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Organic Chemistry

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CHAPTER -

Organic Chemistry

CHAPTER OUTLINE

1.1	Carbon, A Unique Element
1.2	Hydrocarbons
1.3	Aromatics
1.4	Functional Groups
1.5	Biochemical Molecules

1.6 References

1.1 Carbon, A Unique Element

Lesson Objectives

The student will:

- describe the hybridization states available to carbon.
- explain how the hybridization of carbon allows for the formation of large number of compounds containing carbon.
- describe the three primary allotropes of carbon.

Vocabulary

- allotropes
- delocalized electrons

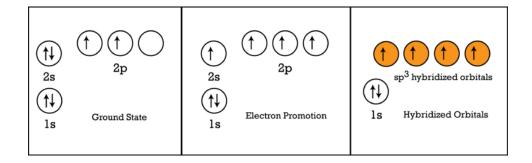
Introduction

Carbon plays a unique role among the chemical elements. You may have heard of life on earth being referred to as "carbon-based." Although the molecules that make up living creatures also contain large amounts of hydrogen, oxygen, nitrogen, phosphorus, and sulfur, these atoms are all generally stitched together by long carbon chains. Due to its four valence electrons, carbon is the smallest element that is able to make covalent bonds to four different atoms in its neutral form. Because of this, large, heavily branched compounds can be made by stringing together carbon and a few other nonmetallic atoms in various arrangements. The almost limitless number of compounds that can be constructed in this way is the focus of organic chemistry.

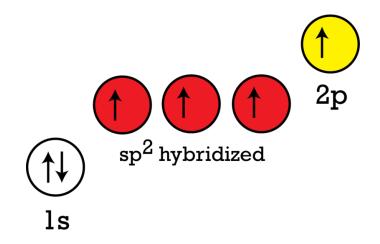
Hybridization

Recall from the chapter "Covalent Bonds and Formulas" that *s* and *p* atomic orbitals can be combined in various ratios to make a set of hybrid orbitals. During hybridization, the number of orbitals combined to make the hybrids is always equal to the number of orbitals created. Thus, carbon will always have a total of four valence orbitals, regardless of how it is hybridized.

When one *s* and three *p* orbitals are combined, it produces a set of four sp^3 orbitals (see figure below). These orbitals are all identical to one another, and they point outward from the carbon atom toward the corners of a tetrahedron. Recall from VSEPR theory that when a central atom is bonded to four different atoms, they are arranged into the shape of a tetrahedron. The shapes of the hybrid orbitals used to make these bonds help explain why this arrangement is chosen.



When one *s* and two *p* orbitals are combined, a set of three identical sp^2 orbitals is created (see below). These orbitals have a trigonal planar arrangement, which is what we would expect from VSEPR theory for a central atom bonded to three other atoms, assuming it has no unshared electron pairs. In addition to the three hybrid orbitals created, the carbon atom will still have one leftover *p* orbital oriented perpendicular to the other three. This orbital is available for side-by-side overlap with other *p* orbitals, forming a pi bond.



Lastly, *sp* orbitals are created by combining one *s* and one *p* orbital, leaving two unchanged *p* orbitals available for pi bonding. The two *sp* orbitals point in opposite directions, which is again what one would expect by looking at VSEPR theory. The number of different hybridization states available to carbon further amplifies the number of organic (carbon-containing) compounds that can be made.

Allotropes of Carbon

Carbon can exist in at least three different forms based on the arrangement of bonds between the atoms. Although these substances are comprised only of carbon atoms, they have quite different properties. When a pure element exists in multiple forms due to different bonding arrangements, these forms are referred to as **allotropes**. Note that different phases (solid, liquid, gas) of an element are not considered to be allotropes; a family of allotropes must all be in the same phase. The three primary allotropes of carbon are diamond, graphite, and fullerenes.

The structure of diamond consists exclusively of sp^3 hybridized carbon atoms. Each one is bound to four other carbon atoms in a tetrahedral array (see **Figure 1.1**). This is a very stable structure, because each atom is held in place by four strong sigma bonds. Consequently, diamonds are extremely hard, and the diamond form of carbon has the highest melting point (>3500°C) of all known elements. Diamond has the rare property that it is a good conductor of heat but a poor conductor of electricity. Electricity is transmitted by the movement of electrons, and since all the valence electrons of diamond are held tightly in localized sigma bonds, very little electric current can flow through the solid.

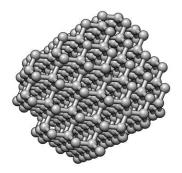


FIGURE 1.1 Diamond lattice structure.

Graphite, most commonly encountered as pencil lead, is clearly a very different substance. The reason for the differing properties has to do with how the atoms are bonded to one another. The structure of graphite is shown in **Figure 1.2**.

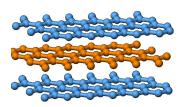


FIGURE 1.2

Graphite structure with multiple layers.

The carbon atoms are sp^2 hybridized, and each carbon makes a strong sigma bond to three other atoms, forming hexagonal sheets. However, this only accounts for three of carbon's four valence electrons. The remaining electron is located in the leftover p orbital. This orbital can overlap with the leftover p orbital from all the adjacent carbon atoms, forming pi bonds. Unlike sigma bonds, where the electrons are held tightly between the two nuclei, pi bonds can interact with adjacent pi bonds, allowing the electrons in those bonds to **delocalize** over all the atoms involved.

Within a sheet of graphite, the carbon atoms are held together by strong sigma bonds. The bond between sheets, however, involves a weaker interaction between the delocalized pi systems of two adjacent sheets. Because of the delocalization, a carbon from one sheet is not rigidly attached to any single carbon from an adjacent sheet, which allows the sheets to slide around freely. For this reason, graphite can be used as a lubricant. When you write with a pencil, the marks left on the paper are sheets of graphite that have slipped all the way off the carbon rod.

Unlike diamond and graphite, which are covalent networks that can extend indefinitely, fullerenes often have a fixed size, forming what are essentially individual molecules made only of carbon. The first fullerene to be discovered was buckminsterfullerene, C_{60} , often referred to as a buckyball (see **Figure 1**.3).

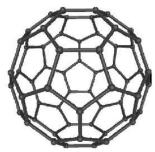




FIGURE 1.3 Buckyball structure (left) compared to soccer ball (right). This allotrope of carbon was not even isolated until 1985, although its possible existence had been postulated in the mid-20th century. A great deal of current research in medicinal chemistry and material science is devoted to the study of this relatively new class of compounds. Examples include carbon nanotubes (fullerenes that fold into a tube instead of a sphere) and superconducting metal-fullerene complexes.

Lesson Summary

- Hybridization is the process of combining atomic orbitals from different subshells to create a new set of orbitals that are all identical to one another. The electrons in these orbitals have equal energy and can all form identical covalent bonds.
- Electrons located in p orbitals that are not used during hybridization are available for side-by-side (pi) bonding.
- Allotropes are the different forms that can be taken by a pure element. Each allotrope is a unique substance with its own chemical properties.
- The differences between allotropes stem from the different bonding arrangements available to those atoms.
- The three primary allotropes of carbon are diamond, graphite, and fullerenes.

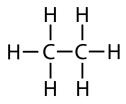
Further Reading / Supplemental Links

The *learner.org* website allows users to view streaming videos of the Annenberg series of chemistry videos. You are required to register before you can watch the videos but there is no charge. The website has one video that relates to this lesson called "Carbon."

• http://learner.org/resources/series61.html

Review Questions

- 1. Carbon is considered to be unique in the periodic table. What property of the carbon atom makes it unique?
- 2. What is the difference between sp, sp^2 , and sp^3 hybridization?
- 3. Which of the following are allotropes of carbon?
 - a. diamond
 - b. buckminsterfullerene
 - c. graphite
 - d. all of the above
- 4. What is the hybridization of the carbon atoms in each of the following molecules:



a. spb. sp^2 c. sp^3

d. dsp^3

1.2 Hydrocarbons

Lesson Objectives

The student will:

- define structural isomers and be able to draw isomers for selected compounds
- differentiate between alkanes, alkenes, and alkynes
- name alkanes, alkenes, and alkynes when given a structure
- draw alkanes, alkenes, and alkynes when given a name
- explain the difference between saturated and unsaturated hydrocarbons

Vocabulary

- alkane
- alkene
- alkyne
- functional group
- · saturated compound
- structural isomers
- unsaturated compound

Introduction

The basic skeleton of any organic molecule consists primarily of carbon and hydrogen atoms bounded to one another in various arrangements. In this section, we will explore various types of organic compounds that include only carbon and hydrogen. In a later section, we will consider the additional possibilities that exist when other atoms are bound to a hydrocarbon backbone.

Alkanes

Alkanes are the simplest hydrocarbons. All carbon atoms are sp^3 hybridized, and each carbon atom makes four sigma bonds. Depending on the size of the chain, alkanes can exist as solids, liquids, or gases at room temperature. Alkanes are non-polar molecules, so they are not soluble in water.

At low temperatures, alkanes are generally not very reactive compared to most other organic molecules. However, when provided with an initial source of energy, alkanes can react with oxygen (a combustion reaction) to produce carbon dioxide and water. Because of this property, many alkanes are used as fuels, including methane (natural gas),

propane (used in gas grills), butane (found in lighters), and octane (found in gasoline). Larger alkanes exist as waxy solids. Since they burn less quickly than their smaller counterparts, they are used to make candles.

Naming Alkanes

Due to the immense variety of possible organic structures that can exist, it is necessary to have a systematic method for naming these compounds so that chemists can communicate with one another. There are a set of fairly straightforward rules that will allow you to name most of the organic compounds you will encounter.

