Chapter 13 – Organic Chemistry

Introduction

Organic chemistry is the study of carbon based compounds. The structural and genetic materials of living organisms are organic compounds. Many of the substances that we encounter on a daily basis are organic compounds: drugs, plastics, textiles, dyes, paper, food, vitamins, etc. Because of the manner in which carbon atoms can bond to one another, the number of organic compounds is enormous. In this chapter, we explore some of the fundamental topics of the structure and reactivity of several classes of organic compounds by applying our knowledge of Lewis structures, resonance, and Lewis acid-base theory.

13.1 Hydrocarbons

Introduction

We begin our study of organic chemistry with two classes of compounds that contain only carbon and hydrogen.

Prerequisites
- 5.8 Formal Charge and Oxidation State (Draw Lewis structures.)

Objectives
- Name and draw the two simplest alkanes.
- Draw line-wedge-dash, Lewis, condensed, and skeletal structures of alkanes.
- Convert skeletal structures into molecular formulas.
- Distinguish between a straight or continuous chain and a branched chain.
- Write the equation for the combustion of an alkane.
- Define an alkene and draw and name the two simplest alkenes.
- Draw the isomers of an alkene.
- Define a polyene and explain why many polyenes absorb visible light.
- Define alkynes and discuss their isomers.
- Distinguish between saturated and unsaturated hydrocarbons.

Alkanes

13.1-1. Definition

Carbon atoms always have four bonds: four single bonds, two single and one double bond, two double bonds, or a single bond and a triple bond. Although carbon is the basic building block, organic compounds usually have hydrogen atoms as well. Oxygen and nitrogen are also common, but almost any other element can be found in organic compounds. In this section, we deal with the class of compounds known as **hydrocarbons**, which are compounds that contain only carbon and hydrogen.

Alkanes are the simplest organic compounds. All of the carbon atoms in an alkane are sp^3 hybridized and tetrahedral, and all bonds are sigma bonds, which makes alkanes relatively unreactive. They have the general formula C$_n$H$_{2n + 2}$, where n is an integer. Table 13.1 shows the three simplest alkanes.

| Alkane	Structure
Methane, CH_4	
Ethane, C_2H_6	
Propane, C_3H_8	

Table 13.1: The Simplest Alkanes

13.1-2. Structures

Carbon atoms always have four bonds in their compounds.

There are times when the line-wedge-dash representation is used to show the three-dimensional structure of organic compounds, but the structures of alkanes are very dynamic because **groups attached by a single bond can rotate relative to one another (much like the wheels on an axle)**. Consequently, other shorthand notations are frequently used. These other methods, shown in Figures 13.1a, 13.1b, 13.1c, and 13.1d, are based on the following points that are common to most organic molecules.

- Carbon atoms form their backbone.
- Carbon atoms always have four bonds to them.
- There are usually many C–H bonds present.
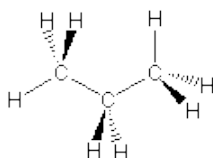
Figure 13.1a: Representations of Propane: Wedge-Dash

Propane is C_3H_8. Figure 13.1a shows the line-wedge-dash representation of the three-dimensional structure.
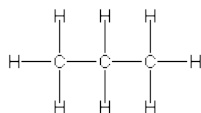
Figure 13.1b: Representations of Propane: Lewis Structure

In a **Lewis structure** of an organic compound, all of the bonds and atoms are shown explicitly, but the bond angles are often shown as 90°.
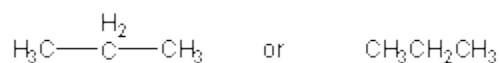
Figure 13.1c: Representations of Propane: Condensed Structure

A **condensed structure** shows the atoms, but not all of the bonds. Sometimes the C–C bonds are shown, but frequently they are not.

Figure 13.1d: Representations of Propane: Skeletal Structure

A **skeletal structure** does not show carbon or hydrogen atoms explicitly, nor does it show the C–H bonds. The positions of the carbon atoms in a skeletal structure are indicated by the ends and intersections of lines. Thus, the structure of propane shows three carbon atoms: one at each end and one at the intersection of the two line segments. The positions of the hydrogen atoms are inferred from the number of bonds shown to each carbon. Each carbon atom must have four bonds (a double bond counts as two bonds and a triple bond counts as three), so *the number of C–H bonds to any carbon atom equals four minus the number of bonds shown to the carbon atom in the skeletal structure*. For example, the skeletal structure shows only one bond to each of the terminal carbon atoms, so there must also be three C–H bonds to each of the end carbons. The structure shows two bonds to the middle carbon, so there must also be two C–H bonds.

13.1-3. Molecular Formulas for Skeletal Structures

Neither carbon nor hydrogen atoms are shown explicitly in a skeletal structure.

Use the following rules to convert the skeletal structures into molecular formulas.

- Carbon atoms are represented as intersections or ends of lines.
- The number of hydrogen atoms attached to a carbon atom is equal to four minus the number of bonds involving the carbon atom because carbon atoms are always involved in four bonds. Note that double and triple bonds count as 2 and 3 bonds, respectively.
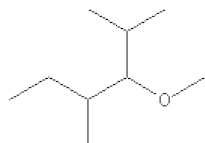

EXERCISE 13.1:

Write the molecular formula for the given skeletal structures. **Note that the order of elements in the formula should be C then H then O**.
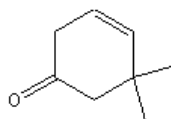

13.1-4. Chains

Isomers are different molecules with the same formula.

There is only one way to connect the carbon atoms in each of the alkanes discussed so far, but there are multiple ways to connect the carbon atoms in all of the alkanes with more than three carbon atoms. The way in which the carbon atoms are connected is called the *connectivity*. The molecules with the same formula but different connectivities are different molecules, and different molecules with the same formula are called *isomers*.

Molecules in which no carbon is connected to more than two other carbons are called ***straight chains*** or ***continuous chains***, while molecules that contain with at least one carbon with three or four carbon atoms attached to it are called ***branched chains***. Butane (C_4H_{10}) exists as two isomers, one straight chain and one branched chain.
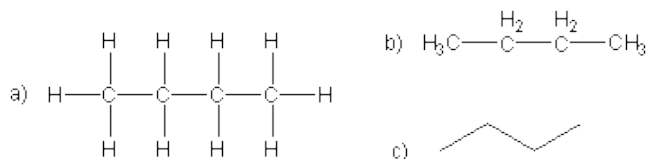
Figure 13.2a: Isomers of Butane: Straight Chain Lewis (a), condensed (b), and skeletal (c) representations of the straight or continuous chain isomer: It is a straight chain isomer because none of the carbon atoms are connected to more than two other carbon atoms.
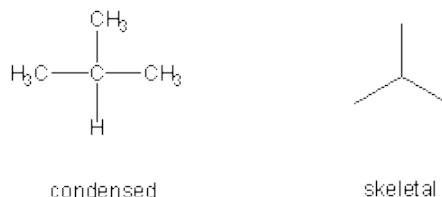
Figure 13.2b: Isomers of Butane: Branched Chain It is a branched isomer because there are three carbon atoms connected to the central carbon atom, so the chain branches at that position.
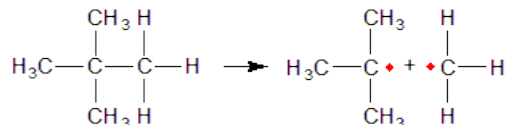
13.1-5. Combustion

Alkanes are found primarily in natural gas (mainly CH_4 and C_2H_6) and petroleum. They are relatively unreactive, but they do burn well. Burning is a rapid combustion, i.e., the reaction with oxygen. The products of the combustion of an alkane are CO_2 and H_2O. Table 13.2 shows the heats of combustion for four common alkanes.

Alkane	Use	Combustion Reaction	Heat of Combustion (kJ/mol)
methane	natural gas furnace	$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O$	-891
propane	propane tank	$C_3H_8 + 5\,O_2 \rightarrow 3\,CO_2 + 4\,H_2O$	-2220
butane	cigarette lighters	$C_4H_{10} + 6.5\,O_2 \rightarrow 4\,CO_2 + 5\,H_2O$	-2855
octane	automobile fuel	$C_8H_{18} + 12.5\,O_2 \rightarrow 8\,CO_2 + 9\,H_2O$	-5494

Table 13.2: Combustion of Some Common Alkanes

13.1-6. Octane Ratings

Each atom in a C–H or C–C bond retains one of the bonding electrons during combustion. The result is two species, called free radicals, that have unpaired electrons. Free radicals are highly reactive, but they are stabilized when the unpaired electron is on an atom that is attached to other carbon-containing groups. Thus, free radicals formed from highly branched carbon atoms are more stable and less reactive than those formed from straight chain hydrocarbons.

Figure 13.3: Free Radicals Bond cleavage of a C–C bond during combusion produces two free radicals. The radicals are stabilized when the carbon atom with the unpaired electron is bound to one or more carbon atoms, so $(CH_3)_3C\cdot$ is more stable and less reactive than $H_3C\cdot$.

Indeed, straight chain hydrocarbons react so fast and violently that they can cause an engine to "knock." The octane rating of a gasoline indicates the extent of knocking it causes. The reference molecules are shown in Figure 13.4. The straight chain hydrocarbon C_7H_{16} causes substantial knocking and is assigned an octane rating of 0, while the highly branched alkane C_8H_{18} (an isomer of octane) causes little knocking and is assigned an octane rating of 100. A gasoline with an octane rating of 87 causes the same knocking as a mixture that is 87% in the branched alkane and 13% of the straight chain alkane.

octane rating = 0   octane rating = 100
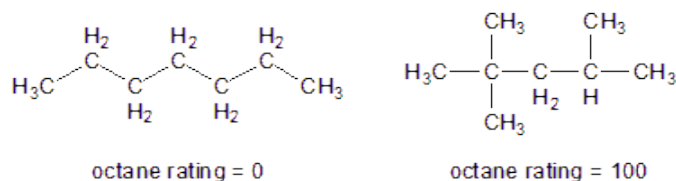
Figure 13.4: Reference Molecules Used to Determine Octane Ratings

Alkenes

13.1-7. Definition

Organic compounds that contain carbon-carbon double bonds are called ***alkenes***. The carbon atoms involved in the double bond are sp^2 hybridized. The two simplest alkenes are ethene (C_2H_4) and propene (C_3H_6).

