15.1 Organic Compounds

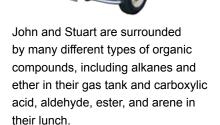
Two co-workers at a pharmaceutical company, John and Stuart, jump into John's car at noon to drive four blocks to get some lunch. The gasoline that fuels the car is

composed of many different organic compounds, including some belonging to the category of organic compounds called alkanes and a fuel additive called methyl t-butyl ether (MTBE). When they get to the restaurant, Stuart orders a spinach and fruit salad. The spinach contains a carboxylic acid called oxalic acid, and the odor from the orange and pineapple slices is due, in part, to the aldehyde 3-methylbutanal and the ester ethyl butanoate. The salad dressing is preserved with BHT, which is an example of an arene. John orders fish, but he sends it back. The smell of the amine called trimethylamine let him know that it was spoiled.

The number of natural and synthetic organic, or carbon-based, compounds runs into the millions. Fortunately, the task of studying them is not so daunting as their

number would suggest, because organic compounds can be categorized according to structural similarities that lead to similarities in the compounds' important properties. For example, you discovered in Section 5.4 that alcohols are organic compounds possessing one or more –OH groups attached to a hydrocarbon group (a group that contains only carbon and hydrogen). Because of this structural similarity, all alcohols share certain chemical characteristics. Chemists are therefore able to describe the properties of alcohols in general, which is simpler than describing each substance individually.

After reading this section, you too will know how to recognize and describe alkanes, ethers, carboxylic acids, aldehydes, esters, arenes, amines, and other types of organic compounds.



Formulas for Organic Compounds

Organic (carbon-based) compounds are often much more complex than inorganic compounds, so it is more difficult to deduce their structures from their chemical formulas. Moreover, many organic formulas represent two or more isomers, each with a Lewis structure of its own (Section 5.5). The formula $C_6H_{14}O$, for example, has numerous isomers, including

butyl ethyl ether

1-hexanol

3-hexanol

Chemists have developed ways of writing organic formulas so as to describe their structures as well. For example, the formula for butyl ethyl ether can be written CH₃CH₂CH₂CH₂CCH₂CH₃, and the formula for 1-hexanol can be written HOCH₂CH₂CH₂CH₂CH₂CH₃ to show the order of the atoms in the structure.

OBJECTIVE 2

OBJECTIVE 2

Formulas such as these that serve as a collapsed or condensed version of a Lewis structure are often called condensed formulas (even though they are longer than the molecular formulas). To simplify these formulas, the repeating $-CH_2$ – groups can be represented by CH_2 in parentheses followed by a subscript indicating the number of times it is repeated. In this convention, butyl ethyl ether becomes $CH_3(CH_2)_3OCH_2CH_3$, and 1-hexanol becomes $HOCH_2(CH_2)_4CH_3$.

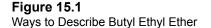
The position of the –OH group in 3-hexanol can be shown with the condensed formula CH₃CH₂CH(OH)CH₂CH₂CH₃. The parentheses, which are often left out, indicate the location at which the –OH group comes off the chain of carbon atoms. According to this convention, the group in parentheses is attached to the carbon that precedes it in the condensed formula.

CH₃CH₂CH(OH)CH₂CH₂CH₃

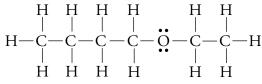
Although Lewis structures are useful for describing the bonding within molecules, they can be time consuming to draw, and they do not show the spatial relationships of the atoms well. For example, the Lewis structure of butyl ethyl ether seems to indicate that the bond angles around each carbon atom are either 90° or 180° and that the carbon atoms lie in a straight line. In contrast, the ball-and-stick and space-filling models in Figure 15.1 on the next page show that the angles are actually about 109° and that the carbons are in a zigzag arrangement. The highly simplified depiction known as a line drawing, introduced in Chapter 13, shows an organic structure's geometry better than a Lewis structure does and takes much less time to draw. Remember that in a line drawing, each corner represents a carbon, each line represents a bond (a double line is a double bond), and an end of a line without another symbol attached also represents a carbon. We assume that there are enough hydrogen atoms attached to each carbon to yield four bonds total.