The basic starting point for learning about organic nomenclature is to look at the straight-chain alkanes. The first ten are compiled in **Table 1.1**. Note that although the structures are drawn in a linear format, the shape around each carbon atom is still tetrahedral. Thus, the actual three-dimensional structure of these compounds would look more like a zig-zag.

TABLE 1.1: First Ten Alkanes

Name methane	Formula CH4	Structural Formula
		H H H H H
ethane	C ₂ H ₆	
		H H H-C-C-H H H
propane	C_3H_8	ннн
		H H H I I I H-C-C-C-H I I I H H H
butane	C_4H_{10}	й й й й
		H H H H I I I H-C-C-C-H I I I H H H H
pentane	C ₅ H ₁₂	H H H H H I I I I I H-C-C-C-C-H I I I I I H H H H
hexane	C ₆ H ₁₄	
		H H H H H H H-C-C-C-C-C-H H H H H H H

TABLE 1.1: (continued)

Name heptane	Formula C ₇ H ₁₆	Structural Formula
		$\begin{array}{cccccccccccccccccccccccccccccccccccc$
octane	C ₈ H ₁₈	
nonane	C ₉ H ₂₀	
		Н Н Н Н Н И И И И H-C-C-C-C-C-C-C-C-C-H
decane	$C_{10}H_{22}$	
		н н н н н н н н н н-с-с-с-с-с-с-с-с-с-с-н н н н н н н н н н н

The names of these simple compounds consist of two parts. As you may be able to deduce from the examples, the suffix "-ane" indicates that these compounds are alkanes. The first part of the name indicates how many carbon atoms are in the chain. The prefixes associated with each number are shown in **Table 1**.2. These should be committed to memory.

TABLE 1.2: Numerical Prefixes for Straight Chain Organic Compounds

Number of C atoms in the longest chain 1	Numerical Prefix meth-
2	eth-
3	prop-
4	but-
5	pent-
6	hex-
7	hept-
8	oct-
9	non-
10	dec-

Example:

Name the following molecule:

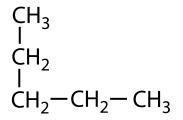
$$CH_3-CH_2-CH_2-CH_2-CH_3$$

Solution:

This is a straight chain hydrocarbon with all single bonds. Therefore, it is an alkane. Since the longest straight chain contains 5 carbon atoms, it is pentane.

You should recognize that the actual molecule does not look like this straight chain picture. The bonding around every carbon atom is a tetrahedron. Therefore, these molecules look more like saw teeth than they do straight chains.

They are drawn in straight lines to make it easier to draw them. If the same molecule is drawn with a bend in it, it is still a straight chain (see below).



This molecule is still a 5-carbon straight chain and is still pentane.

Various side chains of carbon atoms can be attached to the straight chain. When a hydrocarbon side chain is attached to the straight chain, the side chain is named according to the following **Table 1.3**.

Alkyl Groups	Group Name	
$-CH_3$	methyl	
$-CH_2CH_3$	ethyl	
$-CH_2CH_2CH_3$	propyl	
$-CH_2CH_2CH_2CH_3$	butyl	
$-CH_2CH_2CH_2CH_2CH_3$	pentyl	

TABLE 1.3: Alkyl Groups Branches

A side chain can be attached to any carbon but the end carbons in a straight chain. If the chain were attached to an end carbon, it would be part of the straight chain. Here is a straight chain hydrocarbon with a methyl side chain attached.

$$CH_3$$

$$I$$

$$CH_3 - CH_2 - CH - CH_2 - CH_2 - CH_2 - CH_3$$

When naming this compound, we must first identify both the parent chain and the side chain. The parent chain is the longest straight chain of carbon atoms. Be careful, because this chain is not always drawn in a straight line. Additionally, we must indicate the carbon atom to which the side chain is attached. In order to identify the carbon atom to which the side chain is attached, we number the carbon atoms in the parent straight chain. Since it is possible to begin numbering at either end of the straight chain, there is a rule about how the carbon atoms are numbered. The rule is that you must number the carbon atoms in the straight chain so that the side chain is attached to the *lowest* possible numbered carbon atom. Here is the compound again with two possible numbering sequences. In the numbering on the left, the side chain is attached to carbon number 3, whereas on the right, the side chain is attached to carbon number 5. Therefore, the numbering sequence on the right is *wrong*.

$$\begin{array}{c} \mathsf{C}\mathsf{H}_3 \\ \mathsf{C}\mathsf{H}_3 - \mathsf{C}_2\mathsf{H}_2 - \mathsf{C}_3\mathsf{H} - \mathsf{C}_4\mathsf{H}_2 - \mathsf{C}_2\mathsf{H}_2 - \mathsf{C}_2\mathsf{H}_2 - \mathsf{C}_2\mathsf{H}_3 \\ \mathsf{H}_3 - \mathsf{C}_2\mathsf{H}_2 - \mathsf{C}_3\mathsf{H} - \mathsf{C}_4\mathsf{H}_2 - \mathsf{C}_3\mathsf{H}_2 - \mathsf{C}_4\mathsf{H}_2 - \mathsf{C}_4\mathsf{H}_4 - \mathsf{C}_4\mathsf{H}_4$$

To name this compound, we indicate the number of the carbon atom to which the side chain is attached, insert a hyphen after the number (no spaces in between), then name the side chain (again no spaces), and finally name the parent straight chain (again no spaces). Therefore, the correct name of this compound is 3-methylheptane.

1.2. Hydrocarbons

If two or more of the same type of side chain is present, this is indicated with a slightly different set of numerical prefixes. "Mono-" is not used because the prefix is omitted when only one of that particular side chain is present. "Eth-," "prop-," and "but-" are replaced with "di-," "tri-," and "tetra-," respectively. The remaining prefixes are the same as those shown above in **Table 1.3**.

If multiple different types of side chains are present, they are written in alphabetical order. When alphabetizing names, we ignore the secondary prefix that indicates how many of each side chain there are. Therefore, "ethyl" comes before "dimethyl."

Example:

Name the following molecule:

$$CH_{3}$$

 H_{2}
 CH_{2}
 CH_{3}
 CH_{2}
 CH_{2}
 CH_{3}
 CH_{2}
 CH_{2}
 CH_{3}
 CH_{2}
 CH_{2}
 CH_{3}
 CH_{2}
 CH_{3}
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 CH_{3}
 CH_{2}
 CH_{3}
 CH_{3

Step 1: Find the parent chain.

The longest chain in this molecules contains 8 carbon atoms. Therefore, the parent chain is octane.

<u>Step 2:</u> Name the branches and determine the carbon numbers to which they are attached. Looking at the molecule, there are two branches that are not part of the parent chain. Using **Table 1.3**, these branches can be identified as a methyl group and an ethyl group.

$$CH_{3}$$

 I
 $CH_{3} - CH_{2} - CH_{2} - CH_{2} - CH_{2} - CH_{2} - CH_{2} - CH_{3}$

Step 3: Add the name of the branches and their positions to the parent chain name.

5-ethyl-3-methyloctane

Notice that there are no spaces anywhere in the name.

Drawing Alkanes

So far, we have been given the structure of the molecule and asked to provide a name. However, there are also cases where we will be given a name and asked to draw the structure. Converting names to structures is generally easier than converting structures to names.

Example:

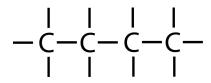
Draw the structure for butane, C_4H_{10} .

Solution:

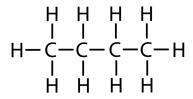
Step 1: Start by drawing the four carbon atoms in a straight chain with all the atoms connected by single bonds.

$$\mathbf{C}-\mathbf{C}-\mathbf{C}-\mathbf{C}$$

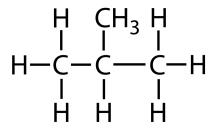
Step 2: Add single bonds until each carbon atom has four possible bonding sites.



Step 3: Add one hydrogen atom to the end of each of the single bonds formed in Step 2.



Prior to this chapter, we have mainly been considering compounds that can be uniquely identified simply by writing their chemical formula. However, this is not the case for organic molecules. In the previous example, you were asked to draw the structure for butane, C4H10. However, this is not the only way that those atoms could be arranged. Drawn below is 2-methylpropane. It is still composed of four carbon atoms and ten hydrogen atoms, but they are arranged in a different way. Two molecules that have the same formula but different bonding arrangements are referred to as **structural isomers**.

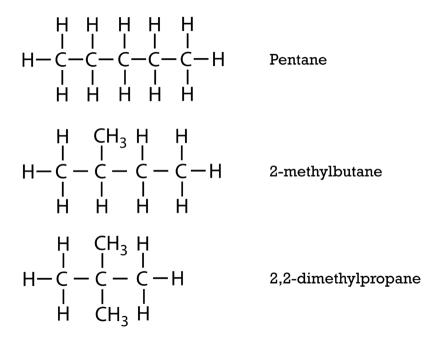


Structural isomers have the same formula, but because they have different structures, they also have different chemical properties. As the number of carbon atoms increases, the number of possible isomers increases. For example, decane has 75 structural isomers, each with its own properties. A compound such as $C_{30}H_{62}$ has 4×10^8 isomers, many of which have not even been isolated yet. With this many possible compounds, you can understand the need for this complex naming system.

Example:

Draw the structural isomers of pentane, C_5H_{12} .

Solution:



Alkenes

Alkanes provide the basic skeleton for organic molecules. Although there are vast numbers of alkanes that could potentially be constructed, the chemistry available to alkanes is quite similar and is relatively limited. Generally, the reactivity of an organic molecule is determined by its functional groups. **Functional groups** include double bonds, triple bonds, and groups that contain atoms other than carbon and hydrogen. The first functional group we will consider is an **alkene**, which is defined as a double bond between two carbon atoms.