Alkenes in which the position of the double bond is different are different molecules. However, care must be taken to be certain that the two positions are indeed different and not just a different view of the same molecule.
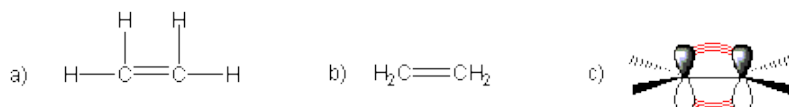

Figure 13.5a: a) Lewis, b) Condensed, and c) Line-Wedge Representations of Ethene
Note that the p orbitals and the pi interaction are shown in the line-wedge structure.

The two carbon atoms are each sp^2 hybridized, and the molecule is planar. Figure 13.5a(c) shows the pi bond (represented in red) as the overlap of the two p orbitals that are not used to make the hybrid orbitals. The electron density of the pi bond lies above and below the molecular plane. Consequently, the pi electrons can attack other substances, i.e., alkenes are weak Lewis bases.
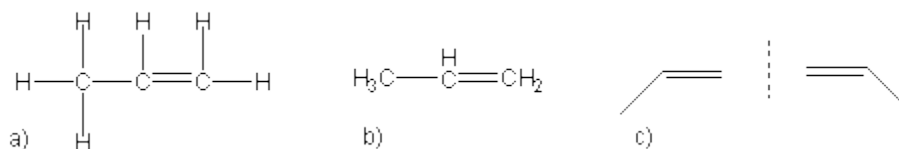

Figure 13.5b: a) Lewis, b) Condensed, and c) Skeletal Structures of Propene

It might appear that the double bond in C_3H_6 could be placed after the first carbon or before the last carbon. However, these two positions are identical because one can be converted into the other by a rotation of the molecule. Thus, the two skeletal structures shown in Figure 13.5b(c) are identical, not isomers. Simply rotate one about the dotted line to get the other.

13.1-8. Butene

The double bond in C_4H_8 can be placed in three different positions (after the first or second carbon in a straight chain or after the first carbon of a branched chain) to produce three isomers. In addition, groups cannot rotate about double bonds like they can about single bonds because the rotation would break the pi bond. Consequently, the butene with two carbon atoms (two CH_3 groups) on the same side of the double bond is different than the one with the two carbon atoms on opposite sides. We will discuss this type of isomer in more detail later.

The four isomers of C_4H_8 are derived below by starting with propene as follows.
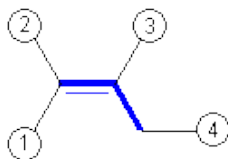
Figure 13.6: Possible Positions of the Fourth Carbon Atom in Butene The skeleton of C_3H_6 is highlighted in blue. The fourth carbon (CH_3 group) of C_4H_8 can be placed in any of the labeled positions to produce a total of four different molecules (isomers).

Position of 4th C	Skeletal Structure	Comments
1		Propane is C_3H_8. This is a straight chain alkene with double bond after the second carbon atom. In this isomer, the two CH_3 groups are on the *same side* of the double bond.
2		This is also a straight chain alkene with double bond after the second carbon atom. In this isomer, the two CH_3 groups are on *opposite sides* of the double bond.
3		This isomer is the only branched isomer.
4		This is the only straight chain isomer in which the double bond involves one of the end carbons.

Table 13.3: The Isomers of Butene

13.1-9. Polyenes

Organic dyes are polyenes with alternating single and double bonds.

The names of alkenes all end in -*ene*, and compounds with many double bonds are called ***polyenes***. An extended pi system results when double bonds of a polyene alternate with single bonds (as in — ═ — ═ — ═ — ═) and the pi electrons are delocalized over the alternating single and double bonds. Recall from our discussion of band theory (Chapter 8.6), that electronic energy levels get closer together as electrons become spread out over many bonds. Also recall from Chapter 6.5 that pi electrons can be delocalized over many carbon atoms. Thus, while most organic compounds are white or colorless because their electronic energy levels are too far apart to absorb visible light, many polyenes with alternating single and double bonds absorb visible light and are colored. Consequently, they are often used to make dyes. As we shall see later in this chapter, it is the absorption of a visible photon by a polyene that initiates the vision process. Two common polyene dyes are considered in Figures 13.7a and 13.7b.
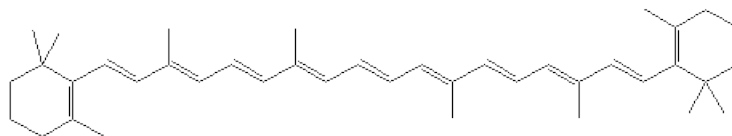
Figure 13.7a: Skeletal Structures of Two Polyenes: Beta Carotene Beta carotene gives carrots their orange color and is oxidized to vitamin A in the body. Its color is due to the large number of alternating single and double bonds (21).
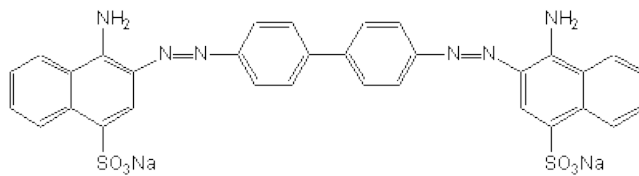
Figure 13.7b: Skeletal Structures of Two Polyenes: Congo Red Congo red was one of the first dyes for cotton. It has 41 bonds involved in the pi system. The polar NH_2 and SO_3^{1-} groups form hydrogen bonds to the cellulose in the cotton fiber, which keeps the dye from washing out.

Alkynes

13.1-10. Definition

Alkynes are hydrocarbons that contain at least one triple bond. The simplest alkyne is C_2H_2, which is ethyne, or more commonly acetylene.
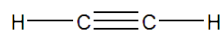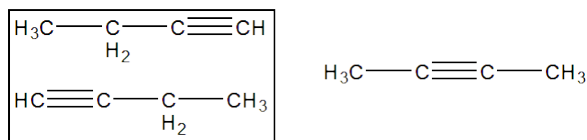

Figure 13.8

Carbon atoms involved in triple bonds have only two electron regions, are sp hybridized, and have 180° bond angles. The presence of π electrons makes them Lewis basic as well, and their chemistry is similar to that described above for alkenes.

13.1-11. Isomers

As with alkenes, different positions of the multiple bond can lead to different isomers. However, the positions must be different viewed from either end of the molecule. For example, there are three ways to draw butyne, but there are only two isomers. The two molecules on the left of
Figure 13.9 are the same molecule as the triple bond in each is located on a terminal carbon atom. The molecule on the right is the isomer of the molecule on the left.


Figure 13.9: Isomers of Butyne

13.1-12. Hydrogenation and Saturation

Carbon atoms with four sigma bonds are **saturated carbons**, while those with less than four sigma bonds are **unsaturated carbons**.

All of the carbon atoms in alkanes are saturated because they have the maximum number of sigma bonds (four). However, carbon atoms involved in multiple (double or triple) bonds are unsaturated because their pi bonds can be replaced with sigma bonds, which increases the number of electron regions. Compounds with many multiple bonds are said to be **polyunsaturated**. An unsaturated compound can be saturated by **hydrogenation**, i.e., by reaction with hydrogen. In a hydrogenation, H_2 adds across the double bond, forming two C–H bonds, i.e., the pi bond between the carbon atom is replaced by two C–H sigma bonds.

unsaturated hydrocarbon	+	hydrogen	→	saturated hydrocarbon

unsaturated alkene

+	3 H$_2$	→

saturated alkane
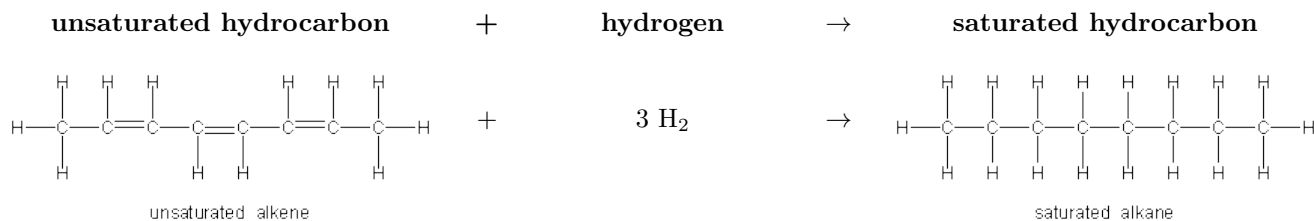
Multiple bonds (double and triple) are unsaturated. The more multiple bonds a compound has, the higher is its degree of unsaturation. Unsaturated compounds can be saturated by hydrogenation.

One H$_2$ is required for each double bond.

All C–C bonds are single bonds in the hydrocarbon above, so it is saturated.

13.2 Naming Simple Hydrocarbons

Introduction

Understanding the nomenclature of alkanes, alkenes, and alkynes will help you understand some of the diversity in organic molecules that will be discussed later in the chapter.

Prerequisites
- 5.8 Formal Charge and Oxidation State (Draw Lewis structures.)
- 6.4: Valence Bond Theory and Hybridization (Determine the hybridization of an atom in a Lewis structure.)

Objectives
- Give the common root names and the endings for alkanes and alkenes.
- Name straight chain alkanes.
- Identify and name the two simplest alkyl groups.
- Name branched alkanes with a single alkyl group.
- Name branched alkanes with two alkyl groups.
- Name straight chain alkenes and alkynes.

13.2-1. Root Names

The name of a hydrocarbon is based on the name of the longest continuous chain it contains.

The name of an organic compound must indicate the number of carbon atoms in the longest continuous chain, which is given by the **root name** of the chain as given in Table 13.4, and the type of compound, which is designated by the ending of the name as shown below.

- Alkanes end in **ane**.
- Alkenes end in **ene**.
- Alkynes end in **yne**.

For example, a hexane is an alkane that contains a six-carbon chain, while a pentene is an alkene with a five-carbon chain, and butyne is an alkyne with a four-carbon chain.

