What is Chemistry all about?

A survey of chemical science

Chemistry is such a broad subject and one so full of detail that it is easy for a newcomer to find it somewhat overwhelming, if not intimidating. The best way around this is to look at Chemistry from a variety of viewpoints:

- How Chemistry relates to other sciences and to the world in general
- What are some of the fundamental concepts that extend throughout Chemistry?
- What are some of the major currents of modern-day Chemistry?

1 The scope of chemical science

Chemistry is too universal and dynamically-changing a subject to be confined to a fixed definition; it might be better to think of chemistry more as a *point of view* that places its major focus on the structure and properties of **substances**— particular kinds of matter— and especially on the changes that they undergo.



In some ways, **physics** might be considered more "fundamental" to the extent that it deals with matter and energy in a more general way, without the emphasis on particular substances.

But the distincion can get pretty fuzzy; it is ultimately rather futile to confine any aspect of human endeavour to little boxes.

Chemistry: the central science

The real importance of Chemistry is that it serves as the interface to practically all of the other sciences, as well as to many other areas of human endeavor. For this reason, Chemistry is often said (at least by chemists!) to be the "central science".

Chemistry can be "central" in a much more personal way: with a solid background in Chemistry, you will find it far easier to migrate into other fields as your interests develop.



Chemistry can enhance any career. Chemistry is so deeply ingrained into so many areas of business, government, and environmental management that some background in the subject can be useful (and able to give you a career edge as a team member having special skills) in fields as varied as product development, marketing, management, computer science, technical writing, and even law.

So just what *is* chemistry?



Do you remember the <u>story</u> about the group of blind men who encountered an elephant? Each one moved his hands over a different part of the elephant's body— the trunk, an ear, or a leg and came up with an entirely different description of the beast.

Chemistry can similarly be approached in different ways, each yielding a different, valid, (and yet hopelessly incomplete) view of the subject.

Thus we can view chemistry from multiple standpoints ranging from the theoretical to the eminently practical:

Mainly theoretical	Mainly practical
Why do particular combinations of atoms hold together, but not others?	What are the properties of a certain compound?
How can I predict the shape of a molecule?	How can I prepare a certain compound?
Why are some reactions slow, while others occur rapidly?	Does a certain reaction proceed to completion?
Is a certain reaction possible?	How can I determine the composition of an unknown substance?

Boiling it down to the basics

At the most fundmental level, chemistry can be organized along the lines shown here.

Dynamics

refers to the details of that rearrangements of atoms that occur during chemical change, and that strongly affect the rate at which change occurs.

Energetics

refers to the thermodynamics of chemical change, relating to the uptake or release of heat. More importantly, this aspect of chemistry controls the direction in which change occurs, and the mixture of substances that results.

Composition and structure

define the substances that are results of chemical change. *Structure* refers specifically to the relative arrangements of the atoms in space. The extent to which a given structure can persist is itself determined by energetics and dynamics.

Synthesis

strictly speaking, refers to formation of new (and usually more complex) substances from simpler ones, but in the present context we use it in the more general sense to denote the operations required to bring about chemical change and to isolate the desired products.

This view of Chemistry is a rather astringent one that is probably more appreciated by people who already know the subject than by those who are about to learn it, so we will use a somewhat expanded scheme to organize the fundamental concepts of chemical science. But if you need a singlesentence"definition of Chemistry, this one wraps it up pretty well:



Chemistry is the study of *substances*; their properties, structure, and the changes they undergo.

Micro-macro: the forest or the trees



Chemistry, like all the natural sciences, begins with the direct observation of nature— in this case, of matter. But when we look at matter in bulk, we see only the "forest", not the "trees"— the atoms and molecules of which matter is composed— whose properties ultimately determine the nature and behavior of the matter we are looking at.

This dichotomy between what we can and cannot directly see constitutes two contrasting views which run through all of chemistry, which we call *macroscopic* and *microscopic*.

- In the context of Chemistry, "microscopic" implies detail at the atomic or subatomic levels which cannot be seen directly (even with a microscope!)
- The macroscopic world is the one we can know by direct observations of physical properties such as mass, volume, etc.

The following table provides a conceptual overview of Chemical science according to the macroscopic/microscopic dichotomy we have been discussing.