When a molecule has only one functional group, sometimes the name of the functional group is used to refer to the entire molecule. For example, the entire 2-hexene molecule can be referred to as an alkene, even though the only double bond is between carbons 2 and 3.

Because the carbons in an alkene are not surrounded by the maximum number of other atoms, alkenes are referred to as **unsaturated**. Conversely, alkanes are referred to as **saturated**, since no additional atoms can be added to any of the carbons without removing some of the ones already present.

As we stated earlier, simple alkanes are generally not very reactive unless enough energy is added to start a combustion reaction. This can be explained by the fact that alkanes contain only C-C and C-H sigma bonds, both of which are relatively strong. In contrast, alkenes contain pi bonds, which are not as strong. Much of the chemistry of alkenes involves breaking this relatively weak bond to create two new sigma bonds between the carbons of the alkene and atoms from other molecules.

Naming Alkenes

The naming of alkenes is very similar to that for alkanes, except for a few key differences:

- 1. The end of the name is changed from "-ane" to "-ene."
- 2. The parent chain should always include the double bond, even if it is no longer the longest chain of carbon atoms.
- 3. Numbering begins at the end of the parent chain closest to the double bond
- 4. The position of the double bond is indicated by inserting the number of the carbon closest to the end just before the name of the parent chain.

Example:

Name the following compound.

$$H_3C - CH = CH - CH_2 - CH_3$$

Solution:

$$H_3 \overset{1}{C} - \overset{2}{C} H = \overset{3}{C} H - \overset{4}{C} H_2 - \overset{5}{C} H_3$$

The parent chain has five (5) carbon atoms. Using **Table 1.2**, the prefix for this compound is "pent-."

There are no branches, but the double bond is between carbons 2 and 3. Therefore the name of the molecule is 2-pentene (using the smaller of the two numbers on the carbon atoms).

Drawing Alkenes

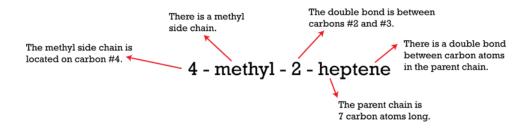
Drawing alkenes also follows the same rules as drawing alkanes. Remember to place the double bond where the name indicates its placement.

Example:

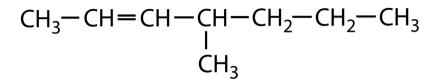
Draw the structural formula for 4-methyl-2-heptene.

Solution:

Looking at the name reveals a great deal about how to draw the structure.



Therefore, the molecule has the structure:



When numbering alkene chains, you always begin with the carbon end nearest to the double bond regardless of what this does to the side chain number.

Alkynes

An **alkyne** is a carbon-carbon triple bond. It can also refer to a molecule containing a carbon-carbon triple bond. Like alkenes, alkynes are considered unsaturated because the carbons in the triple bond are not surrounded by the maximum number of other atoms.

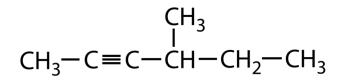
1.2. Hydrocarbons

Naming Alkynes

Alkynes are names in the same way as alkenes, except the suffix at the end of the parent chain is changed to "-yne." For these compounds, the position of the triple bond is indicated in the name of the structure.

Example:

Name the following structure.



Solution:

The parent chain has six carbon atoms. Using Table 1.2, the prefix is "hex-."

There is a triple bond, so the suffix is "-yne."

The triple bond is between carbons 2 and 3.

There is one branch on carbon 4 that is a methyl group.

Therefore the name of the molecule is 4-methyl-2-hexyne.

Drawing Alkynes

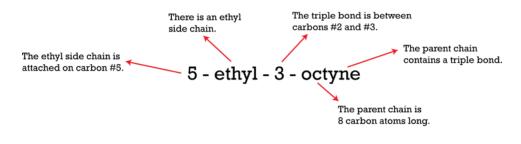
To draw alkynes, again follow the same rules as for alkanes and alkenes. Remember to place the triple bond where the name indicates its placement.

Example:

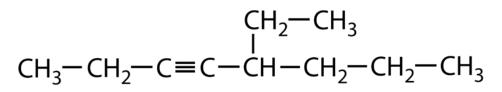
Draw the structural formula for 5-ethyl-3-octyne.

Solution:

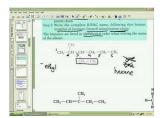
Looking at the name reveals a great deal about how to draw the structure.



Therefore, the molecule has the structure:



This video is an introduction to process of naming hydrocarbons (10d), see http://www.youtube.com/watch?v=c mzHMHw6oeA (9:02).



MEDIA

Click image to the left for more content.

Lesson Summary

- Alkanes are relatively unreactive hydrocarbons that contain only C-C and C-H single bonds.
- Alkenes contain a carbon-carbon double bond.
- Alkynes contain a carbon-carbon triple bond.
- Organic molecules containing only single bonds are referred to as saturated, while those containing double or triple bonds are referred to as unsaturated.

Further Reading / Supplemental Links

The *learner.org* website allows users to view the Annenberg series of chemistry videos. You are required to register before you can watch the videos, but there is no charge to register. The video called "Molecular Architecture" examines isomers (primarily organic molecules) and how the electronic structure of a molecule's elements and bonds affects its shape and physical properties.

• http://www.learner.org/vod/vod_window.html?pid=801

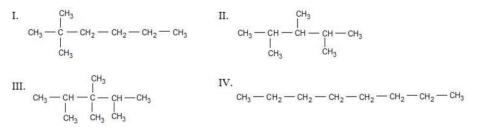
Review Questions

- 1. Define the terms alkane, alkene and alkyne.
- 2. What is the difference between a saturated and an unsaturated compound?
- 3. Which of the following organic compounds is unsaturated?
 - a. ethylcyclobutane
 - b. 3-ethyl-2-methyl-1-pentene
 - c. 2-bromobutane
 - d. 2-methyl-1-chlorohexane
- 4. Which compound is a structural isomer of the compound shown below?

- a. butane
- b. methane
- c. pentane
- d. hexane

1.2. Hydrocarbons

5. Which structures are isomers of one of the other structures?

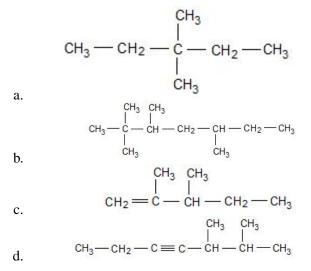


- a. I, II, III
- b. II, III
- c. I, II, IV
- d. They are all isomers.
- 6. Which of the following structures has the shortest parent chain? (There can be more than one correct answers.)

I.
$$CH_{3} - CH_{2} - CH_{2} - CH_{2} - CH_{3}$$

 $CH_{3} - CH_{2} - CH_{2} - CH_{2} - CH_{3}$
II. $CH_{3} - CH_{3} - CH_{3} - CH_{3} - CH_{3} - CH_{3}$
III. $CH_{3} - CH_{3} - CH_{3} - CH_{3} - CH_{3}$
IV. $CH_{3} - CH_{2} -$

- 7. Draw each of the following compounds.
 - a. 2,3,4-trimethylpentane
 - b. 2-chloro-1-propene
 - c. 1-bromo-2-methylbutane
 - d. Ethyne
 - e. 1-bromo-5,5-dimethylheptane
- 8. Name each of the following structures.



9. Name the isomers for C_6H_{14} .

1.3 Aromatics

Lesson Objectives

The student will:

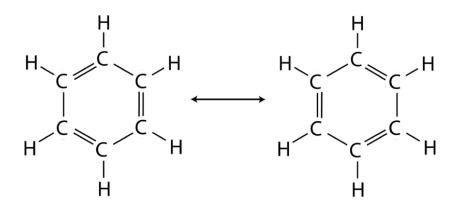
- describe the bonding in benzene.
- define aromatic compounds.
- name simple compounds containing benzene.
- draw simple compounds containing benzene.

Vocabulary

• benzene ring

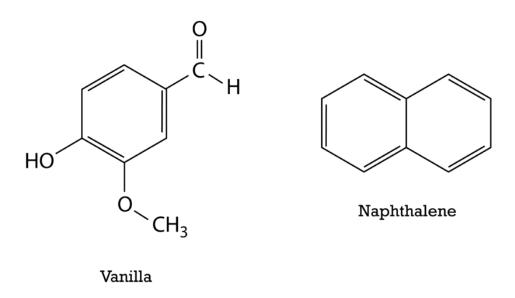
Introduction

In this lesson, we will focus on another category of organic compounds called the aromatics. One common building block of aromatic compounds is benzene. Benzene is composed of a 6-membered carbon ring commonly represented by the resonance structures below.



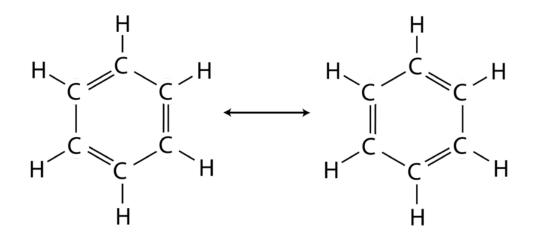
Benzene was discovered in the 1820s by Michael Faraday, but it took more than 40 years to determine the actual structure of benzene. The German organic chemist Friedrich August Kekulé is credited for discovering the benzene structure in 1865. Legend has it that Kekulé discovered the benzene structure upon awaking from a dream of a snake biting the end of its tail.

A compound classified as an aromatic doesn't necessarily have to have a pleasant smell, although many aromatic compounds do have a pleasant odor. Vanilla (structure shown below) is an example of a pleasant-smelling aromatic compound. In comparison, napthalene (structure shown below) is the chemical found in moth balls with an unpleasant smell. In short, aromaticity has to do with structure and not smell.