# C atoms	Root Name	Name of Alkane	Name of Alkene
1	meth	methane	
2	eth	ethane	ethene
3	prop	propane	propene
4	but	butane	butene
5	pent	pentane	pentene
6	hex	hexane	hexene
7	hept	heptane	heptene
8	oct	octane	octene
9	non	nonane	nonene
10	dec	decane	decene

Table 13.4: Root Names for Organic Compounds

13.2-2. Naming Organic Molecules

EXERCISE 13.2:

To name a straight or continuous chain alkane, *__indicate the number of carbon atoms it contains with the appropriate root name and add -ane__*. For example, $C_{10}H_{22}$ contains ten carbon atoms, so its root name is dec, and it is an alkane, so -ane is added to the root name. Thus, $C_{10}H_{22}$ is decane.

Name the following straight or continuous chain alkanes.

_____   _____   _____
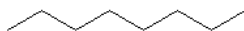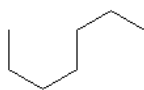
13.2-3. Alkyl Groups

An alkyl group is formed by removing an H atom from an alkane. They are the side chains (not on the longest continuous chain) of a hydrocarbon.

All of the carbon atoms are not in the longest continuous chain of a branched hydrocarbon. Instead, these carbon atoms are in groups called *side chains*, which are attached to the longest continuous chain. Side chains can be any type of group, but we restrict our discussion to *__alkyl groups__*. Alkyl groups are formed by removing one hydrogen atom from an alkane. The resulting alkyl group binds to a longer chain at the position of the removed hydrogen. Alkyl groups are parts of compounds; they are not compounds themselves. The name of the alkyl group is obtained by adding -yl to the root name The two simplest alkyl groups are given in Table 13.5.

Formula of Alkyl Group	Name of Alkyl Group
$-CH_3$	methyl
$-C_2H_5$	ethyl

Table 13.5: The Simplest Alkyl Groups

The dash before the formula indicates where they bond to a longer chain. Propyl, butyl, pentyl, etc., groups also exist, but there are more than one of each of these alkyl groups. For example, there are two different propyl groups that differ by the position of the removed hydrogen, which can come from a terminal carbon atom or from the middle

carbon atom. We restrict our discussion of naming organic compounds to compounds that contain methyl and/or ethyl groups to avoid this complexity.

13.2-4. Naming Alkanes

Branched alkanes have side chains, so the name of a branched alkane specifies the longest continuous chain and the identity and position of the side chains (alkyl groups). Although there can be many side chains of varying lengths, we restrict our discussion of branched alkanes to those with one or two side chains, which will be either a methyl or an ethyl group. The position of the alkyl group is indicated by the number of the carbon atom to which it is attached. Thus, the carbon atoms in the longest chain must be numbered. To number the longest continuous chain, start at the end that produces the smallest number for the side chain.

To name branched alkanes:

1 Identify the longest chain, select the appropriate root name, and add *ane* to indicate an alkane.

2 Number the carbon atoms of the longest continuous chain starting at the end that produces the smaller number for the carbon atom to which the alkyl group is attached.

3 Identify the side chain and its position.

4 Name the alkane as the number of the position of the side chain, a hyphen, and then the name of the alkyl group followed by the name obtained in step 1.

Note that the name of the alkyl group and the name of the longest chain are combined into one word. For example, 2-methylhexane has a six-carbon chain with a CH_3 group attached to the second carbon from the end (either end).

As an example, we will follow the steps above to name the following compound.
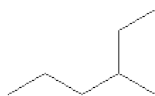
1 Identify the longest continuous chain.
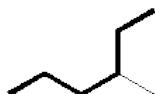
The longest chain contains six carbon atoms, so this is a **hexane**.

2 Number the longest continuous chain so that the side chain has the lowest number.
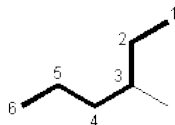
Numbering the chain from left to right places the side chain on carbon 4, but numbering it from right to left puts the side chain on carbon 3. Thus, the chain is numbered from right to left to produce the smaller number for the alkyl group.

3 Identify the side chain and its position.

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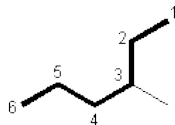
The side chain contains a single carbon atom, so it is a methyl group. It is attached to carbon number 3.

4   Name the compound by combining the name of the longest chain with the position and identity of the side chain.
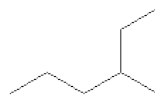
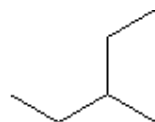
3-methylhexane

13.2-5. Naming Alkanes Exercise

Practice naming branched alkanes by naming the three organic compounds in Exercise 13.3. The root names can be found in Table 13.4.

EXERCISE 13.3:

Answer the questions for each of the branched alkanes.

How many carbon atoms are in the longest continuous chain?

——————————

What is the name of the longest continuous chain?

——————————

What is the name of the alkyl group on the longest chain?

——————————

What is the position of the alkyl group (number of carbon)?

——————————

What is the name of the compound?

——————————

How many carbon atoms are in the longest continuous chain?

——————————

What is the name of the longest continuous chain?

——————————

What is the name of the alkyl group on the longest chain?

_____

What is the position of the alkyl group (number of carbon)?

_____

What is the name of the compound?

_____

How many carbon atoms are in the longest continuous chain?

_____

What is the name of the longest continuous chain?

_____

What is the name of the alkyl group on the longest chain?

_____

What is the position of the alkyl group (number of carbon)?

_____

What is the name of the compound?

_____

13.2-6. Naming Alkanes with Multiple Alkyl Groups

To name alkanes with more than one side chain, simply place the names of the alkyl groups in alphabetical order separated by hyphens in front of the root name. For example, 3-ethyl-2-methylheptane is a seven carbon continuous chain with a C_2H_5 group on the third carbon and a CH_3 group attached to the second carbon. If two identical groups are attached to the same carbon, the number of the position is repeated with a comma separator, and the number of groups is given by a prefix, as in 2,2-dimethylheptane.

EXERCISE 13.4:

Name the following compounds.

_____   _____

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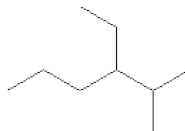
13.2-7. Naming Alkenes and Alkynes

Alkenes are numbered so that the C=C double bond has the lowest number possible.

To name a straight or continuous chain alkene:

1. Number the chain so as to give the carbon atoms in the double or triple bond the lowest number.

2. Specify the chain length with the appropriate root name and add -ene to indicate an alkene or -yne to indicate an alkyne.

3. Indicate the position of the double or triple bond by the number of the carbon atom in the bond with the lower number in the chain.

4. The name is the position of the bond as determined in step 3 followed by a hyphen and then the root name determined in step 2.

For example, 1-pentene is a five-carbon alkene with a double bond between carbon atoms 1 and 2, and 2-hexyne is a six-carbon alkyne with a triple bond between carbons 2 and 3.

EXERCISE 13.5:

Name the following straight or continuous chain alkenes.

_____   _____   _____
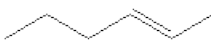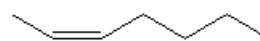
13.3 Isomers

Introduction

We have seen that there can be several organic compounds with the same formula. Compounds with the same formula are called isomers. Isomers can have very different chemical and physical properties. In this section, we introduce two broad classifications of isomers.

Prerequisites
- 6.1 Molecular Shapes

Objectives
- Draw the constitutional isomers with a given molecular formula.
- Draw all of the constitutional isomers of an alkane.
- Identify stereoisomers.
- Name the two types of stereoisomers.
- Distinguish between cis and trans isomers.
- Describe the molecular process responsible for vision.
- Identify stereocenters.
- Identify enantiomers.

Constitutional
13.3-1. Constitutional Isomers

Constitutional isomers differ in their connectivities.

The number of constitutional isomers increases with the number of carbon atoms. C_3H_8O has three constitutional isomers, but there are six isomers of $C_4H_{10}O$ and well over a hundred isomers of $C_{12}H_{26}O$. Constitutional isomers can be the same type of molecule with similar properties. For example, there are over 100 isomers of $C_{10}H_{22}$, but they

are all alkanes. However, constitutional isomers can also be totally different types of molecules with very different properties. As shown in Figure 13.10, there are three isomers of C_3H_8O. Two are alcohols and one is an ether.

- **Ethers** contain the C–O–C connectivity.
- **Alcohols** contain the C–O–H connectivity.

Ethers do not hydrogen bond to one another, while alcohols do because they contain O–H bonds. Consequently, alcohols have much higher boiling points than their corresponding ether isomers. For example, the isomer of C_3H_8O that is an ether boils at $-23\ ^\circ C$, while the two isomers that are alcohols boil at $+78\ ^\circ C$ and $+83\ ^\circ C$.
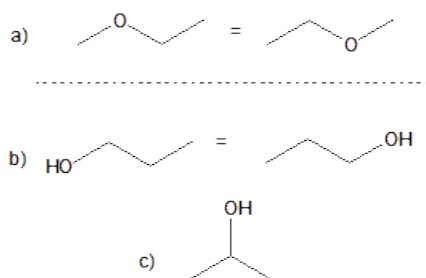
Figure 13.10: Isomers of C_3H_8O The three isomers of C_3H_8O: Isomer (a) is an ether, and isomers (b) and (c) are alcohols.

Now consider the six structures for molecules having the formula $C_4H_{10}O$. Figures 13.11(a) and 13.11(b) contain a C–O–C linkage, so they are ethers, while the remaining structures all contain a hydroxyl group, which makes each of them alcohols. For $C_{12}H_{26}O$, there are well over one hundred isomers! The existence of so many constitutional isomers gives rise to a wealth of structural diversity in organic chemistry. While there is no simple mathematical relationship between the molecular formula and the number of constitutional isomers, you can be certain that molecules with a large number of carbon atoms will have a large number of constitutional isomers.
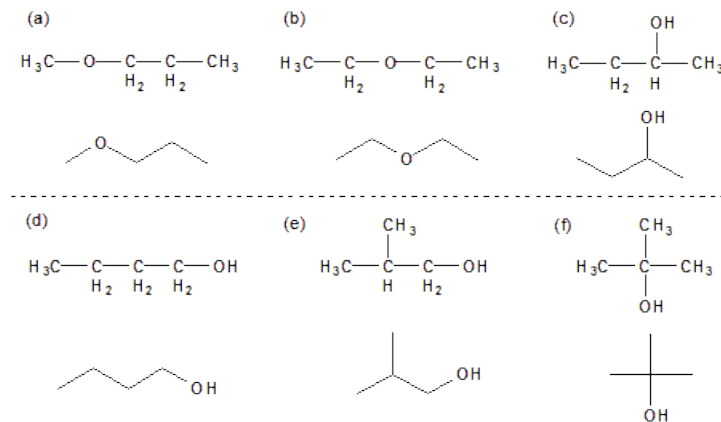
Figure 13.11: Isomers of $C_4H_{10}O$ The six isomers of $C_4H_{10}O$: Isomers (a) and (b) are ethers, but the others are alcohols.