OBJECTIVE 2

Study Figures 15.1, 15.2, and 15.3 and then practice converting Lewis structures into condensed formulas and line drawings, and vice versa.



OBJECTIVE 2



 $CH_3CH_2CH_2CH_2OCH_2CH_3 \ \ or \ \ CH_3(CH_2)_3OCH_2CH_3$





Carbon atoms with two hydrogen atoms attached



Carbon atoms with three hydrogen atoms attached

Figure 15.2

Ways to Describe 1-Hexanol

OBJECTIVE 2

HOCH₂CH₂CH₂CH₂CH₃ or HOCH₂(CH₂)₄CH₃

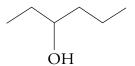


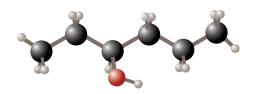


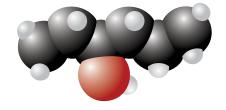
Figure 15.3
Ways to Describe 3-Hexanol

OBJECTIVE 2

CH₃CH₂CH(OH)CH₂CH₂CH₃







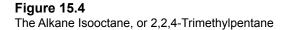
The remainder of this section lays a foundation for your future study of organic chemistry by providing brief descriptions of some of the most important families of organic compounds. Table 15.1 at the end of this section provides a summary of these descriptions.

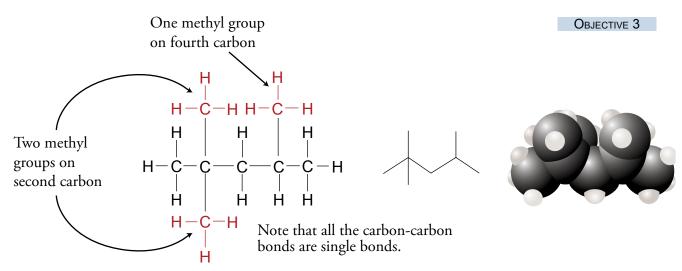
This is not the place to describe the process of naming organic compounds, which is much more complex than for inorganic compounds, except to say that many of the better known organic substances have both a systematic and a common name. In the examples that follow, the first name presented is the one that follows the rules set up by the International Union of Pure and Applied Chemistry (IUPAC). Any alternative names will be presented in parentheses. Thereafter, we will refer to the compound by whichever name is more frequently used by chemists.

Alkanes

Hydrocarbons (compounds composed of carbon and hydrogen) in which all of the carbon-carbon bonds are single bonds are called **alkanes**. An example is 2,2,4-trimethylpentane (or isooctane), depicted in Figure 15.4. To show that two methyl groups, –CH₃, come off the second carbon atom and another comes off the fourth carbon atom, its formula can be described as CH₃C(CH₃)₂CH₂CH(CH₃)CH₃ or (CH₃)₃CCH₂CH(CH₃)₂.

OBJECTIVE 3





Isooctane is used as a standard of comparison in the rating of gasoline. The "octane rating" you see at the gas pump is an average of a "research octane" value, R, determined under laboratory conditions and a "motor octane" value, M, based on actual road operation. Gasoline that has a research octane rating of 100 runs a test engine as efficiently as a fuel that is 100% isooctane. A gasoline that runs a test engine as efficiently (or, rather, inefficiently) as 100% heptane, CH₃(CH₂)₅CH₃, has a zero research octane rating. A gasoline that has a research octane rating of 80 runs a test engine as efficiently as a mixture of 80% isooctane and 20% heptane.



This gasoline pump shows the octane rating for the gasoline it pumps.