It is of course only one of many ways of looking at the subject, but you may find it a helpful means of organizing the many facts and ideas you will encounter in your study of Chemistry. We will organize the discussion in this lesson along similar lines.

realm	macroscopic view	microscopic view
composition	formulas, mixtures	structures of solids, molecules, and atoms
properties	intensive properties of bulk matter	particle sizes, masses and interactions
change (energetics)	energetics and equilibrium	statistics of energy distribution

change (dynamics)	kinetics (rates of reactions)	mechanistics

2 Chemical composition

Mixture or "pure substance" ?

In science it is necessary to know exactly what we are talking about, so before we can even begin to consider matter from a chemical point of view, we need to know something about its *composition*; is the stuff I am looking at a *single substance*, or is it a *mixture*? (We will get into the details of these definitions elsewhere, but for the moment you probably already have a fair understanding of the distinction; think of a sample of crystalline salt (sodium chloride) as opposed to a *solution* of salt in water— a *mixture* of salt and water.)



To a chemist, there is a fundamental distinction between a pure substance and a mixture. But marketers, and through them, the general public, don't hesitate to describe a complex mixture such as peanut butter as "pure". Pure *what*?

Elements and compounds

It has been known for at least a thousand years that some substances can be broken down by heating or chemical treatment into "simpler" ones, but there is always a limit; we eventually get substances known as *elements* that cannot be reduced to any simpler forms by ordinary chemical or physical means. What is our criterion for "simpler"? The most observable (and therefore macroscopic) property is the weight.



The idea of a minimal unit of chemical identity that we call an *element* developed from experimental observations of the relative weights of substances involved in chemical reactions. For example, the compound mercuric oxide can be broken down by heating into two other substances:

$$2 \text{ HgO} \rightarrow 2 \text{ Hg} + \text{O}_2$$

... but the two products, metallic mercury and dioxygen, cannot be decomposed into simpler substances, so they must be elements.

The definition of an element given above is an *operational* one; a certain result (or in this case, a non-result!) of a procedure that might lead to the decomposition of a substance into lighter units will tentatively place that substance in one of the categories, element or compound. Because this operation is carried out on bulk matter, the concept of the element is also a *macroscopic* one.

Painting by Joseph Wright of Derby (1734-97) The Alchymist in Search of the <u>Philosopher's Stone</u> discovers Phosphorus

[image link]



Elements and atoms: what's the difference?

The *atom*, by contrast, is a *microscopic* concept which in modern chemistry relates the unique character of every chemical element to an actual physical particle.

The idea of the atom as the smallest particle of matter had its origins in Greek philosophy around 400 BCE but was controversial from the start (both Plato and Aristotle maintained that matter was infinitely divisible.) It was not until 1803 that John Dalton proposed a rational atomic theory to explain the facts of chemical combination on their ways then linear the size the first to employ mechanism stick and a start of the size of th



of chemical combination as they were then known, thus being the first to employ macroscopic evidence to illuminate the microscopic world.



It took almost until 1900 for the atomic theory to became universally accepted. In the 1920's it became possible to measure the sizes and masses of atoms, and in the 1970's techniques were developed that produced images of individual atoms.

 \leftarrow Cobalt atom imaged by a scanning tunneling microscope [image $\underline{\mathrm{link}}]$

Formula and structure

The *formula* of a substance expresses the relative number of atoms of each element it contains. Because the formula can be determined by experiments on bulk matter, it is a macroscopic concept even though it is expressed in terms of atoms.

What the ordinary chemical formula does *not* tell us is the order in which the component atoms are connected, whether they are grouped into discrete units (*molecules*) or are two- or three dimensional extended structures, as is the case with solids such as ordinary salt. The microscopic aspect of composition is *structure*, which in its greatest detail reveals the relative locations (in two or three dimensional space) of each atom within the minimum collection needed to define the structure of the substance.

	Macroscopic	Microscopic
Substances are defined at the macroscopic level by their formulas or compositions , and at the microscopic level by their structures .	The elements hydrogen and oxygen combine to form a compound whose composition is expressed by the formula H ₂ O.	The molecule of water has the structure shown here.
Chemical substances that cannot be broken down into simpler ones are known as elements . The actual physical particles of which elements are composed are atoms or molecules .	Sulfur-the- element in its orthorhombic crystalline form.	The S ₈ molecule is an octagonal ring of sulfur atoms . The crystal shown at the left is composed of an ordered array of these molecules. (This animation does not properly represent the actual vibrational motions of the molecule.)