13.3-2. Isomers of Hexane

Follow these steps to determine the constitutional isomers of an alkane.

1 Start by drawing the straight chain isomer.

2 Remove one carbon atom from the straight chain produced above and place the removed carbon (methyl group) on each carbon of the resulting chain that produces a different isomer.

- The methyl group cannot be placed on a terminal carbon atom as that would lead to the same chain as in the previous step.
- It does not matter which way the carbon atoms are numbered, so placing a methyl group on each of the carbon atoms that are next to the end carbon produces the same compound.

3 Remove a second carbon atom and place the two methyl groups or one ethyl group on the remaining chain. The ethyl group cannot be placed on a terminal carbon as that would produce the longest chain obtained in step 1, and it cannot be placed on the second carbon as that would produce one of the isomers produced in step 2.

4 Keep removing one carbon atom until you get to a length where no new isomers can be obtained.
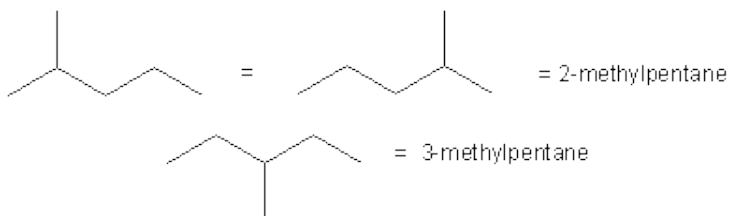

We now follow these steps to draw the constitutional isomers of C_6H_{14}.

1 6-carbon chain

The straight chain isomer is hexane.

2 5-carbon chains

The methyl group can be placed on a carbon that is next to the end or in the middle to produce two isomers.

3 4-carbon chains
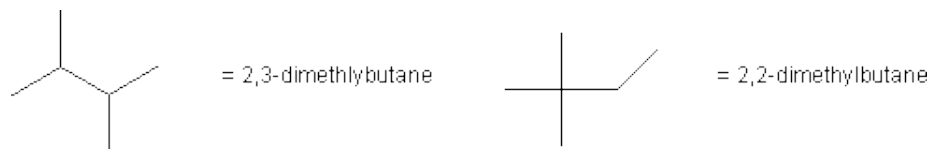
Two carbons must be added to a four-carbon chain. An ethyl group cannot be used because no matter where it is placed, it lengthens the chain and produces one of the isomers of the 5- or 6-carbon chains. The two methyl groups can be placed in two ways: one group on each of the two interior carbons or both groups on the same interior carbon.

4 3-carbon chains

There are no isomers of C_6H_{14} with longest chains of less than four carbons. Thus, there are five isomers of C_6H_{14}.

13.3-3. Isomers of Heptane - an Exercise

Draw the eight isomers of the alkane C_7H_{16} by adding methyl groups to the longest chain.

A video or simulation is available online.

Stereoisomers
13.3-4. Definitions

Stereoisomers have the same connectivities, but they differ in the spatial arrangement of their atoms. There are two types of stereoisomers.

- **Geometric isomers**: Different spatial arrangement of atoms occurs due to the presence of a bond that cannot be twisted completely. We consider only the case of the double bond.
- **Enantiomers**: Different spatial arrangement of atoms occurs due to the presence of a carbon atom that has four different groups attached to it.

We take up geometric isomers first, then turn to a discussion of enantiomers.

13.3-5. Bond Twisting

Groups can rotate relative to one another about a single bond, but not about a double or triple bond.

Sigma bonds are cylindrical, and the groups bound by them rotate around the bond to adopt different relative positions. Figure 13.12(a) shows the rotation about the sigma bond. However, groups connected by double bonds cannot rotate relative to one another without breaking the π bond because the rotation would move the two p orbitals used in the π bond away from one another and remove their overlap.
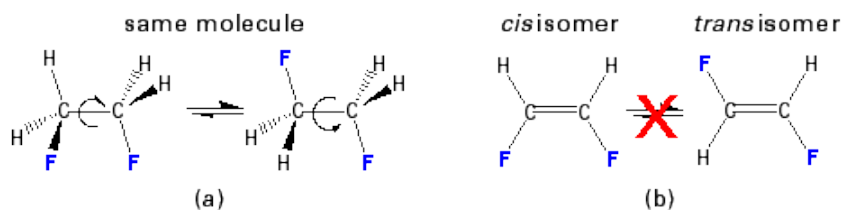
Figure 13.12: Rotation can occur about single bonds, but not about double bonds. (a) The two structures of $C_2H_4F_2$ are not isomers because the groups can rotate around the single bond. (b) The two structures of $C_2H_2F_2$ are isomers because the groups cannot rotate around a double bond.

13.3-6. Cis and Trans Isomers

Two atoms on the same side of a double bond are said to be **cis**, while two atoms on opposite sides of the double bond are said to be **trans**.

EXERCISE 13.6:

Consider the following three isomers of $C_2H_2F_2$.
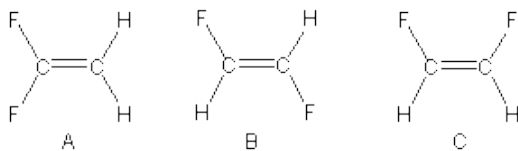
One has no geometric isomer but is a constitutional isomer of the other two. The other two are geometric isomers of one another—one is cis and one is trans. Indicate which is the constitutional isomer and identify the cis and trans geometric isomers.

Isomer A:	Isomer B:	Isomer C:
constitutional	constitutional	constitutional
cis isomer	cis isomer	cis isomer
trans isomer	trans isomer	trans isomer

13.3-7. Retinal

The vision process is initiated by a cis-trans isomerization.

The trans form of an alkene can be twisted into the cis form if the pi bond is broken. Indeed, it is a trans $\rightarrow$ cis conversion that initiates the vision process. Protein molecules in the eye hold retinal molecules in a structure where one double bond is in the less stable cis configuration. The retinal molecule can absorb a photon of visible light due to the presence of alternating single and double bonds. The energy of the photon breaks the pi bond at

the cis double bond. Once the pi bond is broken, the molecule springs back to the more stable trans configuration. This trans → cis conversion initiates a cascade of events that results in vision.
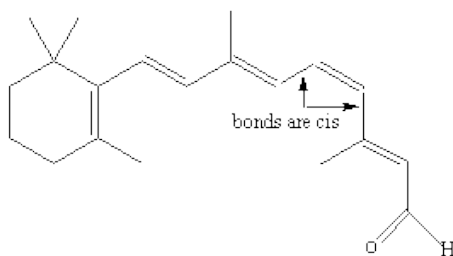
Figure 13.13a: Cis-Trans Isomerization in Retinal: Cis Isomer The cis isomer of retinal is found in the eye when it is dark.
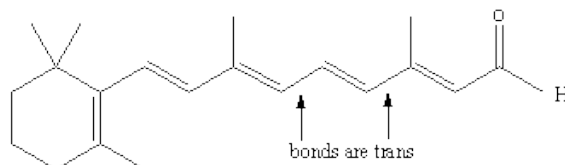
Figure 13.13b: Cis-Trans Isomerization in Retinal: Trans Isomer Absorption of a photon promotes a $\pi \to \pi^*$ transition, so the bond order is reduced in the excited state. The weakened bond can then rotate to convert the cis isomer into the trans isomer shown.

13.3-8. Naming Cis and Trans Isomers Exercise

To indicate the isomer of an alkene, place "cis-" or "trans-" in front of the name of the alkene.

EXERCISE 13.7:

Name the following compounds.

number of carbon atoms in longest chain   position of double bond

———————   ———————

isomer (cis or trans)   name

———————   ———————

number of carbon atoms in longest chain   position of double bond

———————   ———————

isomer (cis or trans)   name

———————   ———————
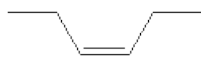
number of carbon atoms in longest chain	position of double bond
————————	————————
isomer (cis or trans)	name
————————	————————

13.3-9. Stereocenters

A carbon atom with four different groups attached to it is called a **stereocenter**.

The atoms attached to a stereocenter do not have to be different, but the groups do. For example, a CH_3 group is different than a C_2H_5 group, but both involve a carbon atom attached to the stereocenter. The following exercise should help.

EXERCISE 13.8:

Is the carbon labeled in red a stereocenter?
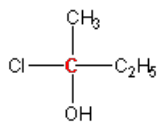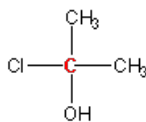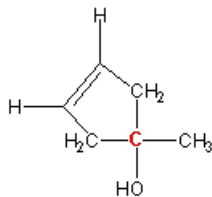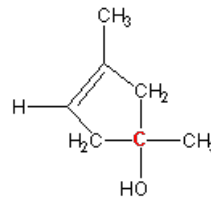
Yes   Yes   Yes   Yes
No   No   No   No

13.3-10. Enantiomers

Enantiomers are isomers that contain stereocenters and are mirror images of one another.