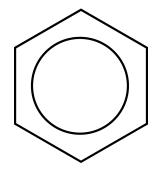


Benzene Structure

As indicated in the introduction, there are two possible structures of the benzene molecule (C_6H_6) .

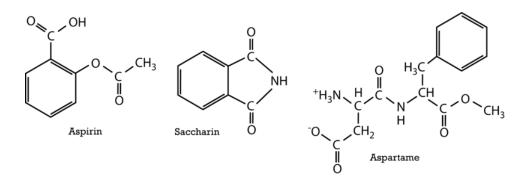


Both of these structures represent resonance structures of the benzene molecule. Recall from the chapter "Covalent Bonds and Formulas" that resonance is the theory that describes compounds whose electronic structure is not represented by any one Lewis structure, but by an average of several structures. This theory, proposed by American chemist Linus Pauling, can be used to explain the structure of benzene. Although the structure shows alternating double and single bonds, all of the bonds are actually the same length. Carbon-carbon single bonds are 154 pm long, while carbon-carbon double bonds are 134 pm in length. For benzene, however, all of the carbon-carbon bonds in benzene are 139 pm in length, so they are neither single nor double bonds. As a result, you may sometimes see a benzene structure represented as follows:



A **benzene ring**, then, is a structure that contains a ring represented by equivalent resonance structures. Benzene is an important compound in organic chemistry because of its properties and the vast number of compounds in which a benzene ring is an integral part of the structure.

Benzene is a part of many everyday items. Examples of structures where the benzene ring is an integral part of the structure include aspirin, saccharin, and aspartame (structures shown below). Aspirin is a common painkiller, while both saccharin and aspartame are artificial sweeteners. Aspartame is commonly used in soft drinks and diet drinks.



Naming Benzene Structures

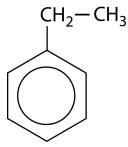
All of the carbon atoms in the benzene ring have one hydrogen atom attached. If we were to replace one of these hydrogens with a branch from **Table** 1.4, the naming is simply the name of the branch plus "benzene."

TABLE 1.4: Branches

Group	Name
$-CH_3$	methyl-
$-CH_2CH_3$	ethyl-
-F	fluoro-
-Cl	chloro-
-Br	bromo-
-I	iodo-
-NO ₂	nitro-

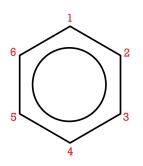
Example:

Name the following structure.

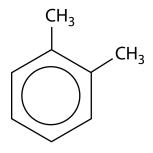


Solution: ethylbenzene

When there is more than one substituent on the benzene ring, then there has to be a way to determine the position of each branch. We number the carbon atoms the same as we had done for the alkanes, alkenes, and alkynes.



By numbering, we have a way to methodically determine the location of each branch on the benzene ring.



- The branches are both methyl groups
- The locations of the methyl groups are on carbons 1 and 2.
- The name of the molecule is 1,2-dimethylbenzene.

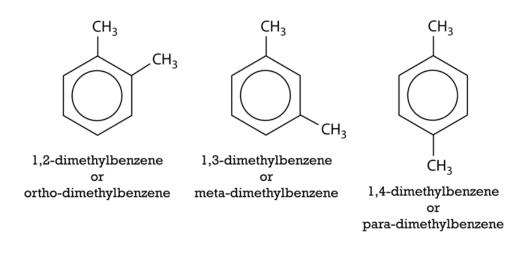
An alternate naming system is given for molecules with two substituent groups (two branches). Alternate names are provided in **Table 1.5**.

TABLE 1.5: Alternate Naming System for Disubstituted Benzene

Location of branches	Prefix	Prefix symbol
carbons 1 and 2	ortho-	0-
carbons 1 and 3	meta-	m-
carbons 1 and 4	para-	p-

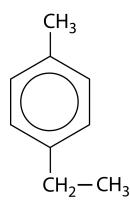
The prefix "ortho-" indicates that the two substituents are on adjacent carbon atoms. The prefix "meta-" indicates that the two substituents are on carbon atoms with one carbon atom between them. The prefix "para-" indicates

that the two substituents are on opposite carbon atoms. Therefore, 1,2-dimethylbenzene could also be named orthodimethylbenzene, 1,3-dimethylbenzene could also be named meta-dimethylbenzene, and 1,4-dimethylbenzene could also be named para-dimethylbenzene



Example:

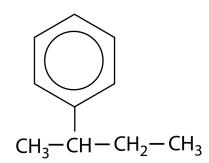
Name the following structure.



Solution:

- The branches are one methyl group and one ethyl group
- The locations of the methyl groups are on carbons 1 and 4.
- The name of the molecule is 1-ethyl-4-methylbenzene or, according to Table 1.5, *p*-ethylmethylbenzene.

You may have noticed that in **Table 1.4**, the number of alkyl groups acting as branches is more limited for benzene than for alkanes, alkenes, and alkynes. When the alkyl group becomes larger, the benzene ring is sometimes considered the branch, and the alkyl group is considered the parent chain. As a branch, benzene is known as a phenyl group.



1.3. Aromatics

In this case, butane is the parent chain, and the benzene ring is a side chain. This molecule would be named 2-phenylbutane.

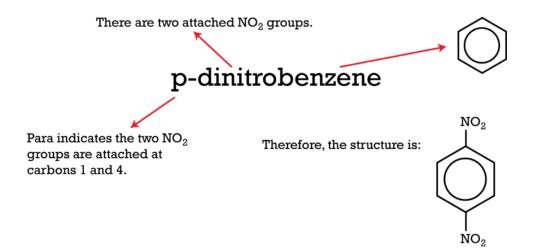
Drawing Benzene Structures

Drawing benzene structures works in a similar way as drawing alkanes, alkenes, and alkynes. Consider the following example.

Example:

Draw the structure of p-dinitrobenzene.

Solution:



Lesson Summary

- A benzene ring is an organic structure that contains a 6-carbon ring with alternating double bonds.
- Resonance refers to a condition occurring when more than one Lewis structure can be written for a particular molecule. The actual electronic structure is not represented by any one of the Lewis structures, but by the average of all of them.
- The electrons in the pi bonds of the benzene molecule are delocalized because they are not confined to a particular pair of carbon atoms.
- As a substituent of a hydrocarbon chain, benzene is known as a phenyl group.

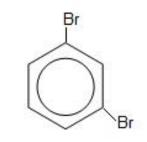
Further Reading / Supplemental Links

• Chemistry and Chemical Reactivity, Kotz, Truchel, Weaver; Thompson, 2006.

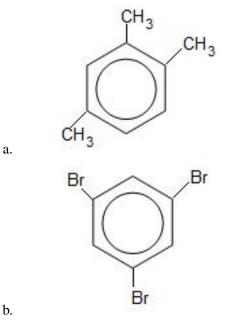
Review Questions

1. Define aromaticity.

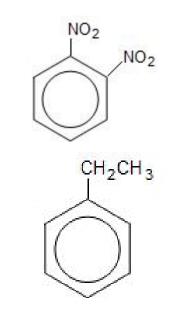
- 2. When is the benzene ring referred to as a phenyl group?
- 3. Name the following structure.



- a. dibromocyclohexene
- b. 1,3-dibromocyclohexatriene
- c. 1,3-dibromobenzene
- d. 2,4-dibromobenzene
- 4. Which formula represents an aromatic compound?
 - a. C_2H_2
 - b. C₆H₆
 - c. C₆H₈
 - d. C₆H₁₄
- 5. How many different possible structures of trichlorobenzene exist?
 - a. 1
 - b. 2
 - c. 3
 - d. 4
- 6. Name the following structures.



a.



d.

c.

7. Draw the following structures.

- a. fluorobenzene
- b. *p*-diethylbenzene
- c. 3-phenylhexane
- d. 2-methyl-1,4-diethylbenzene

1.4 Functional Groups

Lesson Objectives

The student will:

- define and give examples of functional groups.
- identify alcohols, aldehydes, ketones, ethers, organic acids, and esters based on their functional groups.
- name and draw simple alcohols, aldehydes, ketones, ethers, organic acids, and esters.

Vocabulary

- alcohol
- aldehyde
- carbonyl group
- ester
- ether
- hydroxyl group
- ketone
- organic acid

Introduction

Earlier in this chapter, we were introduced to several functional groups, including alkenes and alkynes. Remember that a functional group is an atom or a group of atoms that replaces hydrogen in an organic compound and is responsible for the characteristic properties of the compound. Functional groups can be used to identify different categories of organic compounds. In this lesson, six of these categories will be studied in terms of their functional groups: the alcohols, aldehydes and ketones, ethers, organic acids, and esters.

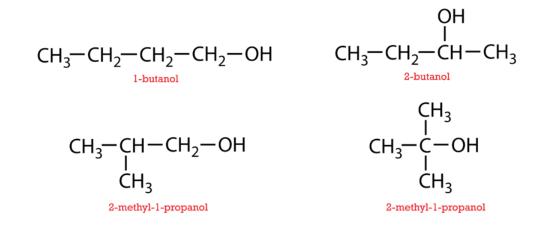
Alcohols

Alcohols have the same general formula as an alkane, but alchols also have the functional group -OH, called the **hydroxyl group**. In terms of solubility, alcohols are soluble in water if the number of carbon atoms is low (three or less). If, however, the number of carbon atoms increases, the solubility decreases accordingly.

The most common alcohol, known as ethanol, is used in alcoholic drinks, as a fuel (gasohol), in thermometers, as a preservative for biological specimens, and as a solvent for paints and drugs. The structure for ethanol is shown below. Notice the hydroxyl group on the end of the two carbon chain.