Alkenes

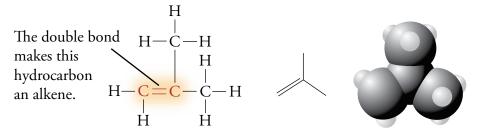
OBJECTIVE 3

Hydrocarbons that have one or more carbon-carbon double bonds are called **alkenes**. The alkene 2-methylpropene (isobutene), $CH_2C(CH_3)CH_3$ or $CH_2C(CH_3)_2$, is used to make many other substances, including the gasoline additive MTBE and the antioxidant BHT (Figure 15.5).

All alkenes have very similar chemical and physical properties, primarily determined by the carbon-carbon double bond. When a small section of an organic molecule is largely responsible for the molecule's chemical and physical characteristics, that section is called a **functional group**.

Figure 15.5The Alkene 2-Methylpropene (Isobutene)

OBJECTIVE 3



Alkynes



The energy necessary to weld metals with an oxyacetylene torch comes from the combustion of acetylene.

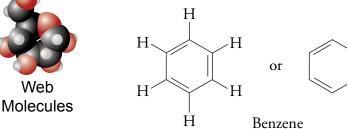
Hydrocarbons that have one or more carbon-carbon triple bonds are called **alkynes**. The most common alkyne is ethyne (acetylene), C_2H_2 (Figure 15.6). It is the gas used in oxyacetylene torches.

Figure 15.6
The Alkyne Acetylene (or Ethyne)

The triple bond makes this hydrocarbon an alkyne. $H-C\equiv C-H$

Arenes (Aromatics)

Benzene, C_6H_6 , has six carbon atoms arranged in a ring.



OBJECTIVE 3

Compounds that contain the benzene ring are called **arenes** or **aromatics**. There are many important arenes, including butylated hydroxytoluene (BHT), which is a common antioxidant added to food containing fats and oils, and trinitrotoluene

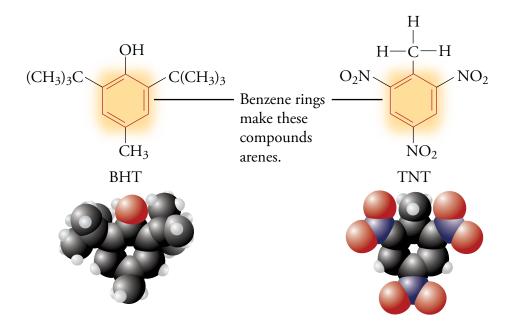


Figure 15.7The Arenes Butylated
Hydroxytoluene, BHT, and
Trinitrotoluene, TNT

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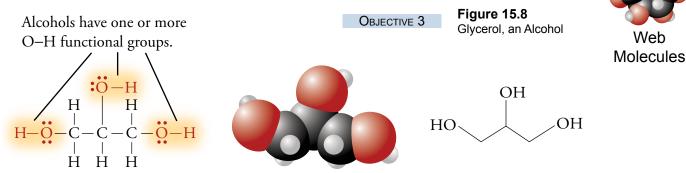
OBJECTIVE 3

Alcohols

As you learned in Chapter 5, **alcohols** are compounds with one or more -OH groups attached to a hydrocarbon group, that is, to a group consisting of only carbon and hydrogen atoms. We have encountered methanol (methyl alcohol), CH_3OH , and ethanol (ethyl alcohol), C_2H_5OH , in earlier chapters; 2-propanol (isopropyl alcohol), $CH_3CH(OH)CH_3$, is a common rubbing alcohol, and 1,2-ethanediol (ethylene glycol), $HOCH_2CH_2OH$, is a common coolant and antifreeze.

OBJECTIVE 3

The alcohol 1,2,3-propanetriol (glycerol or glycerin), HOCH₂CH(OH)CH₂OH, is used as an emollient (smoother) and demulcent (softener) in cosmetics and as an antidrying agent in toothpaste and tobacco (Figure 15.8).