Compounds and molecules

As we indicated above, a *compound* is a substance containing more than one element. Since the concept of an element is macroscopic and the distinction between elements and compounds was recognized long before the existence of physical atoms was accepted, the concept of a compound must also be a macroscopic one that makes no assumptions about the nature of the ultimate .



A *molecule* is an assembly of atoms having a fixed composition, structure, and distinctive, measurable properties.

In its most general meaning, the term *molecule* can describe *any* kind of particle (even a single atom) having a unique chemical identity. Even at the end of the 19th century, when compounds and their formulas had long been in use, some prominent chemists doubted that molecules (or atoms) were any more than a convenient model.

Computer model of the nicotine molecule, $C_{10}H_{14}N_2,$ by Ronald Perry \uparrow



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Molecules suddenly became real in 1905, when Albert Einstein showed that Brownian motion, the irregular microscopic movements of tiny pollen grains floating in water, could be directly attributed to collisions with molecule-sized particles.

•



ordinary salt, NaCl (see below.)

Finally, we get to see one! In 2009, IBM scientists in Switzerland succeeded in imaging a real molecule, using a technique known as <u>atomic force microscopy</u> in which an atoms-thin metallic probe is drawn ever-so-slightly above the surface of an immobilized pentacene molecule cooled to nearly absolute zero. In order to improve the image quality, a molecule of carbon monoxide was placed on the end of the probe.

The image produced by the AFM probe is shown at the very bottom. What is actually being imaged is the surface of the electron clouds of the molecule, which consists of five hexagonal rings of carbon atoms with hydrogens on its periphery. The tiny bumps that correspond to these hydrogen atom attest to the remarkable resolution of this experiment.

The original article was published in *Science magazine*; see here for an understandable account of this historic work.

The atomic composition of a molecule is given by its **formula**. Thus the formulas CO, CH_4 , and O_2 represent the molecules carbon monoxide, methane, and dioxygen.

However, the fact that we can write a formula for a compound does not imply the existence of molecules having that composition. Gases and most liquids consist of molecules, but many solids exist as extended lattices of atoms or ions (electrically charged atoms or molecules.) For example, there is no such thing as a "molecule" of

Confused about the distinction between molecules and compounds?

Maybe the following will help:



Structure and properties

Composition and structure lie at the core of Chemistry, but they encompass only a very small part of it. It is largely the *properties* of chemical substances that interest us; it is through these that we experience and find uses for substances, and much of chemistry-as-a-science is devoted to understanding the relation between structure and properties. For some purposes it is convenient to distinguish between chemical properties and physical properties, but as with most human-constructed dichotomies, the distinction becomes more fuzzy as one looks more closely.

[image link]

Putting it all together

This concept map offers a good overview of the ideas we have developed so far. Take some time to look it over and make sure you understand all the terms and the relations between them.



For a more in-depth treatment of much of the material covered here, please see <u>*The basics of atoms, moles, formulas equations, and nomenclature.*</u>



3 Chemical change

Chemical change is defined macroscopically as a process in which new substances are formed. On a microscopic basis it can be thought of as a re-arrangement of atoms. A given chemical change is commonly referred to as a chemical reaction and is described by a chemical equation that has the form

reactants \rightarrow products

Chemical change vs. physical change

In elementary courses it is customary to distinguish between "chemical" and "physical" change, the latter usually relating to changes in physical state such as melting and vaporization. As with most human-created dichotomies, this begins to break down when examined closely. This is largely because of some ambiguity in what we regard as a distinct "substance".

	Example: sodium chloride, NaCl.
Example: dichlorine, Cl₂. Elemental chlorine exists as the diatomic molecule Cl_2 in the gas, liquid, and solid states; the major difference between them lies in the degree of organization. In the gas the molecules move about randomly, whereas in the solid they are constrained to locations in a 3-dimensional lattice. In the liquid, this tight organization is relaxed, allowing the molecules to slip and slide around each other. Since the basic molecular units remain the same in all three states, the processes of melting, freezing, condensation and vaporization are usually regarded as <i>physical</i> rather than chemical changes.	Solid salt consists of an indefinitely extended 3- dimensional array of Na ⁺ and Cl ⁻ <i>ions</i> (electrically- charged atoms.) When heated above 801°C, the solid melts to form a liquid consisting of these same ions. This liquid boils at 1430° to form a vapor made up of discrete molecules having the formula Na ₂ Cl ₂ . Salt dissolves in water to form a solution containing separate Na ⁺ and Cl ⁻ ions to which are loosely attached varying numbers of H ₂ O molecules. The resulting hydrated ions are represented as Na ⁺ (aq) and Cl ⁻ (aq). Because the ions in the solid, the hydrated ions in the solution, and the molecule Na ₂ Cl ₂ are really different chemical species, the distinction between physical and chemical change becomes a bit fuzzy.