$CH_3 - CH_2 - OH$

Butanol, an alcohol with four carbon atoms, is used in paint thinners and in the cosmetic industry. The four different isomers of butanol are shown in the figure below.



Naming and Drawing Simple Alcohols

In naming alcohols, the suffix "-ol" is added to the parent chain of the alkane name. The position of the -OH functional group is indicated in the name. Remember to start numbering the parent chain on the end closest to where the -OH is located.

Example:

Name the following:

 $CH_3-CH_2-CH_2-OH\\$

Solution:

The carbon chain contains 3 carbon atoms and an -OH group at one end of the chain.

Therefore, the molecule is 1-propanol.

Alcohols can be classified as primary (1°) , secondary (2°) and tertiary (3°) alcohols, as shown below.

$$\begin{array}{c} \mathsf{CH}_{3}-\mathsf{CH}_{2}-\overset{\mathsf{H}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{O}}{\underset{\mathsf{H}}{\overset{\mathsf{O}}{\underset{\mathsf{O}}{\atop\mathsf{O}}{\underset{\mathsf{O}}{\atop\bullet}{\bullet}}}}}}}}}}}}}}}}}}}}}}}} \\{ \mathsf{C}$$

1-propanol is a primary alcohol because the carbon atom that the hydroxyl group is attached to is connected to only one alkyl group. In other words, carbon 1 in 1-propanol is attached to -OH, two hydrogen atoms, and an ethyl group. Therefore, 1-propanol is a 1° alcohol.

An example of a secondary (2°) alcohol is 2-butanol. Notice in 2-butanol that the carbon atom to which the hydroxyl group is bounded to is also connected to a methyl group on the right and an ethyl group on the left.

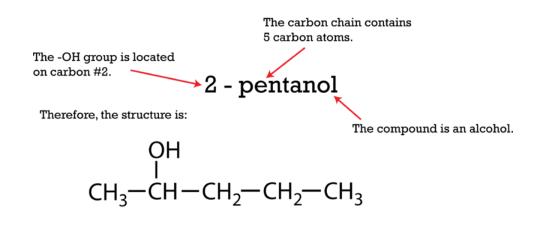
In comparison, 2-methyl-2-propanol is a tertiary (3°) alcohol. If you look at this structure, the carbon atom bounded to the hydroxyl group is also bounded to three methyl groups.

As with the other organic compounds introduced in this chapter, alcohols can be drawn by looking at the name of the compound and analyzing what the name tells about the structure of the compound.

Example:

Draw the structure of 2-pentanol.

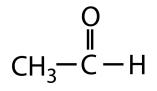
Solution:



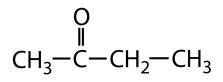
Aldehydes and Ketones

The **aldehydes** and **ketones** contain what is known as the carbonyl group. A **carbonyl group** is a carbon atom double bonded to an oxygen atom (C = O), and the carbon is also bounded to two other atoms or groups. In an aldehyde, the carbonyl group is always on an end carbon. In a ketone, the carbonyl group is never on an end carbon. Look at the diagram below to compare the location of the carbonyl group in ethanal (an aldehyde) and 2-butanone (a ketone).

Ethanal

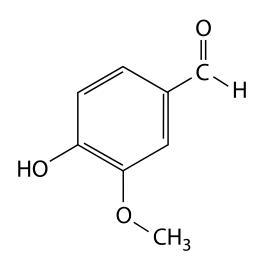


2 - butanone



Aldehydes

Aldehydes play an important role in our everyday lives. Those that have higher molecular masses are responsible for some very pleasant smells that you may have experienced in your own home. Benzaldehyde is an aldehyde responsible for the baking ingredient almond extract, while the smell of vanilla is due partially to an aldehyde component in the structure methoxybenzaldehyde (structure of vanilla is shown below).

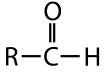


Vanilla (4-hydroxy-3-methoxybenzaldehyde)

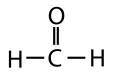
Of course, other aldehydes, such as formaldehyde, do not smell as nice. Formaldehyde is used as a preservative for organs and as an embalming fluid. Acetaldehyde is the oldest known aldehyde (more than 300 years old) and has its use in the preparation of ethanol.

Naming and Drawing Aldehydes

In order to name aldehydes, use the parent chain name of the alkane and add the suffix "–al." Remember that all aldehydes have the general formula shown below.

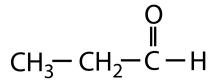


In the general formula above, R represents a hydrogen atom or any alkyl group. The simplest aldehyde is methanal, where R = H.



Example:

Name the following structure:



Solution:

The parent chain contains 3 carbon atoms, and it has a carbonyl group on the end of the chain. Therefore, the name is propanal.

Example:

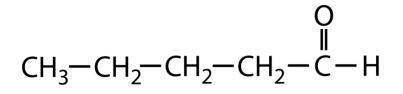
Draw the structure of pentanal.

Solution:

Pentanal has the prefix "pent-," meaning it has five carbon atoms.

Pentanal has the suffix "-al," meaning it has the aldehyde functional group

Therefore, the structure is:



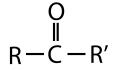
Ketones

Ketones are equally as important as aldehydes in our daily lives. Ketones are present in the body when fat is broken down for energy. A buildup of ketones leads to ketoacidosis, a potentially dangerous condition. Acetone is also a ketone and is the main component in finger nail polish. Carvone is a ketone that is found in many naturally occurring products, such the oils from mandarin oranges, dill seeds, and spearmint. Another example of a useful ketone is isophorone (3,5,5-trimethyl-2-cyclohene-1-one), which is used in some paints to improve the flow and increase the glossiness. Isophorone has the structure shown below.

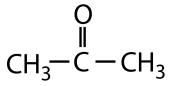


Naming and Drawing Ketones

In order to name compounds that are ketones, use the parent chain name of the alkane and add the suffix "–one." For parent chains more than four carbon atoms, the position of the carbonyl group must be indicated. Remember that all ketones have the general formula shown below.

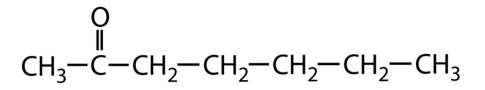


In the general formula above, R and R' are both alkyl groups, which can be the same or different. The simplest ketone is propanone (acetone), where R and R' are both methyl groups.



Example:

Name the following structure.



Solution:

There are alkyl groups attached on both sides of the carbonyl group, therefore the molecule is a ketone. The name of this compound is 2-heptanone.

Example:

Draw the structure of 3-pentanone.

Solution:

The carbon chain will be 5 carbon atoms long, and it will have a carbonyl group at carbon 3. Therefore, the structure is:

$$CH_3 - CH_2 - C - CH_2 - CH_3$$

Ethers

All **ether** compounds have the general formula R - O - R', where R and R' are both alkyl groups, which could either be the same or different. The most common ether is a compound also known as diethyl ether. The structure of diethyl ether is shown below:

 $CH_3-CH_2-O-CH_2-CH_3\\$

In this structure the alkyl groups on either side of the oxygen atom are ethyl groups, hence the name diethyl ether. Diethyl ether was first publicly demonstrated as an anesthetic in 1846 at Massachusetts General Hospital. It was considered at the time to be a great breakthrough because it produced the ability for physicians to provide "painless" surgery. Today it also has other uses, such as a solvent for fats and oils. It is also sometimes used to anesthetize ticks before removing them from the skin. The harmful side effects and highly flammable nature of the compound, however, makes its use less common today than in past eras.

Naming and Drawing Ethers

There are two possible ways to to name ethers. One way is to name the alkyl groups on either side of the ether functional group and then adding the word "ether" on the end. The other possibility is to name the smaller alkyl group, add the suffix "–oxy," and then give the alkane name to the larger alkyl group. The alkyl groups are named in alphabetical order.

Example:

Draw the structure for ethyl methyl ether.

Solution:

The general structure is R - O - R'. Looking at the name of the structure, we can determine what alkyl groups will be the R and the R'.

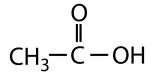
Let $R = CH_3CH_2$ and let $R' = CH_3$, then draw the structure.

$CH_3 - CH_2 - O - CH_3$

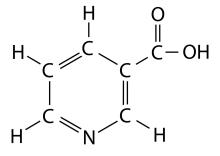
Note this structure is also called methoxy ethane.

Organic Acids

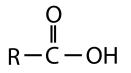
The **organic acids** (or carboxylic acids) contain the carboxyl group. A **carboxyl group** is a carbon atom double bonded to an oxygen atom (C = O), a hydroxyl group (-OH), and either a hydrogen atom or an alkyl group. Carboxylic acids are often found in nature and often combined with other functional groups. Many of these compounds are liquids or solids with low melting points. Carboxylic acids are also highly soluble in water and have a relatively low pH. Vinegar is a water solution containing 5% of the common carboxylic acid acetic acid (shown below).



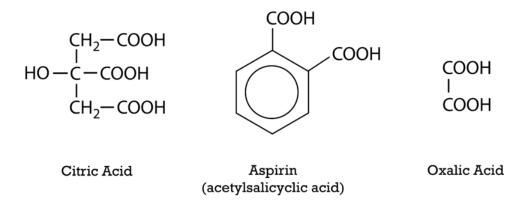
Another common carboxylic acid is niacin (Vitamin B_3). Niacin (shown below) is found in carrots, green leafy vegetables, milk, eggs, and some fish. It is used by the body to aid metabolism, DNA repair, and the functioning of the adrenal gland.



The formula for the carboxyl group is written as R - COOH, where R is a hydrogen atom or an alkyl group. The general formula for the organic acid is found in the diagram below.