There is additional complexity in the structures of organic molecules that possess carbon atoms with four different groups attached to them. Such carbon atoms are said to be stereocenters. The central carbon shown in red in molecule A in Figure 13.14 is a stereocenter because it contains four different groups: H, OH, CH_3, and Cl. Molecule B in Figure 13.14 is its mirror image. Molecules A and B are different molecules! That they are different can be seen by rotating molecule B by 180° about the C–C bond ($B_1 \rightarrow B_2$). The rotation makes the OH and CH_3 groups of the two molecules (A and B_2) superimposable. However, the H and the Cl groups are still reversed in the two molecules. Consequently, molecules A and B are not superimposable. Note that your right and left hands are also mirror images that are not superimposable. Molecules with a stereocenter cannot be superimposed on their mirror images. Pairs of molecules that are nonsuperimposable mirror images are called enantiomers. Enantiomers are stereoisomers because their spatial arrangements are different while their connectivities are identical. Molecules A and B are enantiomers.
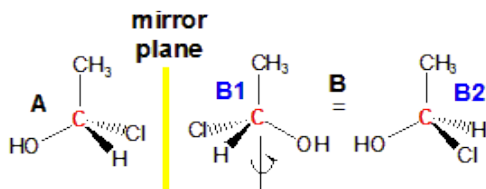
Figure 13.14: Enantiomers The two molecules each contain a stereocenter, and they are mirror images of one another. Consequently, they are enantiomers.

13.3-11. Enantiomer Exercise

EXERCISE 13.9:

The following molecule has a stereocenter.
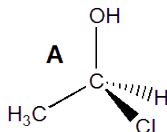
Indicate whether each of the following molecules is the same molecule or its enantiomer.
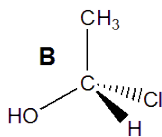

same
enantiomer
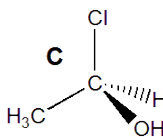
same
enantiomer

13.3-12. Enantiomeric Compounds

Enantiomers have the same melting and boiling points, but they often have dramatically different biological activities because biological activities are often based on the structures of the reacting molecules. Thus, one compound may cause one effect, but its enantiomer may cause a very different effect or have no effect at all. All of the biologically active amino acids except one have stereocenters, and in each case, only one enantiomer is active. The following are a couple of examples.
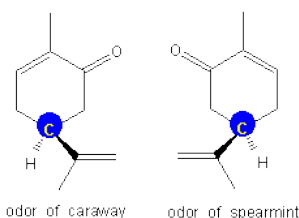
Figure 13.15: Carvone Carvone contains one stereocenter (the yellow carbon on a blue field). The enantiomer on the left is recognized by the olfactory receptors in the nose as the odor of caraway, while the one on the right is recognized as the odor of spearmint.
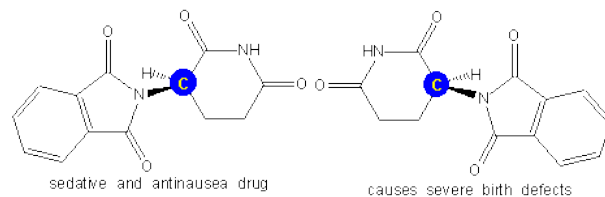
Figure 13.16: Thalidomide Thalidomide contains one stereocenter (the yellow carbon on a blue field). One stereoisomer acts as a sedative and antinausea drug, while the other causes severe birth defects. A drug that contained both enantiomers was marketed in Europe between 1959 and 1962 and resulted in thousands of badly deformed babies. Today, the enantiomer that caused birth defects is being studied as a possible treatment for leprosy, AIDS, and cancer.

13.3-13. Counting Mirror Images

A large structural diversity can occur in molecules that contain several stereocenters. In general, there are 2^n stereoisomers of a molecule with n stereocenters. Thus, there are 2 stereoisomers of a molecule with only one stereocenter, $2^2 = 4$ stereoisomers of a molecule with two stereocenters, and $2^{15} = 32{,}768$ stereoisomers of a molecule with 15 stereocenters.

EXERCISE 13.10:

Consider the sucrose molecule, table sugar. The red highlight of one carbon atom is there for discussion purposes only. It is not special in any other way.
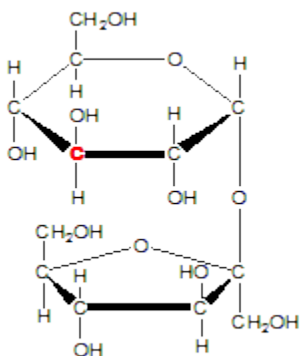
How many stereocenters does a molecule of sucrose contain?

_____

How many stereoisomers of sucrose are there?

_____

13.4 Functional Groups
Introduction

Organic molecules are designed with specific sizes, shapes, and functional groups to perform specific functions (e.g., a better drug or a stronger plastic). Once a molecule is designed, organic chemists develop procedures to make it. These procedures, which can involve many steps, can be developed because so many organic reactions proceed by a few well understood mechanisms. Organic mechanisms are based on the principles of the octet rule, resonance, and Lewis acid-base theory. Reactions occur at specific groups within the molecule called **functional groups**. Functional groups have specific reactivities that can be utilized to produce desired reactions. In this section, we introduce some of the functional groups and the fundamental types of reactions they undergo.

Objectives
- Identify some common functional groups.

13.4-1. Alcohols

Alcohols can behave as Brønsted acids because they contain a hydrogen atom attached to an electronegative atom, but they are also Lewis bases because the oxygen atom contains two lone pairs. Alkyl groups are usually electron donating, so alcohols in which R is an alkyl group function more as Lewis bases than acids.

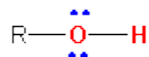*Alcohols* have the general formula R–OH, where R is a generic group of atoms and OH is the hydroxyl group.

Figure 13.17: Generic Alcohol

Alcohols in which R is an alkyl group are named by adding -anol to the root name of the alkyl group. The position of the hydroxyl group is indicated with the number of the carbon atom to which it is attached.
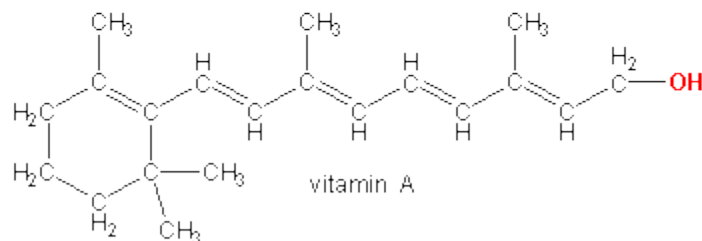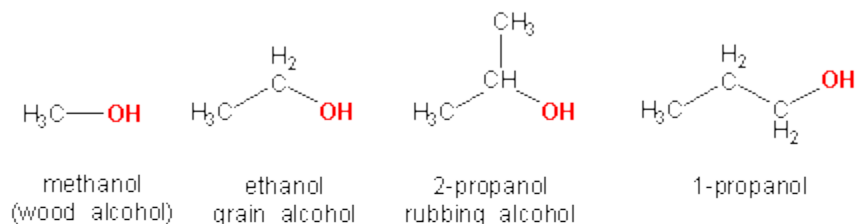
Figure 13.18: Some Common Alcohols

13.4-2. Carbonyls

The *carbonyl group* is C=O.

The carbon atom is sp^2 hybridized and is surrounded by only three electron regions. In addition, the electronegative oxygen places a partial positive charge on the carbon atom. These two properties make the carbon atom of a carbonyl a Lewis acid. In Figure 13.19, the one on the left shows the resonance form of a carbonyl that describes the bonding, and the one on the right describes the reactivity of the carbonyl—the carbon atom of the carbonyl can be attacked by the lone pair of a Lewis base. The Lewis acidity of carbonyl groups gives rise to dozens of types of chemical reactions that differ only in the species serving as the Lewis base.
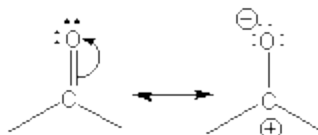
Figure 13.19: Resonance Forms of a Carbonyl Group

13.4-3. Carboxylic Acids

A ***carboxyl group*** is the combination of a carbonyl and a hydroxyl group.
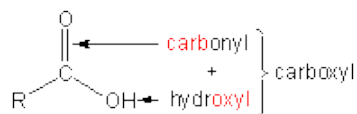
Figure 13.20: Carboxylic Acid

The carbonyl oxygen removes electron density from the O–H bond, which makes carboxyl groups acidic.

A molecule with a carboxyl group is called a ***carboxylic acid*** (RCOOH).
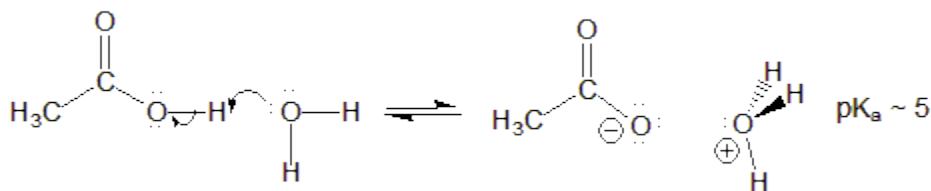
Figure 13.21: Acidity of Acetic Acid

Carboxylic acids in which R is an alkyl group are named by identifying the longest continuous chain that contains the carboxyl carbon and adding "anoic" to the root name of the chain. For example, HCOOH is methanoic (or formic) acid, CH_3COOH is ethanoic (or acetic) acid, and C_2H_5COOH is propanoic acid. The conjugate base of the acid is named by changing the "ic" to "ate." Thus, $C_2H_5COO^{1-}$ is the propanoate ion.

Replacing the O–H hydrogen of a carboxylic acid with an alkyl group results in an ***ester*** (RCOOR').

Esters are named as the name of the alkyl group followed by the name of the group to which it is attached. Consider Figure 13.22, which shows the example of acetic acid (active ingredient of vinegar), which loses a proton to form the acetate ion. Adding an ethyl group to the acetate ion produces the ester ethyl acetate (active ingredient of fingernail polish remover).
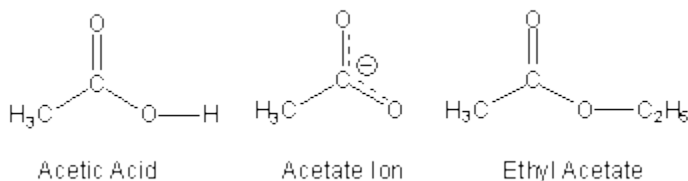
Figure 13.22

The carbon atom of a carbonyl is Lewis acidic, so both carboxylic acids and esters are Lewis acids. In addition, the carbonyl group is electron withdrawing (electronegative oxygen atom), so the O–H bond in a carboxyl group is weakened, which makes carboxylic acids Brønsted acids.

