

KEY ASPECTS OF ORGANIC CHEMISTRY IN ASSORTED DOMAINS

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Abstract

Organic compounds form the basis of all earthly life and constitute the majority of known chemicals. The bonding patterns of carbon, with its valence of four—formal single, double, and triple bonds, plus structures with delocalized electrons—make the array of organic compounds structurally diverse, and their range of applications enormous. They form the basis of, or are constituents of, many commercial products including pharmaceuticals; petrochemicals and agrichemicals, and products made from them including lubricants, solvents; plastics; fuels and explosives. The study of organic chemistry overlaps organometallic chemistry and biochemistry, but also with medicinal chemistry, polymer chemistry, and materials science. Organic chemistry is a branch of chemistry that studies the structure, properties and reactions of organic compounds, which contain carbon in covalent bonding. Study of structure determines their chemical composition and formula. Study of properties includes physical and chemical properties, and evaluation of chemical reactivity to

understand their behavior. The study of organic reactions includes the chemical synthesis of natural products, drugs, and polymers, and study of individual organic molecules in the laboratory and via theoretical (in silico) study. The range of chemicals studied in organic chemistry includes hydrocarbons (compounds containing only carbon and hydrogen) as well as compounds based on carbon, but also containing other elements, especially oxygen, nitrogen, sulfur, phosphorus (included in many biochemicals) and the halogens. Organometallic chemistry is the study of compounds containing carbon–metal bonds. In addition, contemporary research focuses on organic chemistry involving other organometallics including the lanthanides, but especially the transition metals zinc, copper, palladium, nickel, cobalt, titanium and chromium.

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Introduction

Organic chemistry is the study of the structure, properties, composition, reactions, and preparation of carbon-containing compounds, which include not only hydrocarbons but also compounds with any number of other elements, including hydrogen (most compounds contain at least one carbon–hydrogen bond), nitrogen, oxygen, halogens, phosphorus, silicon, and sulfur. This branch of chemistry was originally limited to compounds produced by living organisms but has been broadened to include human-made substances such as plastics. The range of application of organic compounds is enormous and also includes, but is not limited to, pharmaceuticals, petrochemicals, food, explosives, paints, and cosmetics [1].

Organic compounds are all around us. They are central to the economic growth of the United States in the rubber, plastics, fuel, pharmaceutical, cosmetics, detergent, coatings, dyestuff, and agricultural industries, to name a few. The very foundations of biochemistry, biotechnology, and medicine are built on organic compounds and their role in life processes. Many modern, high-tech materials are at least partially composed of organic compounds.

Organic chemists spend much of their time creating new compounds and developing better ways of synthesizing previously known compounds.

Organic chemists at all levels are generally employed by pharmaceutical, biotech, chemical, consumer product, and petroleum industries. Chemists in industry mainly work in development, while chemists in academia are involved in more basic research. The federal (e.g., Food and Drug Administration, Patent and Trademark Office) state, and local governments also hire organic chemists [2].

Biotechnology (“biotech” for short) is a field of applied biology that involves using living organisms and bioprocesses to create or modify products for a specific use. The cultivation of plants has been viewed as the earliest example of biotechnology and the precursor to modern genetic engineering and cell and tissue culture technologies. Virtually all biotechnology products are the result of organic chemistry [3].

Biotechnology is used in health care, crop production and agriculture, nonfood uses of crops and other products (e.g., biodegradable plastics, vegetable oil, biofuels), and environmental applications.

The chemical industry is crucial to modern world economies and works to convert raw materials such as oil, natural gas, air, water, metals, and minerals into more than 70,000 different products. These base products are then used to make consumer products in addition to manufacturing, service, construction, agriculture, and other industries.

Over three-fourths of the chemical industry’s output worldwide is polymers and plastics. Chemicals are used to make a wide variety of consumer goods, as well as thousands of products that are inputs to the agriculture, manufacturing, construction, and service industries. The chemical industry itself consumes about a quarter of its own output. Major industrial customers include rubber and plastic products, textiles, apparel, petroleum refining, pulp and paper, and primary metals [4].