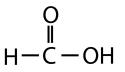


Organic acids play a key role in many aspects of our lives. For example, citric acid is the taste you experience when you drink citrus drinks such as orange juice or put lemon juice on fish. Aspirin (acetylsalicylic acid or ASA) is a widely used pain killer. Oxalic acid is a naturally occurring organic acid found in the leaves of, among other plants, rhubarb, star fruit, black pepper, and parsley. The structures of these organic acids are shown below.



Naming and Drawing Organic Acids

The simplest of organic acids is one where the R group is hydrogen.



When R = H in the general formula, the organic acid is methanoic acid. Methanoic acid (or formic acid) is commonly used in the recycling industry, especially for recycling rubber. It is found in the venom of bees and ants and is released when an insect bites.

When naming organic acids, use the parent chain name of the alkane and add the suffix "-oic acid."

Example:

Name the following structure.

$$CH_3 - CH_2 - CH_2 - C - OH$$

Solution:

This molecule is a 4-carbon chain ending with a carboxylic acid group. Therefore, the name is butanoic acid.

Example:

Draw the structure of 2-methyl propanoic acid.

Solution:

Methyl (CH_3) is a branch found on carbon 2.

Propanoic has the prefix "prop-," meaning it has three carbon atoms in the parent chain. The suffix "–oic acid" means that it has the organic acid functional group. Therefore, the structure is:

Esters

Have you ever wondered why an orange has such a wonderful aroma, or where the smell from a freshly cut pineapple comes from? Most fruits get their rich aroma from molecules known as **esters**. Octyl ethanoate is responsible for the smell for oranges, while butyl butanoate is best known for the smell of pineapple.

Octyl ethanoate (orange flavor)

$$CH_3 - CH_2 -$$

Butylbutanoate (pineapple flavor)

Actually, quite a few of the scents that we are familiar with can be traced back to an ester. Look at **Table 1.6** at some of the common scents and the ester for which the scent can be attributed to.

Scent	Ester
Apples	Methylbutanoate
Pears	Propylethanoate
Raspberries	2-methylpropylethanoate
Peach	Ethylbutanoate
Banana	3-methylbutylethanoate
Orange	Octylacetate
Jasmine	Benzylethanoate

TABLE 1.6: Scents and Their Esters

Naming and Drawing Esters

The general formula for esters is found below.

0 || R-C-O-R'

Notice that the general formula looks similar to the organic acid, but in the case of the ester, the carboxylic acid hydrogen has been replaced with a second alkyl group. This is because esters can be produced by a reaction between an organic acid and an alcohol. This general reaction can be represented as:

$$\begin{array}{c} O \\ H \\ R - C - O - H \\ H \\ H \\ O \\ R' \longrightarrow R - C - O - R' \\ H_2 \\ O \\ R' \longrightarrow R - C \\ O \\ R' + H_2 \\ O \\ R' \\ H_2 \\ H$$

A specific example of this type of reaction is:

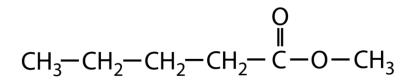
$$\begin{array}{c} O \\ \blacksquare \\ CH_3 - CH_2 - C - O - H + HO - CH_2 - CH_3 \longrightarrow CH_3 - CH_2 - C - O - CH_2 - CH_3 + H_2O \end{array}$$

Since esters have an alkyl group on either side of the functional group, the name of the ester will be in two pieces. As was described earlier, esters are formed from organic acids and alcohols. The alkyl group from the organic acid is R. The alkyl group from the alcohol is R'. The name of an ester is composed of the name of the alkyl group from the alcohol, then of the alkyl group from the organic acid, and finally the suffix "–oate." A sample reaction for a general reaction and then a specific reaction to demonstrate this principal is shown below.

To draw an ester, remember that the first alkyl group is attached to the oxygen and the alkyl group with the suffix "-oate" is part of the C = O chain.

Example:

Name the following structure:



Solution:

The name of this compound is methyl pentanoate (the odor of apple).

Example:

Draw the structure of ethyl heptanoate (the odor of red grapes).

Solution:

Ethyl (CH₃CH₂) is listed first and is therefore from the alcohol, so it will be attached to the oxygen.

Heptanoate is named second and is therefore from the organic acid. Heptanoate has the prefix "hept-," meaning that it has seven carbon atoms in the parent chain. Heptanoate also has the suffix "-oate," meaning it has the ester functional group

Therefore, the structure is:

$$CH_3 - CH_2 - CH_3$$

This video shows an example of naming some compounds containing functional groups (**10e**), see http://www.youtu be.com/watch?feature=player_profilepage&v=nuLxS4SZ4zU (4:38).



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Categories of Organic Compounds

In the table below is a summary of the organic compounds studied in this chapter. **Table 1.7** lists the general formula and the functional groups for the alkanes, the alkenes, the alkynes, and the substituted halogens along with the aromatics, as well as the six new categories introduced in this lesson. An example from each category is also provided.

TABLE 1.7: Summary of the Categories of Organic Compounds

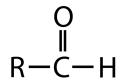
Category	General Formula	Distinguishing Fea-	Example Formula	Name
		ture		
Alkane	NA	All single $C - C$	CH ₃ CH ₂ CH ₃	propane
		bonds		
Alkenes	NA	One $C = C$ bonds	$CH_2 = CH_2$	Ethene
Alkynes	NA	One $C \equiv C$ bond	$HC \equiv CH$	Ethyne

TABLE 1.7: (continued)

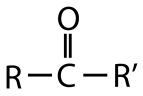
Category	General Formula	Distinguishing Fea- ture	Example Formula	Name
Aromatic	NA	Benzene ring part of structure, Benzene- like structure	NO ₂	Nitrobenzene (floor polish)
Substituted Halogens	R - X	One or more of halogens attached to organic compound	CH ₂ FCl	Chlorofluoromethane (Freon)
Alcohol Ether Aldehydes	$\begin{array}{l} \mathbf{R}-\mathbf{OH}\\ \mathbf{R}-\mathbf{O}-\mathbf{R}' \end{array}$	Hydroxyl group C - O - C	$\begin{array}{c} CH_3CH_2-OH\\ CH_3-O-C_2H_5 \end{array}$	Ethanol Methyl ethyl ether Ethanal
	0 R - C - H	О —С—Н	О II СН ₃ — С - Н	
Ketone				Butanone
	0 R – C – R'	O II – C – (Carbonyl group)	О II CH ₃ - C - C ₂ H ₅	
Organic Acids		<u>,</u>		Ethanoic acid
	0 II R - C - OH	O II – C - OH (Carboxyl group)	О И СН ₃ – С - ОН	
Ester	0 II R – C – O – R'	0 - C - O -	0 Ⅱ C ₃ H ₇ – C – O – C ₄ H ₉	Butyl butyrate (pineapple)

Lesson Summary

- Alcohols have the same general formula as an alkane, except alcohols have the functional group –OH, called the hydroxyl group.
- Primary (1°)alcohols have a carbon atom attached to a hydroxyl group and one alkyl group. Secondary (2°) alcohols have a carbon atom that is attached to a hydroxyl group and two alkyl groups. Tertiary (3°) alcohols have a carbon atom that is attached to a hydroxyl group and three alkyl groups.
- All aldehydes have the general formula below:

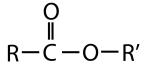


- In order to name aldehydes use the parent chain name of the alkane and add the suffix "-al."
- All ketones have the general formula below:



- To name ketones, use the parent chain name of the hydrocarbon and add the suffix "-one."
- A carbonyl group is a carbon atom double bonded to an oxygen atom (C = O) and to two other atoms or groups.
- All ether compounds have the general formula R O R', where R and R' are alkyl groups.
- Ethers can either be named by naming the alkyl groups on both sides of the ether functional group and then adding the word "ether" on the end. The other possibility is to name the smaller alkyl group, add the suffix "-oxy," and then giving the alkane name to the larger alkyl group.
- The organic acids (or carboxylic acids) contain the carboxyl group (C = O), a hydroxyl group (-OH), and either a hydrogen atom or an alkyl group. The formula for the carboxyl group is written as R COOH, where R is a hydrogen atom or an alkyl group.
- The general formula for the organic acid is below:

- When naming organic acids use the parent chain name of the alkane and add the suffix "-oic acid."
- The general formula for an ester is shown below:



• When naming an ester, the name is composed of the alkyl group from the alcohol, then the alkyl group from the organic acid, and then the suffix "-oate."

Further Reading / Supplemental Links

The *learner.org* website allows users to view streaming videos of the Annenberg series of chemistry videos. You are required to register before you can watch the videos but there is no charge. The website has one video that relates to this lesson called "Carbon." The versatility of carbon's molecular structures and the enormous range of properties of its compounds are presented.

• http://www.learner.org/vod/vod_window.html?pid=813

Review Questions

1. Complete the following chart (**Table** 1.8).

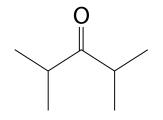
TABLE 1.8:

Group Alcohol	Distinguishing Feature	Draw Example (with Name)
Aldehyde		
Ketone		
Ether		
Organic Acid		
Ester		

- 2. What is the difference between the carbonyl group in the aldehydes and the carbonyl group in the ketones? Give an example to illustrate your answer.
- 3. Which of the following compounds is an alcohol?
 - a. CH₃COOCH₃
 - b. CH₃CH₂OH
 - c. CH₃COOH
 - d. CH₃COCH₃

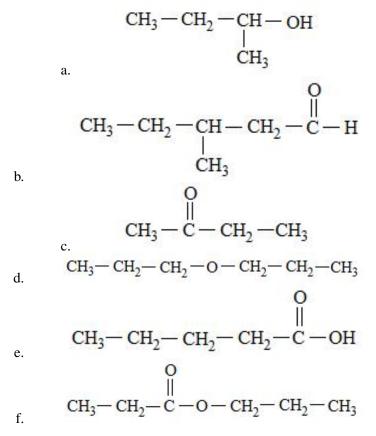
4. To which family of organic compounds does CH₃COCH₂CH₃ belong?