When R is a long alkyl chain, the acid is a **fatty acid**. Fatty acids are found in cells. The R group in fatty acids derived from animal cells is saturated, but those obtained from vegetables are unsaturated (they contain double bonds). Stearic acid (Figure 13.23), a fatty acid derived from animals (it is saturated), is used in making soaps and candles.

Stearic acid - $CH_3(CH_2)_{16}COOH$
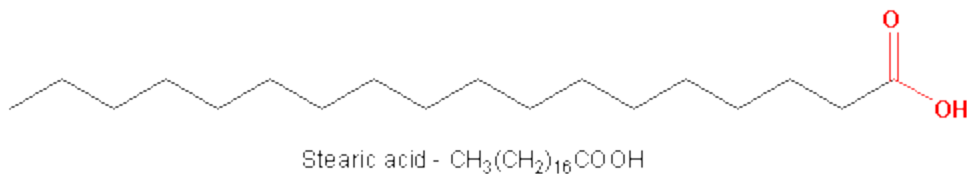
Figure 13.23

13.4-4. Amines and Amides

An ***amine*** is an ammonia molecule in which one or more of the hydrogens have been replaced with R groups. If the nitrogen is attached to a carbonyl, the group becomes an ***amide*** group.

Organic derivatives of ammonia that are not bound to a carbonyl group are called amines. Two examples of simple amines are methyl amine, CH_3NH_2, and dimethyl amine, $(CH_3)_2NH$, are shown in Figure 13.24.
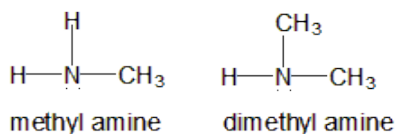
Figure 13.24

Compounds in which a nitrogen atom is bound to a carbonyl carbon are called amides. The groups around the N atom in amides are coplanar, so the N is sp^2 hybridized. The planarity of the amide group is accounted for with the resonance structure in Figure 13.25.
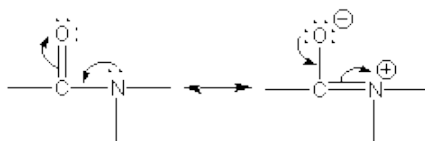
Figure 13.25: Amides

Caffeine contains two amide nitrogens (red), one amine nitrogen (blue), and one nitrogen that is neither an amine nor an amide because it is involved in a double bond.
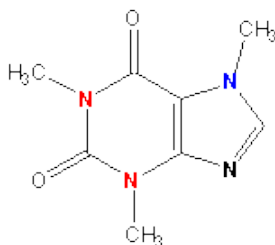
Figure 13.26: Caffeine

13.4-5. Amino Acids

Amino acids contain an amine and a carboxylic acid.

The amine is a good Lewis base, so it can react with the carboxylic acid to produce a charge-separated species, which is the most common form of amino acids in the human body. For example, consider the structure of alanine in Figure 13.27.
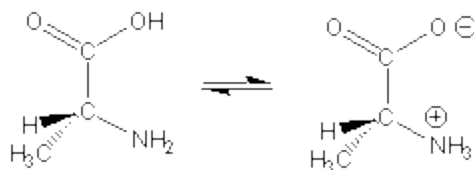
Figure 13.27: Alanine, an Amino Acid Note that the carbon atom in alanine that is connected to both the amine and carboxyl groups is a stereocenter. This is the case in almost all amino acids found in the human body. However, only one enantiomer is biologically active.

13.5 Introduction to Organic Reactions

Introduction

A good amount of organic chemistry can be understood with Lewis acid-base theory. Several mechanisms for different reactions are presented in this section, but all are Lewis acid-base reactions.

Prerequisites
- 5.6 Determining Lewis Structures (Draw Lewis structures.)
- 5.8 Formal Charge and Oxidation State (Determine formal charge.)
- 12.1-7 Curved Arrows in a Mechanism (Represent the mechanism of a Lewis acid-base reaction with curved arrows.)
- 12.1 Lewis Acids and Bases (Determine Lewis acidic and basic sites.)

Objectives
- Identify the Lewis acidic and basic sites involved in an organic reaction.
- Describe an addition reaction.
- Describe a condensation reaction and use curved arrows to show the mechanism for the reaction of a carboxylic acid and an alcohol.
- Use curved arrows to show the attack of an amine on an ester and predict the product of the reaction.

13.5-1. Addition Reactions of Alkenes

Addition reactions are reactions in which two reactants combine to form a single product. We use the addition of a hydrogen halide across a C=C double bond as an example.

A video or simulation is available online.

Alkenes are weak Lewis bases due to their pi electrons, and hydrogen halides are strong Brønsted acids. Hydrogen halides can add across the double bond in two Lewis acid-base reactions.
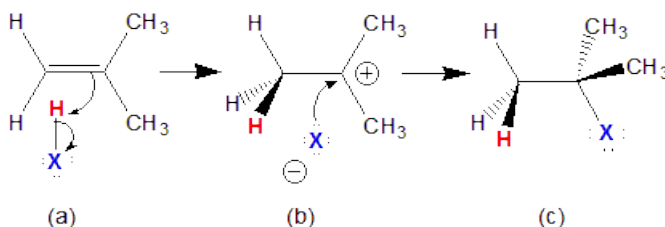
Figure 13.28: The Addition of a Hydrogen Halide Across a Double Bond

1   The pi electrons of the double bond attack the hydrogen of the hydrogen halide to produce a C–H bond, a halide ion, and a carbocation.

2   A lone pair on the halide ion attacks the strong Lewis acidic carbocation to form a C–X bond.

Note that the hybridization of each carbon changes from sp^2 (planar) to sp^3 (tetrahedral) as a result of the addition reaction.

13.5-2. Esterification

In **condensation reactions**, two reactants combine to form two products (one of which is often a small molecule such as water). A carboxylic acid and an alcohol can undergo a condensation reaction called **esterification** to produce an ester and water.
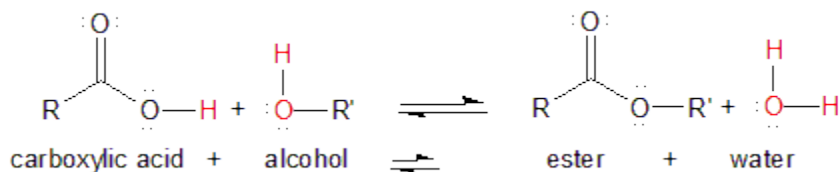

Figure 13.29: Esterification R and R' are usually two different alkyl groups.

The mechanism of esterification is very similar to the one we used to explain the reaction of SO_3 and H_2O in Chapter 12. Indeed, only the identities of the Lewis acid and base have changed.

A video or simulation is available online.

The reaction can be viewed as occurring in three steps.

1 In the first step, the lone pair on the oxygen of the alcohol (the Lewis base) attacks the carbonyl carbon of the acid (the Lewis acid) in a Lewis acid-base reaction. The lone pair becomes a C–O bond, and the pi electrons of the C=O double bond of the carbonyl become a lone pair on the oxygen.

2 A water molecule from the solvent (shown in green) assists in a proton transfer. It first accepts a proton from the oxygen with positive formal charge and then donates a proton to the oxygen involved in the O–H bond.

3 The proton transfer in the second step produces an OH_2 group with a positive formal charge on the oxygen. Electron density moves out onto the oxygen with positive formal charge to produce a water molecule. The water molecule is lost and the C–O pi bond reforms, resulting in a molecule with no formal charge. Loss of small molecules such as water is common in condensation reactions.
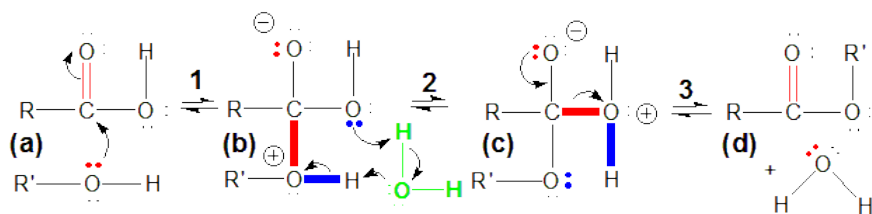

Figure 13.30: Esterification Mechanism

13.5-3. Amide Formation

Amides can be formed in a Lewis acid-base reaction of an amine (base) and an ester (acid). The other product of this condensation reaction is an alcohol.
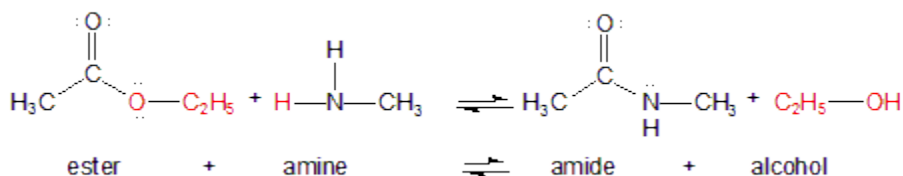
Figure 13.31: Amide Formation

The mechanism of the reaction is identical to esterification.

A video or simulation is available online.

The reaction can be viewed as occurring in three steps.

1 The lone pair on the nitrogen atom of the amine (the Lewis base) attacks the carbonyl carbon of the ester (the Lewis acid) in a Lewis acid-base reaction. The lone pair becomes a C–N bond, and the pi electrons of the C=O double bond of the carbonyl become a lone pair on the oxygen.

2 A water molecule from the solvent assists in a proton transfer. It first accepts a proton from the nitrogen with positive formal charge and then donates a proton to the oxygen involved in the O–R' bond.