4 Energetics of chemical change

You have probably seen chemical reaction equations such as the "generic" one shown below:

$\mathsf{A} + \mathsf{B} \to \mathsf{C} + \mathsf{D}$

An equation of this kind does *not* imply that the reactants A and B will change entirely into the products C and D, although in many cases this will be what appears to happen. Most chemical reactions proceed to some inermediate point that yields a mixture of reactants and products.

For example, if the two gases phosphorus trichloride and chlorine are mixed together at room temprature, they will combine until about half of them have changed into phosphorus pentachloride:

$$PCI_3 + CI_2 \rightarrow PCI_5$$

At other temperatures the extent of reaction will be smaller or greater. The result, in any case, will be an *equilibrium mixture* of reactants and products.

The most important question we can ask about any reaction is "what is the equilibrium composition"?

- If the answer is "all products and negligible quantities of reactants", then we say the reaction can takes place and that it "goes to completion ".
- If the answer is "negligible quantities of products", then we say the reaction cannot take place in the forward direction, but that the reverse reaction can occur.
- If the answer is "significant quantities of all components" (both reactans and products) are present in the equilibrium mixture, then we say the reaction is "reversible" or "incomplete".

The aspect of "change" we are looking at here is a *property of a chemical reaction*, rather than of any one substance. But if you stop to think of the huge number of possible reactions between the more than 15 million known substances, you can see that it would be an impossible task to measure and record the equilibrium compositions of every possible combination.

Fortunately, we don't need to do this. One or two directly measurable properties of the individual reactants and products can be combined to give a number from which the equilibrium composition at any temperature can be easily calculated. There is no need to do an experiment!

This is very much a macroscopic view because the properties we need to directly concern ourselves with are those of the reactants and products. Similarly, the equilibrium composition— the measure of the extent to which a reaction takes place — is expressed in terms of the quantities of these substances.

Chemical Thermodynamics

Virtually all chemical changes involve the uptake or release of energy, usually in the form of heat. It turns out that these energy changes, which are the province of *chemical thermodynamics*, serve as a powerful means of predicting whether or not a given reaction can proceed, and to what extent. Moreover, all we need in order to make this prediction is information about the energetic properties of the reactants and products; there is no need to study the reaction itself. Because these are bulk properties of matter, chemical thermodynamics is entirely macroscopic in its outlook.

[image link] 1





5 Dynamics of chemical change

The energetics of chemical change that we discussed immediately above relate to the *end result* of chemical change: the composition of the final reaction mixture, and the quantity of heat liberated or absorbed.

Energetics determine *whether, and to what extent* a reaction can take place; *dynamics* of chemical change are concerned with **how** (and *how repidly*) the reaction takes place

- What has to happen to get the reaction started (which molecule gets bumped first, how hard, and from what direction?)
- Does the reaction take place in a single step, or are multiple steps and intermediate structures involved?

Mechanism of chemical change

These details constitute what chemists call the *mechanism* of the reaction.

For example, the reaction between nitric oxide and hydrogen (identified as the net reaction at the bottom left), is believed to take place in the two steps shown here. Notice that the nitrous oxide, N_2O , is formed in the first step and consumed in the second, so it does not appear in the net reaction equation. The N_2O is said to act as an *intermediate* in this reaction. Some intermediates are unstable species, often distorted or incomplete molecules that have no independent existence; these are known as *transition states*.





of what happens when the atoms in the reacting species re-arrange themselves into the configurations they have in the products.

[image link]

Mechanisms, unlike energetics, cannot be predicted from information about the reactants and products; chemical theory has not yet advanced to the point were we can do much more than make educated guesses. To make matters even more complicated (or, to chemists, *interesting!*), the same reaction can often proceed via different mechanisms under different conditions.