- a. alcohol
- b. aldehyde
- c. ketone
- d. carboxylic acid
- 5. Which of the following classes of organic compounds contain a carbon-oxygen double bond: i. alcohols, ii. aldehydes, iii. ketones, iv. ethers, v. organic acids, vi. esters?
 - a. i, iii, and iv only
 - b. ii, iv, and vi only
 - c. i, iii, iv, and v only
 - d. ii, iii, v, and vi only
- 6. What is the name of the compound represented below?



- a. heptanone
- b. 2,3-dimethyl-3-pentanone
- c. 2,3-dimethylpentanone
- d. diisopropyl ketone

7. Name the following compounds



- 8. Draw the following compounds.
 - a. 3-ethyl-2-hexanol
 - b. 2,2-dimethylpropanal
 - c. 2-propanone
 - d. dibutyl ether
 - e. methanoic acid
 - f. methyl butanoate

1.5 Biochemical Molecules

Lesson Objectives

The student will:

- describe the basic structure of fatty acids, monosaccharides, and proteins.
- identify the chemical purpose fulfilled by lipids, carbohydrates, and enzymes.
- describe the biological function of hemoglobin and DNA.

Vocabulary

- amino acid
- biochemistry
- carbohydrate
- dipeptide
- DNA
- enzyme
- fatty acid
- lipids
- phospholipid
- polymer
- polypeptide
- protein
- steroid

Introduction

Biochemistry is the study of the structure and properties of molecules in living organisms. In a full course in biochemistry, you would study how those molecules are made, changed, and broken down. Examples of the types of molecules important to biochemistry are proteins, hormones, and nucleosides.

This video details the discovery of organic molecules on extrasolar planets (**11 IE**): http://www.youtube.com/watch ?v=Lxs9Pmxy5MA (5:04).



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Lipids

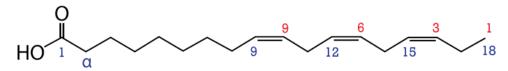
Otherwise known as fats and oils (triglycerides), **lipids** are produced for the purpose of storing energy. One of the best known lipids is cholesterol, which is used in the body to construct cell membranes and as a building block for some hormones. High levels of cholesterol are linked to coronary disease.

There are many categories of lipids, but the three main categories are:

- 1. fatty acids
- 2. steroids
- 3. phospholipids

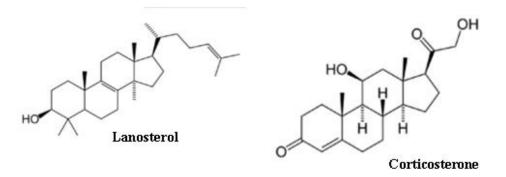
Fatty acids are molecules with a carboxylic acid group at one end, while the remainder of the molecule is a hydrocarbon chain having anywhere from four to thirty-six carbon atoms. They can be saturated or unsaturated, and they generally occur as unbranched chains. As with all biochemical molecules, there are good fatty acids as well as bad.

Omega-3 fatty acid (linolenic acid) is a beneficial fatty acid, cited as slowing the buildup of atherosclerotic plaques. Omega-3 fatty acids have been shown to regulate the immune system and to lower blood pressure. The structure of omega-3 is shown below. It is found in seed oils, fish, and in egg yolks. Since the body cannot produce these particular fatty acids, food is the only source of this type of lipid. Therefore, omega-3 is known as an essential fatty acid.



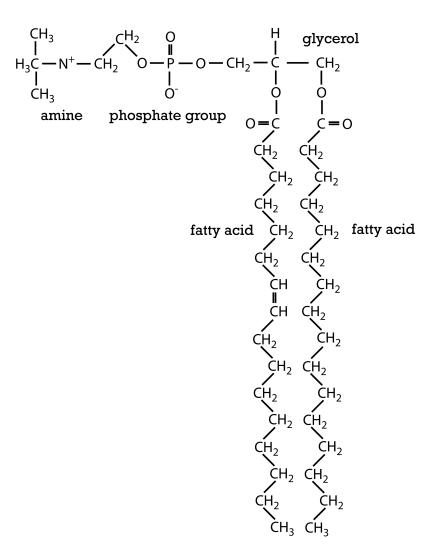
Notice that omega-3 fatty acid has a carboxylic acid functional group on one end and a terminal methyl group on the other end. It also has three double bonds, one at carbon 9, one at carbon 12, and one at carbon 15, giving this fatty acid its unique structure.

Steroids are compounds where four carbon rings are bounded together with branches and functional groups bounded to the rings. Depending on the combinations of the rings, branches, and functional group, different steroids can be formed with different functions in the body. The diagram below shows the structures of lanosterol and corticosterone. In lanosterol, notice that the four rings, the hydroxyl group, and the number of branches from the carbon rings. Lanosterol has 30 carbon atoms in total and acts as the basic building block for all steroids. Corticosterone is a steroid hormone important in mobilizing the immune system to fight infection. Notice the similarity in the structures to lanosterol.



Phospholipids are a combination of fatty acids, glycerol, and a phosphate group joined together. Phospholipids play a major role in cell membranes. The figure below shows phosphatidyl choline, which is the major component of

lecithin. Lecithin is present in egg yolk and soy beans, among other foods. Notice the position of the links between the amine, the phosphate group, the glycerol, and the fatty acids.



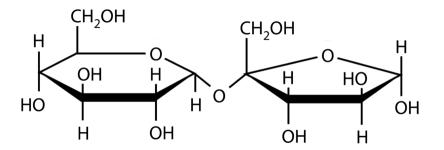
Carbohydrates

Carbohydrates supply the necessary energy living systems need to survive. All carbohydrates contain carbon, hydrogen, and oxygen and have the general formula $C_x(H_2O)_y$. These molecules are also known as sugars or sugar chains that perform specific functions depending on their structure. Carbohydrates can be classified into three different categories:

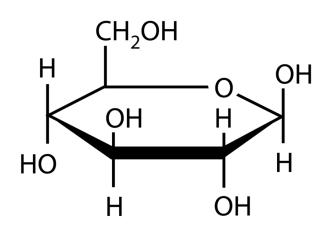
- 1. monosaccharides
- 2. disaccharides
- 3. polysaccharides

Monosaccharides and disaccharides are also known as simple sugars. Refined white sugar commonly found in the home is an example of a simple sugar. More precisely, refined white sugar is the simple sugar sucrose. Sucrose is a disaccharide formed when two monosaccharides (glucose and fructose) join. A **monosaccharide** is a single sugar unit whereas a **disaccharide** has two sugar units. Illustrations of sucrose, glucose, and fructose are shown below. Notice that the bond joining the two monosaccharide units in sucrose. The molecule on the left in sucrose is

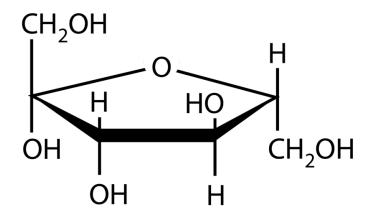
a glucose molecule, while the molecule on the right is a fructose molecule. As the two monosaccharides join, both glucose and fructose will lose a hydrogen atom and one of the molecules will also lose an oxygen atom when they join to form the disaccharide.



Sucrose: a disaccharide



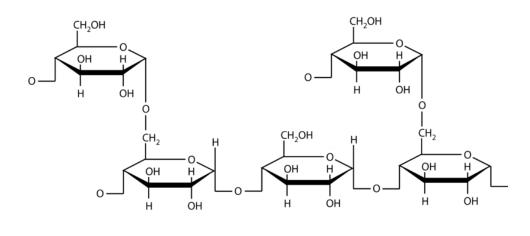
Glucose: a monosaccharide



Fructose: a monosaccharide

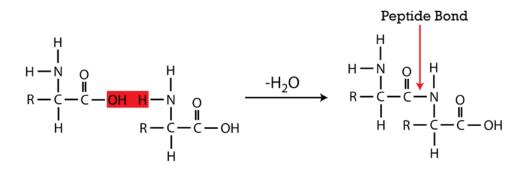
Within polysaccharides, there are numerous individual sugar units. Starches, for example, are polymers where a large number of glucose monosaccharides join together. Starches have the general formula $(C_6H_{10}O_5)_n$, where *n* is dependent on the type of starch formed. For example, glycogen is an animal starch that is made up of approximately 60,000 glucose units. Glycogen is important as a source of energy storage in both the liver and in muscles. When an organism needs that energy, degradation enzymes release the glucose units. Notice in the diagram below how the glucose molecules are linked together in glycogen.

1.5. Biochemical Molecules



Proteins

A **polymer** is a large organic molecule that contains hundreds or even thousands of atoms. **Amino acids** are molecules that contain an amine group $(-NH_2)$ and a carboxylic acid group (-COOH). There are twenty different naturally occurring amino acids that differ only in the R group that separates the amino group from the carboxyl group. When amino acids join together, the link that joins them is called a peptide bond. The diagram below shows the formation of the dipeptide bond.



Two amino acids joining is a **dipeptide**. When many amino acids combine together, a **polypeptides** will form. A **protein** is a combination of these polypeptides or long chains of amino acids. Proteins are essential to the structure and function of all biological cells. **Figure 1.4** shows a 3D model of the protein myoglobin, which is a marker for damaged muscle tissue. It is released when the muscle tissue is damaged. It is a polypeptide made from a chain of 153 linked amino acids.