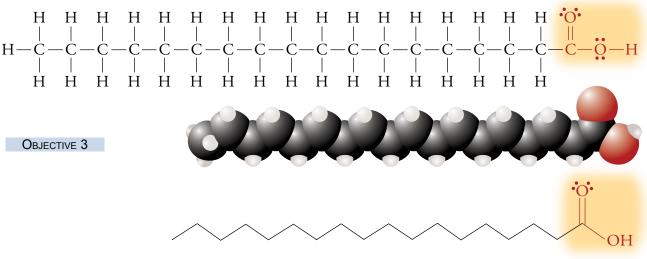


Carboxylic Acids

OBJECTIVE 3 Carboxylic acids are organic compounds that have the general formula

in which R represents either a hydrocarbon group (with all carbon and hydrogen atoms) or a hydrogen atom. The carboxylic acid functional group can be written as -COOH or $-\text{CO}_2\text{H}$. Methanoic acid (formic acid), HCOOH or HCO₂H, is the substance that causes ant bites to sting and itch. Ethanoic acid (acetic acid), written as CH_3COOH , $\text{CH}_3\text{CO}_2\text{H}$, or $\text{HC}_2\text{H}_3\text{O}_2$, is the substance that gives vinegar its sour taste. Butanoic acid (butyric acid), $\text{CH}_3\text{CH}_2\text{CH}_2\text{COOH}$ or $\text{CH}_3\text{CH}_2\text{CH}_2\text{CO}_2\text{H}$, is the substance that gives rancid butter its awful smell. Oxalic acid, HOOCCOOH or $\text{HO}_2\text{CCO}_2\text{H}$, which has two carboxylic acid functional groups, is found in leafy green plants such as spinach. Stearic acid, $\text{CH}_3(\text{CH}_2)_{16}\text{COOH}$ or $\text{CH}_3(\text{CH}_2)_{16}\text{CO}_2\text{H}$, is a natural fatty acid found in beef fat (Figure 15.9).

Figure 15.9 Stearic Acid, a Carboxylic Acid





Molecules

The Lewis structure for stearic acid can be condensed to

$$H - C + C + C - O - H$$

$$H - C + C + C - O - H$$

$$H + H + H$$

Ethers

Ethers consist of two hydrocarbon groups surrounding an oxygen atom. One important ether is diethyl ether, $CH_3CH_2OCH_2CH_3$, used as an anesthetic. A group with a condensed formula of CH_3CH_2 — is called an ethyl group and is often described as C_2H_5 —, so the formula of diethyl ether can also be $C_2H_5OC_2H_5$ or $(C_2H_5)_2O$ (Figure 15.10).

OBJECTIVE 3

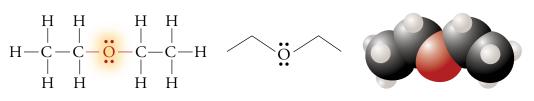


Figure 15.10 Diethyl Ether

OBJECTIVE 3

The ether tert-butyl methyl ether (methyl t-butyl ether or MTBE), $CH_3OC(CH_3)_3$, can be added to gasoline to boost its octane rating.



Web Molecules

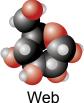
Aldehydes

Compounds called aldehydes have the general structure

OBJECTIVE 3



R can be a hydrogen atom or a hydrocarbon group. An aldehyde's functional group is usually represented by –CHO in condensed formulas. The simplest aldehyde is formaldehyde, HCHO, which has many uses, including the manufacture of polymeric resins.



Web Molecules

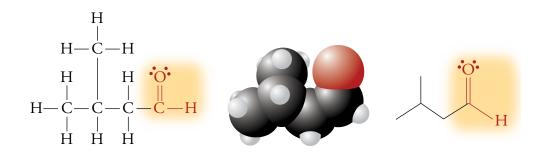
Formaldehyde

Natural aldehydes contribute to the pleasant odors of food. For example, 3-methylbutanal (isovaleraldehyde), (CH₃)₂CHCH₂CHO, is found in oranges, lemons, and peppermint. In the line drawing for aldehydes, it is customary to show

the hydrogen in the aldehyde functional group (Figure 15.11).