The multiple-step synthesis of complex organic compounds is called total synthesis. Total synthesis of complex natural compounds increased in complexity to glucose and terpineol. For example, cholesterol-related compounds have opened ways to synthesize complex human hormones and their modified derivatives. Since the start of the 20th century, complexity of total syntheses has been increased to include molecules of high complexity such as lysergic acid and vitamin B12 [5].

The discovery of petroleum and the development of the petrochemical industry spurred the development of organic chemistry. Converting individual petroleum compounds into types of compounds by various chemical processes led to organic reactions enabling a broad range of industrial and commercial products including, among (many) others: plastics, synthetic rubber, organic adhesives, and various property-modifying petroleum additives and catalysts. The majority of chemical compounds occurring in biological organisms are carbon compounds, so the association between organic chemistry and biochemistry is so close that biochemistry might be regarded as in essence a branch of organic chemistry. Although the history of biochemistry might be taken to span some four centuries, fundamental understanding of the field only began to develop in the late 19th century and the actual term biochemistry was coined around the start of 20th century. Research in the field increased throughout the twentieth century, without any indication of slackening in the rate of increase, as may be verified by inspection of abstraction and indexing services such as BIOSIS Previews and Biological Abstracts, which began in the 1920s as a single annual volume, but has grown so drastically that by the end of the 20th century it was only available to the everyday user as an online electronic database [6].

Since organic compounds often exist as mixtures, a variety of techniques have also been developed to assess purity; chromatography techniques are especially important for this application, and include HPLC and gas chromatography. Traditional methods of separation include distillation, crystallization, and solvent extraction.

Organic compounds were traditionally characterized by a variety of chemical tests, called "wet methods", but such tests have been largely displaced by spectroscopic or other computer-intensive methods of analysis. Listed in approximate order of utility, the chief analytical methods are [7]:

Nuclear magnetic resonance (NMR) spectroscopy is the most commonly used technique, often permitting the complete assignment of atom connectivity and even stereochemistry using correlation spectroscopy. The principal constituent atoms of organic chemistry – hydrogen and carbon – exist naturally with NMR-responsive isotopes, respectively ^1H and ^{13}C .

Mass spectrometry indicates the molecular weight of a compound and, from the fragmentation patterns, its structure. High-resolution mass spectrometry can usually identify the exact formula of a compound and is used in place of elemental analysis. In former times, mass spectrometry was restricted to neutral molecules exhibiting some volatility, but advanced ionization techniques allow one to obtain the "mass spec" of virtually any organic compound.

Crystallography can be useful for determining molecular geometry when a single crystal of the material is available. Highly efficient hardware and software allows a structure to be determined within hours of obtaining a suitable crystal [8].

Traditional spectroscopic methods such as infrared spectroscopy, optical rotation, and UV/VIS spectroscopy provide relatively nonspecific structural information but remain in use for specific applications. Refractive index and density can also be important for substance identification [9].

The physical properties of organic compounds typically of interest include both quantitative and qualitative features. Quantitative information includes a melting point, boiling point, and

index of refraction. Qualitative properties include odor, consistency, solubility, and color [10].

Organic compounds typically melt and many boil. In contrast, while inorganic materials generally can be melted, many do not boil, and instead tend to degrade. In earlier times, the melting point (m.p.) and boiling point (b.p.) provided crucial information on the purity and identity of organic compounds. The melting and boiling points correlate with the polarity of the molecules and their molecular weight. Some organic compounds, especially symmetrical ones, sublime. A well-known example of a sublimable organic compound is para-dichlorobenzene, the odiferous constituent of modern mothballs. Organic compounds are usually not very stable at temperatures above 300 °C, although some exceptions exist.

Neutral organic compounds tend to be hydrophobic; that is, they are less soluble in water than in organic solvents. Exceptions include organic compounds that contain ionizable groups as well as low molecular weight alcohols, amines, and carboxylic acids where hydrogen bonding occurs. Otherwise, organic compounds tend to dissolve in organic solvents. Solubility varies widely with the organic solute and with the organic solvent.