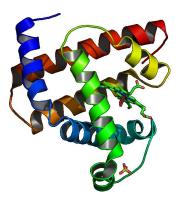
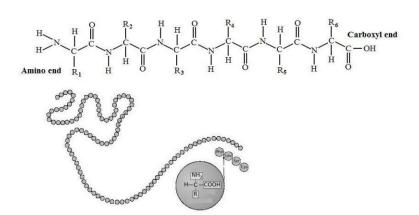


FIGURE 1.4 Representation of a 3D model of a protein. Other proteins that are essential to our life include keratin, collagen, actin, myosin, and hemoglobin. Hair and nails contain keratin, tooth enamel and bones are made from collagen, and muscle tissue contains actin and myosin. Hemoglobin is the most complex of the human proteins and is used to transport oxygen in the blood.

There are four different types of structures that proteins form in the body:

- 1. primary (1°) structures
- 2. secondary (2°) structures
- 3. tertiary (3°) structures
- 4. quaternary (4°) structures

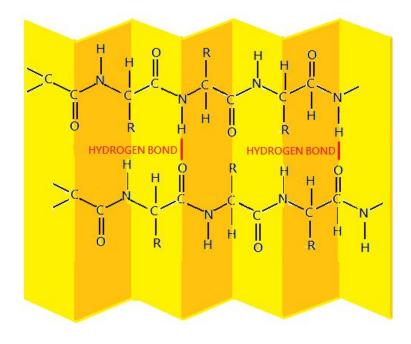
Primary (1°) structures are linear chains of amino acids where the peptide bonds link the amino acids together in long chains or sheets. An example of the primary structure of protein is shown in **Figure 1.5**.

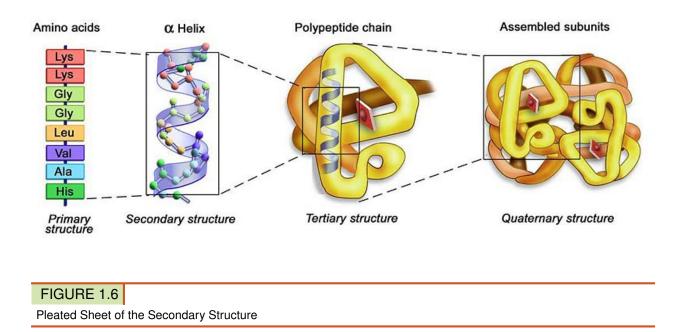




Secondary (2°) structures can form pleated sheets where hydrogen bonds are formed between the amine groups and the carboxylic acid groups of the amino acids in the peptide link (see **Figure 1.6**).

These structures can also form alpha-helix formations where hydrogen bonds connect the amino acids in the peptide link and the carboxylic acid groups in amino acids further down the protein chain. The diagram below shows the structure for the alpha helix. Notice the coiled structure versus the more straightened structure of the pleated sheet.



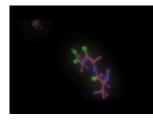


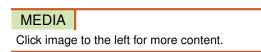
Tertiary (3°) structures form helical structures as pleated sheets and alpha-helices join together in the same molecule. The structure of myoglobin shown above (in **Figure** 1.4) shows the strings of the pleated sheets and the coils of the alpha-helix structures. There is hydrogen bonding between amino hydrogen atoms and carbonyl oxygen atoms with the secondary structures, as well as bonding between the amino acids.

Lastly, quaternary (4°) structures occur when two or more polypeptides join together. The quaternary structure of hemoglobin, (**Figure 1.7**) the principal oxygen-carrying protein found in red blood cells, is a combination of four structural units similar to the tertiary structure of myoglobin.

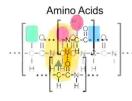
FIGURE 1.7 Hemoglobin

This video shows an animation of the formation of a protein (**10a**, **10c**; **11 IE Stand.**): http://www.youtube.com/w atch?v=w-ctkPUUpUc (4:00).





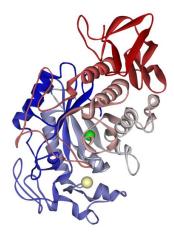
This video explains how amino acids form the polypeptide backbone structure of proteins (**10f; 1l IE Stand.**): http://www.youtube.com/watch?v=0_WaQniUU-g (2:22).



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Enzymes

Proteins are essential to life, and there are over 10,000 different kinds of proteins in the body. **Enzymes** are a subset of proteins. They are a specific type of protein that speed up chemical reactions, thus acting as biological catalysts. Recall that a catalyst is a substance which accelerates the rate of a chemical reaction without itself undergoing any net change. There are more than 4,000 enzyme reactions that occur in biological systems. One of the earliest known enzymes, known as amylase, was first identified by Anselme Payen in 1833. This enzyme is used in digestion to convert starch to sugar in the body. If you were to chew on a cracker, you would notice that after a while it would start to taste a little sweet in the mouth. This is the enzyme in the saliva beginning to do its job. **Figure 1.8** shows an illustration of amylase. Notice the similarity in structure between enzymes and proteins.

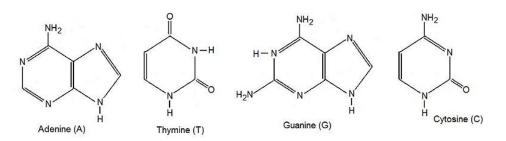


Amylase

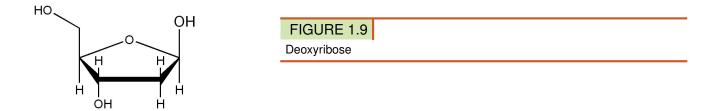
DNA

After a discussion of proteins, the next logical step is to learn about nucleic acids. **DNA** (short for deoxyribonucleic acid), is a polynucleotide found primarily in the nucleus of the cell that maintains our genetic coding. Its function is to direct the body in the synthesis of proteins. The DNA molecule is a large polynucleotide with a molecular weight in the range of 6 million amu. Ribonucleic acids, like RNA, are smaller with molecular weights in the realm of 20,000 to 40,000 amu. A DNA nucleotide consists of one sugar (deoxyribose), a phosphate group, and one of four nitrogen bases. These four nitrogen bases are:

- 1. adenine (A)
- 2. thymine (T)
- 3. guanine (G)
- 4. cytosine (C)



Looking at the structure for deoxyribose (the sugar in the DNA molecule, structure shown in **Figure 1.9**), the phosphate will react and form a link with the hydroxyl groups, forming an outer layer of phosphate-deoxyribose chains. The inner structure of the DNA molecule contains the nitrogen bases. Each nitrogen base has linked to the deoxyribose via a hydroxyl group on the sugar unit, and through hydrogen bonding, these nitrogen bases have complementary linkages to each other (A exclusively links to T, and C connects only to G).



It is interesting to note that the two strands form a double helix (see **Figure ??**), which adds flexibility to the structure, easy storage, and availability of genetic material in addition to ease in the integrity of replication. In order to copy the DNA in cell replication, the double helix unwinds, resulting in two complementary strands, each of which can construct a daughter double helical DNA structure of its own.

Lesson Summary

- Lipids are used for the storage of energy.
- Carbohydrates are also known as sugars or sugar chains, and they supply the necessary energy for living systems.

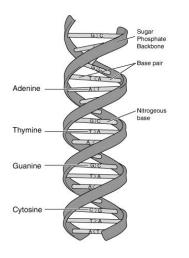


FIGURE 1.10 Illustration of DNA as a double helix.

- Amino acids are building blocks for proteins.
- Enzymes are a special type of protein that speed up chemical reactions and thus act as catalysts.
- DNA contains our genetic coding, its function is to direct the body in synthesizing proteins.

Further Reading / Supplemental Links

The *learner.org* website allows users to view streaming videos of the Annenberg series of chemistry videos. You are required to register before you can watch the videos but there is no charge. The website has one video that relates to this lesson called "Proteins: Structures and Function."

• http://www.learner.org/vod/vod_window.html?pid=815

This video is a ChemStudy film called "Synthesis of an Organic Compound." The film is somewhat dated but the information is accurate.

http://www.youtube.com/watch?v=ToSmwYgbvI0

Review Questions

1. Fill in the following table (**Table 1.9**).

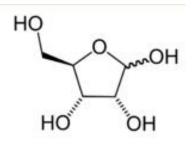
TABLE 1.9:

Compound	Main Purpose
Carbohydrate	
Lipid	
Protein	
Enzyme	
DNA	

- 2. For which biochemical molecule do the triglycerides belong?
 - a. carbohydrates
 - b lipids

1.5. Biochemical Molecules

- 5. Starch is a member of what biochemical molecular group?
 - a. carbohydrates
 - b. lipids
 - c. proteins
 - d. enzymes
- 6. The structure for ribose is shown below. What is the difference between this sugar and the sugar commonly found in DNA?



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1.6 References

- 1. Diamond lattice structure. CC-BY 3.0
- 2. Benjah-bmm27. Graphite structure with multiple layers. Public domain
- 3. Michael Ströck (http://commons.wikimedia.org/wiki/File:C60a.png), http://en.wikipedia.org/wiki/File:Fussball. . GNU Free Documentation License, GNU Free Documentation License
- 4. Aza Toth. Representation of a 3D model of a protein.. Public Domain
- 5. National Human Genome Research Institute. Primary structure of a protein. Public domain
- 6. . Secondary structure of a protein.. CC-BY-SA
- 7. Richard Wheeler. Hemoglobin. GNU Free Documentation
- 8. . Amylase. Public Domain
- 9. . Deoxyribose. GNU Free Documentation
- 10. Courtesy of National Institutes of Health. DNA Illustration as a double helix. Public domain