Figure 15.11 Isovaleraldehyde, or 3-Methylbutanal

OBJECTIVE 3



Ketones

Ketones have the general formula

OBJECTIVE 3



Web Molecules

Ketone

The hydrocarbon groups represented by R and R' can be identical or different. The most common ketones are 2-propanone (acetone), CH₃COCH₃, and 2-butanone (methyl ethyl ketone or MEK), CH₃COCH₂CH₃. Both compounds are solvents frequently used in nail polish removers (Figure 15.12).

Methyl ethyl ketone (MEK)

Figure 15.12 Acetone, a Ketone

OBJECTIVE 3

Esters

Esters are pleasant smelling substances whose general formula is

OBJECTIVE 3

$$\begin{array}{c|c} & & & \\ & & & \\ R - C - O - R' \end{array}$$

with R representing either a hydrocarbon group or a hydrogen atom, and R'

representing a hydrocarbon group. In condensed formulas, the ester functional group is indicated by either –COO– or –CO₂–. Ethyl butanoate (or ethyl butyrate), CH₃CH₂CH₂COOCH₂CH₃ or CH₃CH₂CO₂CH₂CH₃, is an ester that contributes to pineapples' characteristic odor (Figure 15.13).



Web Molecules

Amines

Amines have the general formula

OBJECTIVE 3

in which the R's represent hydrocarbon groups or hydrogen atoms (but at least one of the groups must be a hydrocarbon group). The amine 1-aminobutane (or n-butylamine), $CH_3CH_2CH_2CH_2NH_2$, is an intermediate that can be converted into pharmaceuticals, dyes, and insecticides. Amines can have more than one amine functional group. Amines often have distinctive and unpleasant odors. For example, 1,5-diaminopentane (cadaverine), $H_2N(CH_2)_5NH_2$, and 1,4-diaminobutane (putrescine), $H_2N(CH_2)_4NH_2$, form part of the odor of rotting flesh and in much smaller quantities, bad breath.

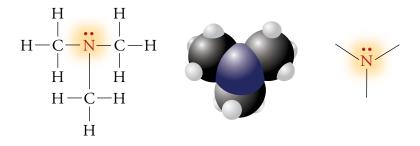


Web Molecules

Trimethylamine, (CH₃)₃N, is partly responsible for the smell of spoiled fish (Figure 15.14).

Figure 15.14 Trimethylamine, an Amine

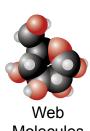
OBJECTIVE 3



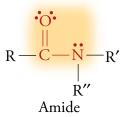
Amides

OBJECTIVE 3

Amides have the following general formula



Molecules



with the R's representing hydrocarbon groups or hydrogen atoms. In condensed formulas, the amide functional group is indicated by -CON-. The amide ethanamide (acetamide), CH3CONH2, has many uses, including the production of explosives (Figure 15.15).

Figure 15.15 Acetamide, an Amide

OBJECTIVE 3



Organic Compounds with More Than One Functional Group

Many organic compounds have more than one functional group. For example, 4-aminobutanoic acid (more often called gamma aminobutanoic acid, gamma aminobutyric acid, or GABA), H₂N(CH₂)₃COOH, has an amine functional group on one end and a carboxylic acid functional group on the other (Figure 15.16). GABA inhibits nerve cell activity in the body, as described in Special Topic 5.1: *Molecular Shapes, Intoxicating Liquids, and the Brain*.



The compound 3-hydroxybutanal (aldol), CH₃CH(OH)CH₂CHO, contains both an alcohol and an aldehyde functional group. Aldol is used to make perfumes, fungicides, and dyes (Figure 15.17).

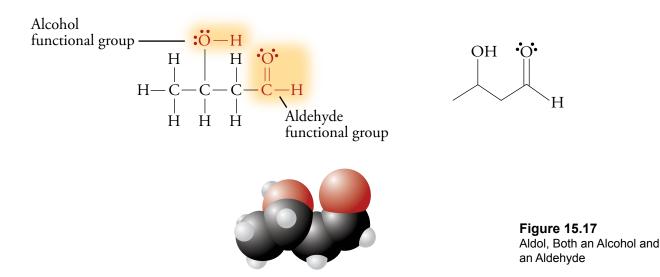


Table 15.1, on the next page, summarizes the ways in which you can recognize organic compounds.