3 The proton transfer in the second step produces a R'OH group with a positive formal charge on the oxygen. Electron density moves out onto the oxygen with positive formal charge to produce an alcohol molecule (R'OH), which is lost as the C–O pi bond reforms, resulting in a molecule with no formal charge. Loss of small molecules such as alcohols is common in condensation reactions.
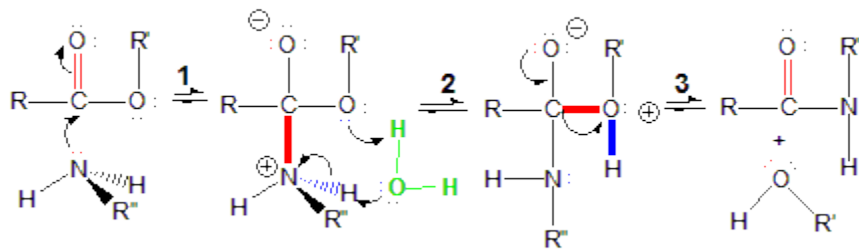
Figure 13.32: Amide Formation Mechanism

13.6 Polymers

Introduction

Natural polymers, such as carbohydrates, proteins, and nucleic acids, are part of living tissue and are responsible for increasing the rates of reactions and giving structural characteristics like strength and flexibility. Others store our genetic code. When most of us think of polymers, however, we think of man-made polymers like PVC, teflon, polyethylene, or polyesters. In this section, we examine both natural and man-made polymers.

Prerequisites
- 7.3-10 Hydrogen Bonding (Describe the hydrogen bond and state the requirement for it.)

Objectives
- Define monomer, dimer, trimer, and polymer.
- Identify the monomer upon which a polymer is based.
- Recognize some common polymers.
- State the requirement for the reactants used to produce a condensation polymer.
- Distinguish between a polyamide and a polypeptide.
- Explain why proteins frequently form α-helices.
- Describe a base pair, explain why they are important, and identify the hydrogen bonding sites in a base pair.
- Describe the double helix structure of DNA and explain its origin.

Addition
13.6-1. Polymers

Polymers are large molecules consisting of many single unit building blocks called *monomers*.

"Mer" is used to indicate a building block. How the term mer is used is demonstrated in Figure 13.33, which shows a **mono**mer (single mer), a **di**mer (two mers), a **tri**mer (three mers), and a **poly**mer (many mers). The polymer grows as the result of successive reactions of the monomers that lengthen the polymer chain. They typically have many kinks and folds because the single bonds are flexible. Although polymers can be formed by several different mechanisms, we consider only those reactions that occur by mechanisms like those that we have already discussed. Synthetic polymers are classified as condensation or addition polymers depending on the type of reaction that is used to form them.
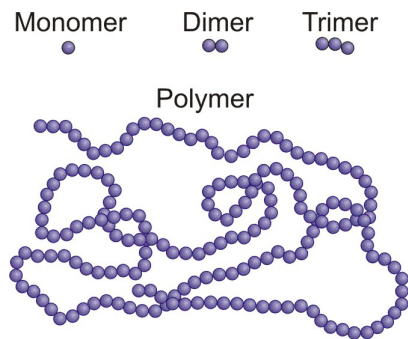
Figure 13.33: Several Mers

13.6-2. Addition Polymers

Addition polymers are formed in addition reactions.

Addition polymers based on alkenes include some of the most common polymers. The polymerization process is summarized in Figure 13.34. Note that the "x" in the figure is a large number typically in the thousands.
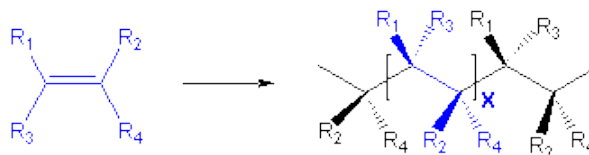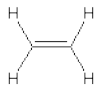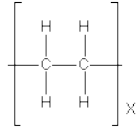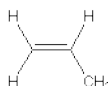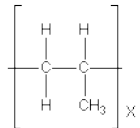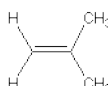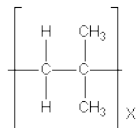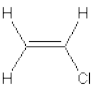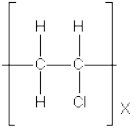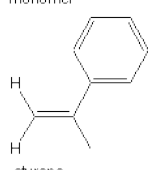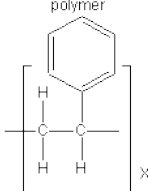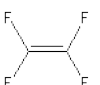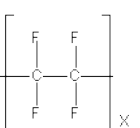

Figure 13.34: Alkene Polymerization

Polymer	Structure	Uses
polyethylene	monomer: ethylene (ethene); polymer: polyethylene	plastic bottles and bags
propylene	monomer: propylene (propene); polymer: polypropylene	carpets
isobutylene	monomer: isobutylene; polymer: polyisobutylene	tires
poly(vinyl chloride)(PVC)	monomer: vinyl chloride; polymer: poly(vinyl chloride)	plumbing and hoses
polystyrene	monomer: styrene; polymer: polystyrene	insulation
tetrafluoroethylene(teflon)	monomer: tetrafluoroethylene; polymer: polytetrafluoroethylene	cooking utensils and nonstick cooking surfaces

**Table 13.6: Structures and Uses of Some Common Polymers**

13.6-3. Isobutylene

The reaction of isobutylene with hydrogen halides was used as an example of an addition reaction in the previous section. We now examine the mechanism of the reaction.

A video or simulation is available online.

In the first step of that reaction, the pi electrons attacked the hydrogen of HX to produce a C–H bond and a carbocation on the carbon (the carbon with more alkyl groups). The carbocation is a strong Lewis acid, which was immediately attacked by the strongest base in the vicinity, the halide ion. However, only trace amounts of HX are used in the polymerization, so there is no halide ion close to the carbocation. Consequently, the next strongest base (another isobutylene molecule) reacts with the cation. Reaction of an isobutylene molecule with the carbocation

produces a dimer that still contains a carbocation. The dimer then reacts with a third isobutylene to form a trimer, and so on to produce poly(isobutylene). A typical poly(isobutylene) chain consists of from 2,000 to 20,000 monomer units.
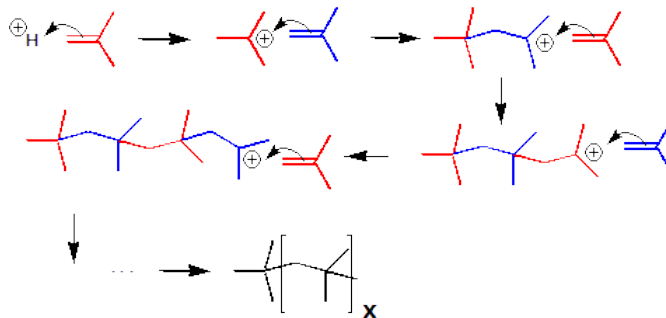
Figure 13.35: Polymerization of Isobutene into Isobutylene

Natural rubber is a polymer of isoprene (see Figure 13.36) that can now be made in the chemistry laboratory. Butyl rubber is a polymer made from isobutylene and isoprene. The United States produces over 500 million pounds of butyl rubber each year.
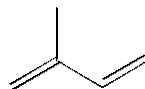

Figure 13.36: Isoprene

Condensation Polymers
13.6-4. Condensation Polymers

*Condensation polymers* are produced in condensation reactions.

The requirement for polymerization is that the reactants must each have two reacting centers. The formation of an ester from a carboxylic acid and an alcohol was used in the previous section as an example of a condensation reaction, and the formation of a **polyester** from a diacid and a diol (compounds with two carboxyl and two hydroxyl groups) is demonstrated in Figures 13.37a, 13.37b, and 13.37c.

$$x \text{ diacid} + x \text{ diol} \rightarrow \text{polyester}$$
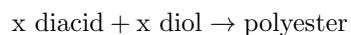
The polyester poly(ethylene terephthalate) or PET is used in clothing, upholstery, tires, and other products. It is marketed as Mylar, Dacron, and Terylene. 4.5 billion pounds of PET are produced in the U.S. every year.
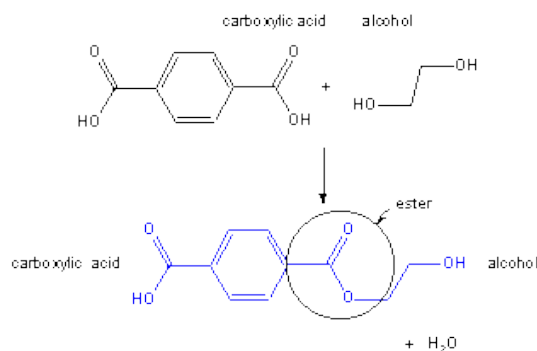
Figure 13.37a: Polyester Poly(ethylene terephthalate) or PET: Step 1 The reaction of a diacid and a diol produces an ester that contains a hydroxyl group at one end and a carboxyl group at the other.
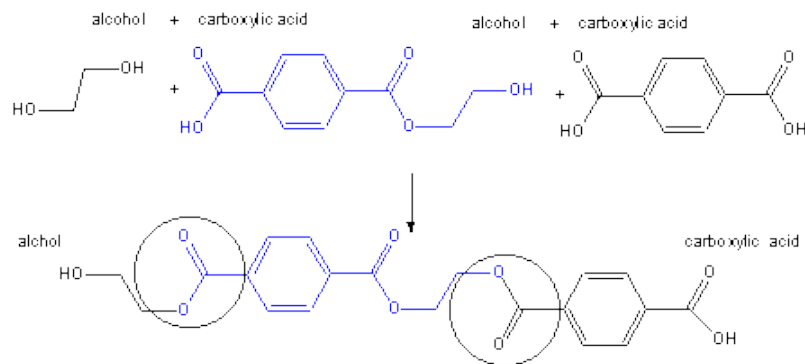
Figure 13.37b: Polyester Poly(ethylene terephthalate) or PET: Step 2 The ester formed in step 1 can react with another diacid molecule and another diol molecule to produce a compound with three ester linkages (the original one and two new ones, which are circled). The product still contains a hydroxyl group at one end and a carboxyl group at the other end, which can react with more diacid and diol molecules.
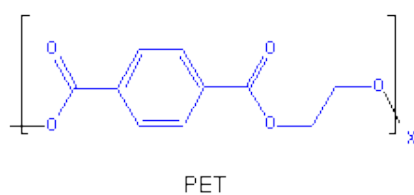

Figure 13.37c: Polyester Poly(ethylene terephthalate) or PET: Product Continued reaction increases the number of ester linkages, but maintains one hydroxyl group and one carboxyl group that can react. The monomer unit of the PET polymer is shown.