Kinetics of chemical change

Because we cannot directly watch the molecules as they react, the best we can usually do is to infer a reaction mechanism

from experimental data, particularly that which relates to the rate of the reaction as it is influenced by the concentrations of the reactants. This entirely experimental area of chemical dynamics is known as *kinetics*.

Reaction rates, as they are called, vary immensly: some reactions are completed in microseconds, others may take years; many are so slow that their rates are essentially zero. To make things even more interesting, there is no relation between reaction rates and "tendency to react" as governed by the factors in the top half of the above diagram; the latter can be accurately predicted from energetic data on the substances (the properties we mentioned in the previous screen), but reaction rates must be determined by experiment.

Catalysts

Catalysts can make dramatic changes in rates of reactions, especially in those whose un-catalyzed rate is essentially zero. Consider, for example, this rate data on the decomposition of hydrogen peroxide. H_2O_2 is a by-product of respiration that is poisonous to living cells which have, as a consquence, evolved a highly efficient *enzyme* (a biological catalyst) that is able to destroy peroxide as quickly as it forms. Catalysts work by enabling a reaction to proceed by an alternative mechanism.

$H_2O_2 \rightarrow 2 H_2O + O_2$	
	relative rate
no catalyst	1
platimum catalyst	24,000
catalase enzyme	2,900,000,000

In some reactions, even *light* can act as a catalyst. For example, the gaseous elements hydrogen and chlorine can remain mixed together in the dark indefinitely without any sign of a reaction, but in the sunlight they combine explosively.



6 Currents of modern Chemistry

In the preceding section we looked at chemistry from a conceptual standpoint. If this can be considered a "macroscopic" view of chemistry, what is the "microscopic" view? It would likely be what chemists actually do. Because a thorough exploration of this would lead us into far more detail than we can accommodate here, we will mention only a few of the areas that have emerged as being especially important in modern chemistry.

Separation science in Chemistry

A surprisingly large part of chemistry has to do with isolating one component from a mixture. This may occur at any number of stages in a manufacturing process, including the very critical steps involved in removing toxic, odiferous, or otherwise undesirable by-products from a waste stream. But even in the research lab, a considerable amount of effort is often devoted to separating the desired substance from the many components of a reaction mixture, or in separating a component from a complex mixture (for example, a drug metabolite from a urine sample) prior to measuring the amount present.

Distillation

is used to separate liquids having different boiling points. This ancient technique (believed to have originated with <u>Arabic alchemists</u> in 3500 BCE), is still one of the most widely employed operations both in the laboratory and in industrial processes such as <u>oil refining</u>.

Solvent extraction -

Separation of substances based on their differing solubilities. A common laboratory tool for isolating substances from plants and chemical reaction mixtures. Practical uses include processing of radioactive wastes and decaffienation of coffee beans. The separatory funnel shown here is the simplest apparatus for liquid-liquid extraction; for solid-liquid extraction, the <u>Soxhlet apparatus</u> is commonly used.





Chromatography

This extremely versatile method depends on the tendency of different kinds of molecules to adsorb (attach) to different surfaces as they travel along a "column" of the adsorbent material. Just as the progress of



people walking through a shopping mall depends on how long they spend looking in the windows they pass, those molecules that adsorb more strongly to a material will emerge from the chromatography column more slowly than molecules that are not so strongly adsorbed.

Paper chromatography of plant juice [link] \rightarrow

Gel electrophoresis

is a powerful method for separating and "fingerprinting" macromolecules such as nucleic acids or proteins on the basis of physcal properties such as size and electric charge.

Identification and assay in Chemistry

What do the following people have in common?

- A plant manager deciding on whether to accept a rail tank car of vinyl chloride for manufacture into plastic pipe
- An agricultural chemist who wants to know about the vitamin content of a new vegetable hybrid
- The manager of a city water-treatment plant who needs to make sure that the carbonate content of the water is maintained high enough to prevent corrosion, but low enough to prevent scale build-up

The answer is that all depend on **analytical techniques** — measurements of the nature or quantity ("assays") of some substance of interest, sometimes at very low concentrations.



"In the early 1900's a chemist could analyze about 200 samples per year for the major rock-forming elements. Today, using modern tools, two chemists can perform the same type of analyses on 7,000 samples per year."