Table 15.1 OBJECTIVE 3

Types of Organic Compounds (Unless stated otherwise, R represents either a hydrocarbon group or a hydrogen atom.)

		General		
Type of	0 10	Condensed	F 1	
Compound	General Structure	Formula	Example	
Alkane	R R	CR₃CR₃	Propane, CH ₃ CH ₂ CH ₃ , in liquid petroleum (LP) gas	H H H
Alkene	$\begin{array}{ccc} R-C=C-R \\ \mid & \mid \\ R & R \end{array}$	CR ₂ CR ₂	2-Methylpropene (isobutene), CH ₂ C(CH ₃) ₂ used to make butyl rubber, BHT (an antioxidant), and MTBE (a gasoline additive)	H H-C-H H-C=C-C-H H H
Alkyne	$R-C\equiv C-R$	CRCR	Ethyne (acetylene), C ₂ H ₂ used in oxyacetylene torches	H−C≡C−H
Arene (aromatic)	R R R R R	C ₆ R ₆	Trinitrotoluene (TNT), $CH_3C_6H_2(NO_2)_3$, an explosive	H H C H O_2N NO_2
Alcohols	R— <mark>Ö</mark> —H R≠H	ROH	Ethanol (ethyl alcohol), C ₂ H ₅ OH in intoxicating beverages	$\begin{array}{cccc} H & H \\ H - C - C - & - & - & - \\ & & H & H \end{array}$
Carboxylic acids	; ; ;; 	RCOOH or RCO ₂ H	Ethanoic acid (acetic acid), CH ₃ COOH in vinegar	H H−C−C−Ω−H H
Ethers	R—Ö—R′ R's≠H	ROR	Diethyl ether, CH ₃ CH ₂ OCH ₂ CH ₃ , an anesthetic	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
Aldehyde	⊷ H R—C—H	RCHO	Ethanal (acetaldehyde), CH ₃ CHO used to make acetic acid; created from ethanol in the human body	Н 'Ö' H—С—С—Н Н
Ketone	*O* R—C—R' R's ≠ H	RCOR	2-Propanone (acetone), CH ₃ COCH ₃ , a solvent	H *** H H-C-C-C-H H H

Ester	* ⊙ • R—C— Ö —R' R'≠H	RCOOR or RCO ₂ R	Ethyl butanoate (ethyl butyrate), CH ₃ CH ₂ CH ₂ COOCH ₂ CH ₃ smells like pineapples; used in artificial flavorings	H H H H O H H H H H H H H H H H H H H H
Amine	R—N—R' R" At least one R is a hydrocarbon group.	R ₃ N	1-Aminobutane (n-butyl amine), NH ₂ CH ₂ CH ₂ CH ₂ CH ₃ intermediate in the production of pharmaceuticals, dyes, and insecticides	H H H H H-N-C-C-C-C-H H H H H H
Amide	**************************************	RCONR ₂	Ethanamide (acetamide), CH ₃ CONH ₂ used to make explosives	H H — C — C — N — H H H

Exercise 15.1 - Organic Compounds

Identify each of these structures as representing an alkane, alkene, alkyne, arene (aromatic), alcohol, carboxylic acid, ether, aldehyde, ketone, ester, amine, or amide.

OBJECTIVE 3



Molecules

Exercise 15.2 - Condensed Formulas

OBJECTIVE 2

Write condensed formulas to represent the Lewis structures in parts a through l of Exercise 15.1.

EXERCISE 15.3 - Line Drawings

OBJECTIVE 2

Make line drawings that represent the Lewis structures in parts a through j of Exercise 15.1.

