive range of reactions that serve both to functionalize and to eliminate functional groups. Regardless of the size of a molecule, most hurdles to its synthesis arise from the presence of unwanted functional groups rather than from its size per se. The success of an organic synthesis relies on careful consideration of the chemical properties of the functional groups present and on methodical isolation of the reactive functionality that determines the type of reaction. This requires an understanding of not only molecular structure but also of electronic and molecular structure, for both are reflected in the chemical properties of functional groups. As organic molecules continue to increase in size and complexity, the basic concepts of organic chemistry, which are founded on the characteristics of atoms and on the interplay between structure and properties, will assume an even greater importance.

Organic chemistry is the chemistry of carbon compounds. The importance of organic chemistry extends far beyond the study of carbon compounds. Most chemical compounds-from simple salts to ceramics-are not organic compounds. Organic compounds have carbon atoms, potentially a few hydrogen atoms to satisfy valence requirements, and a variety of other elements. All other chemical compounds can be grouped into the “inorganic” category. The terms organic and inorganic are, however, historical and have lost most of their original significance. The importance of organic chemistry lies not in the carbon atoms per se but in the fact that bonded carbon atoms tend, in general, to form molecular compounds. The other major element present in organic compounds is hydrogen, and it cannot form molecular compounds. Consequently, even a small hydrocarbon-an ethyl radical, CH3CH2-possesses the general characteristics of the majority of organic compounds. This notion is best developed by examining the individual atoms present in organic compounds and the electronic structure that influences their bonding.

The structure of an organic compound largely determines its properties, and its properties-physical and chemical-determine its behavior. By structure, we refer not only to the spatial arrangement of atoms but also to the distribution of electrons. A complete knowledge of structure enables one to predict one's properties and behavior. Conversely, detailed knowledge of the chemical and physical properties helps the determination of structure. The notion that structure and properties are intimately connected is one of the central themes of organic chemistry.

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