[image from the U.S. Geological Survey]

A large amount of research is devoted to finding more accurate and convenient means of identifying substances. Many of these involve sophisticated instruments; among the most widely used are the following:

Spectrophotometry

examines the ways that light of various wavelengths is absorbed, emitted, or altered by atomic and molecular species, providing clues to their structures, and also as a means of "fingerprinting" a substance. In the example shown here, the light is in the infrared range, which excites spring-like motions of chemically-bonded atoms. This provides a quick way of identifying the kind of chemical bonds present in a molecule an important tool in determining its structure.

[image link]





Atomic emission spectrophotometry , another widelyemployed spectroscopy method, analyzes the light emitted by the various atoms in a substance. When any atom is heated to a very high temperature, electrons are raised in energy to short-lived "excited" states, which emit light as they decay back to the "ground" state. Each kind of atoms produces a characteristic line spectrum that uniquely identifies it. This serves as an important tool in the laboratory, where exitation is provided by a flame or an electrical discharge. But is also essential to astronomers as a means of identifying both the compositions and distances of stars.

More on atomic line spectra

You have probably observed everal of these spectra without even knowing it! Na (sodium) emits visible light only in the yellow region; this accounts for the yellow color of sodium-vapor street lights. Mercury-vapor lamps (Hg), also used in outdoor lighting, have their strongest emission lines in the blue region, accounting for their characteristic hue. Finally, tubes filled with neon (Ne) gas are widely seen in advertising signs.

Mass spectrometers

break up molecules into fragments that can be characterized by fragmenting them into ions which are then accelerated through an electric field. The resulsing beam passes through a magnetic field which deflectes them into individual components according to their charge-to-mass ratios. A detector at the end of the beam then measures the intensity of each component and sends this information to a computer which plots out the mass spectrum.

> The red lines at the right show how this molecule was broken into the ionized fragments that resulted in the spectrum shown at the left.

Black Body and Line Spectra









NMR spectrometry

analyzes the action of radio waves and magnetic fields on atomic nuclei in order to examine the nature of the chemical bonds attached to a particular kind of atom. NMR is one of the most commonly employed tools for determining the structure of a molecule.

> Shown here is the NMR spectrum of ethanol, CH_3-CH_3-OH . The three peaks in the spectrum represent the three environments of hydrogen atoms in the molecule. The rightmost peak, representing CH_3 hydrogens, is three times as high as the leftmost peak, reflecting the smaller abundance of -OH hydrogens. [<u>mage link</u>] \rightarrow fermation: PSC With Witheredie

More information: <u>RSC Wiki</u> - <u>Wikipedia</u>

X-ray fluorescence (XRF)

This widely-used technique is similar to atomic emission spectrometry (described above), but has the important advantage of not destroying the sample. XRF and other non-destructive methods now allow art historians to determine the kinds of pigments used in old paintings and ancient pottery. $[link] \rightarrow$

How it works. X-rays temporarily knock electrons out of atomic orbitals; when the electrons fall back into the atoms, they produce new X-rays that reflect the various electron energy levels characteristic of that particular element. XRF can detect elements present over an extraordinarily wide concentration range, from 100% to sub-ppb levels.





Materials, polymers, and nanotechnology chemistry

<u>Materials science</u> attempts to relate the physical properties and performance of engineering materials to their underlying chemical structure with the aim of developing improved materials for various applications. <u>*The Role of Chemistry in Materials Science*</u> (a non-technical overview)

Polymer chemistry

develops polymeric ("plastic") materials for industrial uses. Connecting individual polymer molecules by cross-links (red) increases the strength of the material. Thus ordinary polyethylene is a fairly soft material with a low melting point, but the cross-linked form is more rigid and resistent to heat. [link]-

Wikipedia article

Organic semiconductors

offer a number of potential advantages over conventional metalloid-based devices.

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Fullerenes, nanotubes and nanowires

Fullerenes were first identified in 1985 as products of experiments in which graphite was vaporized using a laser, work for which R. F. Curl, Jr., R. E.

Smally, and H. W. Kroto shared the 1996 Nobel Prize in Chemistry. Fullerene research is expected to lead to new materials, lubricants, coatings, catalysts, electro-optical devices, and medical applications.

Nanodevice chemistry

constructing molecular-scale assemblies for specific tasks such as computing, producing motions, etc.

> This "molecular motor" was developed at the vrije Universiteit Amsterdam. It is powered by the thermal energy in the environment.

> > [image link]







Biosensors and biotransporters

the surfaces of metals and semiconductors "decorated" with biopolymers can serve as extremely sensitive detectors of biological substances and infectious agents.