SPECIAL TOPIC 15.1 Rehabilitation of Old Drugs and Development of New Ones

Imagine that you are a research chemist hired by a large pharmaceutical company to develop a new drug for treating AIDS. How are you going to do it? Modern approaches to drug development fall into four general categories.

Old Drug, New Use One approach is to do a computer search of all of the drugs that have been used in the past to try to find one that can be put to a new use. For example, imagine you want to develop a drug for combating the lesions seen in Kaposi's sarcoma, an AIDS related condition. These lesions are caused by the abnormal proliferation of small blood vessels. A list of all of the drugs that are thought to inhibit the growth of blood vessels might include some that are effective in treating Kaposi's sarcoma.

One of the drugs on that list is thalidomide, originally developed as a sedative by the German pharmaceutical company Chemie Gruenenthal in the 1950s. Thalidomide was considered a safe alternative to other sedatives, which are lethal in large doses; but when it was also used to reduce the nausea associated with pregnant women's "morning sickness," it caused birth defects in the babies they were carrying. Thalidomide never did receive approval in the United States, and it was removed from the European market in the 1960s. About 10,000 children were born with incompletely formed arms and legs owing to thalidomide's effects.

Thalidomide is thought to inhibit the formation of limbs in the fetus by slowing the formation of blood vessels, but what can be disastrous for unborn children can be lifesaving for others. Today the drug is being used as a treatment for Kaposi's sarcoma and may be helpful in treating AIDS related weight loss and brain cancer as well.

Old Drug, New Design Another approach to drug development is to take a chemical already known to have a certain desirable effect and alter it slightly in hopes of enhancing its potency. The chemists at the Celgene Corporation have taken this approach with thalidomide. They have developed a number of new drugs similar in structure to thalidomide that appear to be 400 to 500 times more potent.

Rational Drug Design In a third, more direct, approach, often called rational drug design, the researcher first tries to determine what chemicals in the body are leading to the trouble. Often these chemicals are enzymes, large molecules that contain an active site in their structure where other molecules must fit to cause a change in the body. Once the offending enzyme is identified, isolated, and purified,

it is "photographed" by x-ray crystallography, which in combination with sophisticated computer analysis reveals the enzyme's three-dimensional structure, including the shape of the active site. The next step is to design a molecule that will fit into the active site and deactivate the enzyme. If the enzyme is important for the replication of viruses like the AIDS virus or a flu virus, the reproduction of the virus will be slowed.

Combinatorial Chemistry The process of making a single new chemical, isolating it, and purifying it in quantities large enough for testing is time-consuming and expensive. If the chemical fails to work, all you can do is start again and hope for success with the next. Thus chemists are always looking for ways to make and test more new chemicals faster. A new approach to the production of chemicals, called combinatorial chemistry, holds great promise for doing just that.

Instead of making one new chemical at a time, the strategy of combinatorial chemistry is to make and test thousands of similar chemicals at the same time. It therefore requires highly efficient techniques for isolating and identifying different compounds. One way of easily separating the various products from the solution in which they form is to run the reaction on the surface of tiny polymer beads that can be filtered from the reaction mixture after the reaction takes place. The beads need to be tagged in some way, so the researcher can identify which ones contain which new substance. One of the more novel ways of doing this is to cause the reaction to take place inside a tiny capsule from which a microchip sends out an identifying signal.

After a library of new chemicals has been produced, the thousands of compounds need to be tested to see which have desirable properties. Unfortunately, the procedures for testing large numbers of chemicals are often less than precise. One approach is to test them each in rapid succession for one characteristic that suggests a desired activity. A secondary library is then made with a range of structures similar to the structure of any substance that has that characteristic, and these new chemicals are also tested. In this way, the chemist can zero in on the chemicals that are most likely to have therapeutic properties. The most likely candidates are then made in larger quantities, purified more carefully, and tested in more traditional ways. Combinatorial chemistry has shown promise for producing pharmaceuticals of many types including anticancer drugs and drugs to combat AIDS.