Various specialized properties of molecular crystals and organic polymers with conjugated systems are of interest depending on applications, e.g. thermo-mechanical and electro-mechanical such as piezoelectricity, electrical conductivity (see conductive polymers and organic semiconductors), and electro-optical (e.g. non-linear optics) properties. For historical reasons, such properties are mainly the subjects of the areas of polymer science and materials science [11].

The names of organic compounds are either systematic, following logically from a set of rules, or nonsystematic, following various traditions. Systematic nomenclature is stipulated by specifications from IUPAC. Systematic nomenclature starts with the name for a parent structure within the molecule of interest. This parent name is then modified by prefixes,

suffixes, and numbers to unambiguously convey the structure. Given that millions of organic compounds are known, rigorous use of systematic names can be cumbersome. Thus, IUPAC recommendations are more closely followed for simple compounds, but not complex molecules. To use the systematic naming, one must know the structures and names of the parent structures. Parent structures include unsubstituted hydrocarbons, heterocycles, and mono functionalized derivatives thereof [12].

Nonsystematic nomenclature is simpler and unambiguous, at least to organic chemists. Nonsystematic names do not indicate the structure of the compound. They are common for complex molecules, which include most natural products. Thus, the informally named lysergic acid diethylamide is systematically named (6aR,9R)-N,N-diethyl-7-methyl-4,6,6a,7,8,9-hexahydroindolo-[4,3-fg] quinoline-9-carboxamide.

With the increased use of computing, other naming methods have evolved that are intended to be interpreted by machines. Two popular formats are SMILES and InChI.

Organic molecules are described more commonly by drawings or structural formulas, combinations of drawings and chemical symbols. The line-angle formula is simple and unambiguous. In this system, the endpoints and intersections of each line represent one carbon, and hydrogen atoms can either be notated explicitly or assumed to be present as implied by tetravalent carbon.

By 1880 an explosion in the number of chemical compounds being discovered occurred assisted by new synthetic and analytical techniques. Grignard described the situation as "chaos le plus complet" (complete chaos) due to the lack of convention it was possible to have multiple names for the same compound. This led to the creation of the Geneva rules in 1892.

The aliphatic hydrocarbons are subdivided into three groups of homologous series according to their state of saturation:

alkanes (paraffins): aliphatic hydrocarbons without any double or triple bonds, i.e. just C-C, C-H single bonds

alkenes (olefins): aliphatic hydrocarbons that contain one or more double bonds, i.e. di-olefins (dienes) or poly-olefins.

alkynes (acetylenes): aliphatic hydrocarbons which have one or more triple bonds.

The rest of the group is classed according to the functional groups present. Such compounds can be "straight-chain", branched-chain or cyclic. The degree of branching affects characteristics, such as the octane number or cetane number in petroleum chemistry.

Both saturated (alicyclic) compounds and unsaturated compounds exist as cyclic derivatives. The most stable rings contain five or six carbon atoms, but large rings (macrocycles) and smaller rings are common. The smallest cycloalkane family is the three-membered cyclopropane ((CH₂)₃). Saturated cyclic compounds contain single bonds only, whereas aromatic rings have an alternating (or conjugated) double bond. Cycloalkanes do not contain multiple bonds, whereas the cycloalkenes and the cycloalkynes do.

Benzene is one of the best-known aromatic compounds as it is one of the simplest and most stable aromatics. Aromatic hydrocarbons contain conjugated double bonds. This means that every carbon atom in the ring is sp² hybridized, allowing for added stability. The most important example is benzene, the structure of which was formulated by Kekulé who first proposed the delocalization or resonance principle for explaining its structure. For "conventional" cyclic compounds, aromaticity is conferred by the presence of 4n + 2 delocalized pi electrons, where n is an integer. Particular instability (antiaromaticity) is conferred by the presence of 4n conjugated pi electrons.

The characteristics of the cyclic hydrocarbons are again altered if heteroatoms are present, which can exist as either substituents attached externally to the ring (exocyclic) or as a member of the ring itself (endocyclic). In the case of the latter, the ring is termed a heterocycle. Pyridine and furan are examples of aromatic heterocycles while piperidine and tetrahydrofuran are the corresponding alicyclic heterocycles. The heteroatom of heterocyclic molecules is generally oxygen, sulfur, or nitrogen, with the latter being particularly common in biochemical systems.