A single strand of DNA is attached to this gold nanoparticle. If other agents are also attached to the gold, the DNA allows the assembly to target specific cells for drug delivery, tumor detection and gene therapy. link

More: Uses in medical research (Wikipedia) - Properties and applications - Development of engineered polymers and sensors (Duke U.)



Biochemistry and Molecular biology

wide

from



fundamental studies on the chemistry of gene expression and enzyme-substrate interactions to drug design. Much of the activity in this area is directed to efforts in *drug discovery*.

Drug discovery and screening

began as a largely scattershot approach in which a pathogen or a cancer cell line was screened against hundreds or thousands of candidate substances in the hope of finding a few "leads" that might result in a useful therapy.

This field is now highly automated and usually involves combinatorial chemistry (see below) combined with innovative separation and assay methods.

But this is only the first step; a promising drug lead must then be intensely studied to make sure that it can actually be turned into a practical drug. Its molecular structure can often be modified in order to optimize properties such as solubility, toxicity, and potency. This process can take years, and failure rates are very high; the cost of bringing a new drug to market is often as much as \$100 million.



Once a drug candidate has been found, its molecular structure can often be modified in order to ohydrate structure. Computer-modeling is an essential tool in this work.

Wikipedia article on drug development

"Intelligent" drug design

begins by identifying the particular protein or other target that must be attacked or modified in order to alleviate a disease. By means of computerized molecular modeling, a candidate drug molecule is developed that can bind to the target and, in so doing, modify its behavior.

In this example, the drug (the small molecule at the "ligand binding site") is specifically engineered to fit into that location on the large protein it is to modify.

Proteomics

This huge field focusses on the relations between structure and function of proteins— of which there are about 400,000 different kinds in humans. Proteomics is related to genetics in that the DNA sequences in genes get decoded into proteins which eventually define and regulate a particular organism.





Chemical genomics

explores the chain of events in which signalling molecules regulate gene expression.



Chemical synthesis

In its most general sense, this word refers to any reaction that leads to the formation of a particular molecule. It is both one of the oldest areas of chemistry and one of the most actively persued. Some of the major threads are:

New-molecule synthesis

Chemists are always challenged to come up with molecules containing novel features such as new shapes or unusual types of bonds.

This particular molecule, galantamine, is found in certain plants that have been long used in Eastern Euroean folk medicine. It is now approved for treatment of dementia.

Its systematic name (which uniquely describes its structure) is (4a S,6R,8a S)-5,6,9,10,11,12-Hexahydro-3-methoxy-11-methyl-4a H-[1]benzofuro[3a,3,2-ef][2]benzazepin-6-ol.



Combinatorial chemistry

refers to a group of largely-automated techniques for generating tiny quantities of huge numbers of different molecules ("libraries") and then picking out those having certain desired properties. Although it is a major drug discovery technique, it also has many other applications.

Green chemistry

develops synthetic methods that focus on reducing or eliminating the use or release of toxic or non-biodegradable chemicals or byproducts.





Process chemistry

bridges the gap between chemical synthesis and chemical engineering by adapting synthetic routes to the efficient, safe, and environmentally-responsible methods for large-scale synthesis. (The design and construction of working plants is the province of <u>Chemical Engineering</u>.)

[image link]

Congratulations! You have just completed a whirlwind tour of the world of Chemistry, condensed into one quick and painless lesson— the world's shortest Chemistry course! Yes, we left out a lot of the details, the most important of which will take you a few months of happy discovery to pick up. But if you keep in mind the global hierarchy of composition/structure, properties of substances, and change (equilibrium and dynamics) that we



have developed in both macroscopic and microscopic views, you will find it much easier to assemble the details as you encounter them and to see where they fit into the bigger picture.

What you should be able to do

Make sure you thoroughly understand the following essential concepts that have been presented above.

- Distinguish beween *chemistry* and *physics*;
- Suggest ways in which the fields of engineering, economics, and geology relate to Chemistry;

• Define the following terms, and classify them as primarily *microscopic* or *macroscopic* concepts: element, atom, compound, molecule, formula, structure.

• The two underlying concepts that govern chemical change are *energetics* and *dynamics*. What aspects of chemical change does each of these areas describe?

Concept Map



 $\ensuremath{\mathbb{C}}$ 2004-2018 by Stephen Lower - last modified 2018-06-04

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