Heterocycles are commonly found in a wide range of products including aniline dyes and medicines. Additionally, they are prevalent in a wide range of biochemical compounds such as alkaloids, vitamins, steroids, and nucleic acids (e.g. DNA, RNA).

Rings can fuse with other rings on an edge to give polycyclic compounds. The purine nucleoside bases are notable polycyclic aromatic heterocycles. Rings can also fuse on a "corner" such that one atom (almost always carbon) has two bonds going to one ring and two to another. Such compounds are termed spiro and are important in several natural products.

One important property of carbon is that it readily forms chains, or networks, that are linked by carbon-carbon (carbon-to-carbon) bonds. The linking process is called polymerization, while the chains, or networks, are called polymers. The source compound is called a monomer.

Two main groups of polymers exist synthetic polymers and biopolymers. Synthetic polymers are artificially manufactured, and are commonly referred to as industrial polymers. Biopolymers occur within a respectfully natural environment, or without human intervention.

Biomolecular chemistry is a major category within organic chemistry which is frequently studied by biochemists. Many complex multi-functional group molecules are important in living organisms. Some are long-chain biopolymers, and these include peptides, DNA, RNA

and the polysaccharides such as starches in animals and celluloses in plants. The other main classes are amino acids (monomer building blocks of peptides and proteins), carbohydrates (which includes the polysaccharides), the nucleic acids (which include DNA and RNA as polymers), and the lipids. Besides, animal biochemistry contains many small molecule intermediates which assist in energy production through the Krebs cycle, and produces isoprene, the most common hydrocarbon in animals. Isoprenes in animals form the important steroid structural (cholesterol) and steroid hormone compounds; and in plants form terpenes, terpenoids, some alkaloids, and a class of hydrocarbons called biopolymer polyisoprenoids present in the latex of various species of plants, which is the basis for making rubber.

Fullerenes and carbon nanotubes, carbon compounds with spheroidal and tubular structures, have stimulated much research into the related field of materials science. The first fullerene was discovered in 1985 by Sir Harold W. Kroto of the United Kingdom and by Richard E. Smalley and Robert F. Curl, Jr., of the United States. Using a laser to vaporize graphite rods in an atmosphere of helium gas, these chemists and their assistants obtained cage-like molecules composed of 60 carbon atoms (C₆₀) joined together by single and double bonds to form a hollow sphere with 12 pentagonal and 20 hexagonal faces—a design that resembles a football, or soccer ball. In 1996 the trio was awarded the Nobel Prize for their pioneering efforts. The C₆₀ molecule was named buckminsterfullerene (or, more simply, the buckyball) after the American architect R. Buckminster Fuller, whose geodesic dome is constructed on the same structural principles.

Conclusion

Organic reactions are chemical reactions involving organic compounds. Many of these reactions are associated with functional groups. The general theory of these reactions involves careful analysis of such properties as the electron affinity of key atoms, bond strengths and steric hindrance. These factors can determine the relative stability of short-lived reactive intermediates, which usually directly determine the path of the reaction. Synthetic organic chemistry is an applied science as it borders engineering, the "design, analysis, and/or

construction of works for practical purposes". Organic synthesis of a novel compound is a problem-solving task, where a synthesis is designed for a target molecule by selecting optimal reactions from optimal starting materials. Complex compounds can have tens of reaction steps that sequentially build the desired molecule. The synthesis proceeds by utilizing the reactivity of the functional groups in the molecule. For example, a carbonyl compound can be used as a nucleophile by converting it into an enolate, or as an electrophile; the combination of the two is called the aldol reaction. Designing practically useful syntheses always requires conducting the actual synthesis in the laboratory. The scientific practice of creating novel synthetic routes for complex molecules is called total synthesis. Strategies to design a synthesis include retrosynthesis, popularized by E.J. Corey, which starts with the target molecule and splices it to pieces according to known reactions. The pieces, or the proposed precursors, receive the same treatment, until available and ideally inexpensive starting materials are reached. Then, the retrosynthesis is written in the opposite direction to give the synthesis. A "synthetic tree" can be constructed because each compound and also each precursor has multiple syntheses.

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