13.6-5. Nylon 66

Nylons are polyamides formed from the reaction of a diester and a diamine.

Just as reacting an ester and an amine produces an amide, reacting a diester and a diamine produces a ***polyamide***. Polyamides produced in this manner are also called ***nylons***. Each step of the polymerization produces an amide bond, but the product always contains an amine or an ester at each end, so it can react with another diester and/or another diamide.

$$x \text{ diamide} + x \text{ diester} \rightarrow \text{polyamide (nylon)}$$
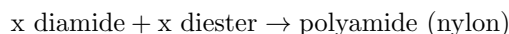
Mechanism:

1 Lone pairs on N atoms of diamines (red and blue in Figure 13.38a) attack carbonyl carbon of diester to form C–N bonds.

2 Proton transfers (shown in circles in Figure 13.38a) from diamine nitrogens to oxygens of diesters produce CH_3OH groups that leave as methanol molecules.

The produced amide also contains two amines, which can each attack another diester. The product of those reactions would contain four amide linkages and two ester groups, each of which could be attacked by another diamine. Each reaction lengthens the polymer chain.
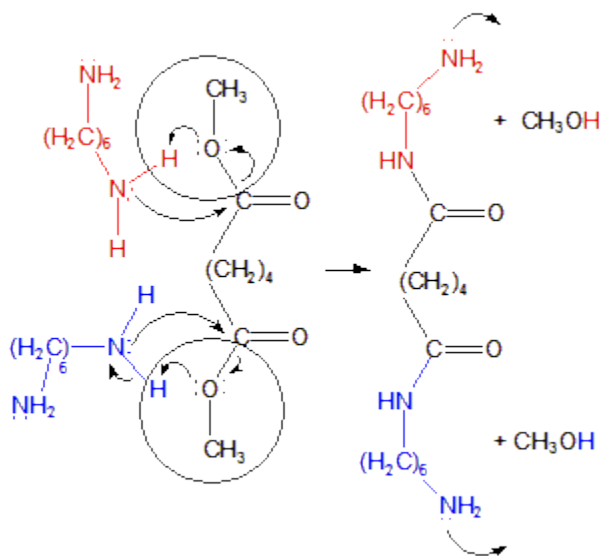
Figure 13.38a: Nylon

One monomer building block for a polyamide is shown in Figure 13.38b. Note that it contains six carbons from the diester between amide linkages (shown in blue) and six carbons from the diamine (shown in red), so the product is named Nylon 66.
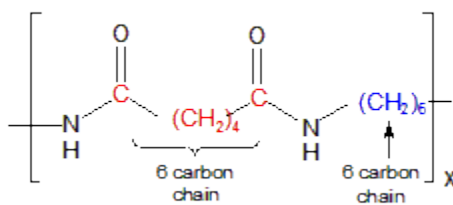

Figure 13.38b: Nylon 66
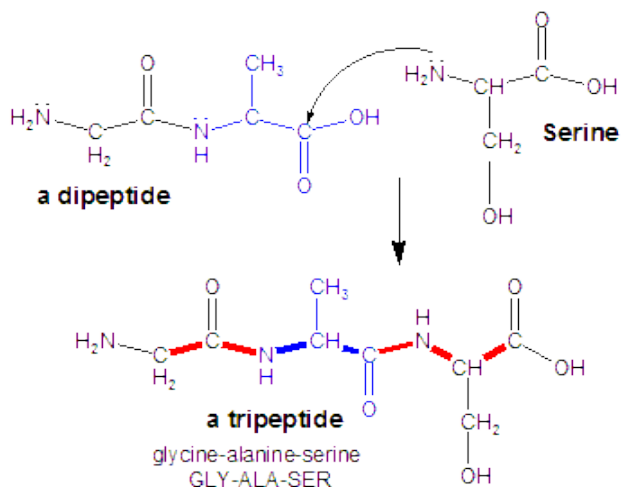
13.6-6. Polypeptides

Polypeptides are polyamides formed by the reaction of amino acids.

Polyamides can also form when each reactant contains both a carboxylic acid and an amine rather than two acids or two amines, i.e., polyamides can also be produced in the reaction of amino acids. Amides produced by the reaction of amino acids are called **peptides**, and the polyamides made from amino acids are called **polypeptides**. The resulting peptide always has two reactive sites, and continued reaction with other amino acids leads to a polypeptide or eventually a protein.

The structure of a polypeptide can be envisioned as a backbone of amide linkages, from which extend various side chains that characterize the various amino acids. Indeed, the amide backbone is frequently represented by thick bonds from which hang the side chains from the amino acids (methyl group from alanine and ethyl group from serine).
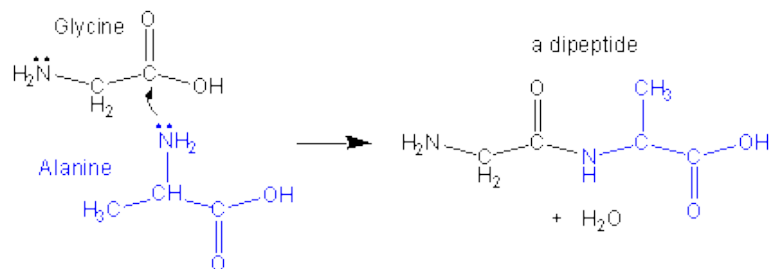
Figure 13.39a: Polypeptides: Dipeptide Two amino acids (glycine and alanine or GLY-ALA) combine to form a dipeptide. The resulting dipeptide still has a reactive site at each end (an amine and a carboxylic acid).


Figure 13.39b: Polypeptides: Tripeptide Three amino acids (glycine, alanine, and serine or GLY-ALA-SER) combine to form a tripeptide. Alternatively, a serine molecule reacts with the dipeptide formed in the first step.

13.6-7. H-Bonding in Proteins

Proteins are large polypeptides.

Proteins are high molecular weight polypeptides that often contain over 100 amino acids (called **residues**). Hydrogen bonding and dipole-dipole interactions between groups within a polypeptide are responsible for the **secondary structure** of a polypeptide. The strongest interaction is hydrogen bonding between an N–H group and a C=O group that is four residues away.

This interaction results in the α-**helix** structure of proteins. The nature and position of the amino acids around the core of the α-helix are responsible for the specific function of the protein.
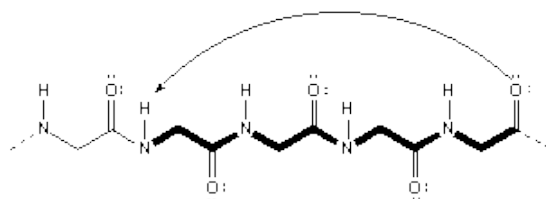
Figure 13.40: H-Bonds Responsible for the α-helix Structure

13.6-8. Protein Structure

An α-helix is shown in Figure 13.41. Color code: red = oxygen, blue = nitrogen, gray = carbon, white = hydrogen, and yellow = sulfur. Note only those hydrogen atoms involved in hydrogen bonding are shown.

(a) Space-filling model

(b) Ball-and-stick model with green ribbon to show polypeptide backbone

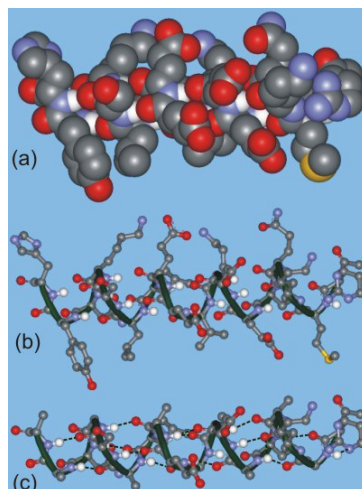(c) Ball-and-stick model in which the side chains have been removed, and hydrogen bonds are shown as dashed lines

Figure 13.41: Representations of an α-Helix

DNA

13.6-9. Nucleotides

A *nucleotide* consists of a phosphate, a sugar, and an N-containing base.
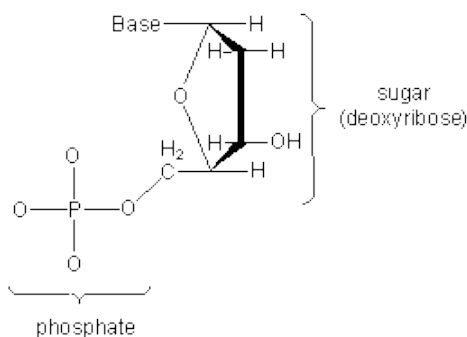

Figure 13.42 The sugar in this nucleotide is called deoxyribose.

Nucleic acids are polymers formed from nucleotide residues. If the sugar in the nucleotide is deoxyribose, then the nucleic acid is a **D**eoxyribo**N**ucleic **A**cid, or simply DNA.
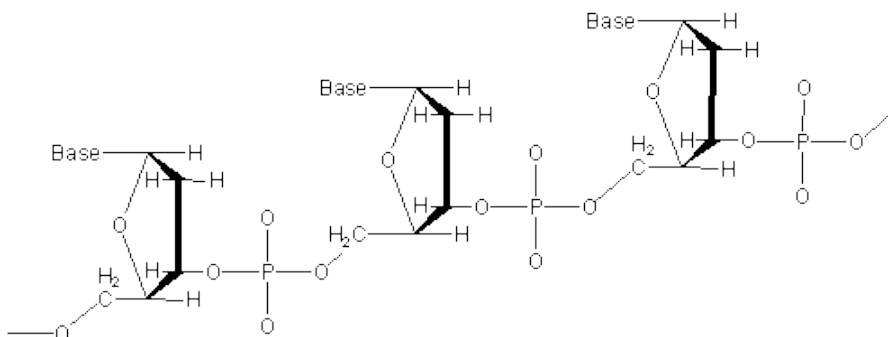

Figure 13.43: Three Residues of a DNA Molecule

13.6-10. Bases

Only four bases, which exist in two base pairs, are found on the nucleotides that form DNA.

Each nucleotide of DNA contains one of the following four bases. The location marked "backbone" indicates the position where each base bonds to the sugar in the nucleotide.

adenine (A)   thymine (T)
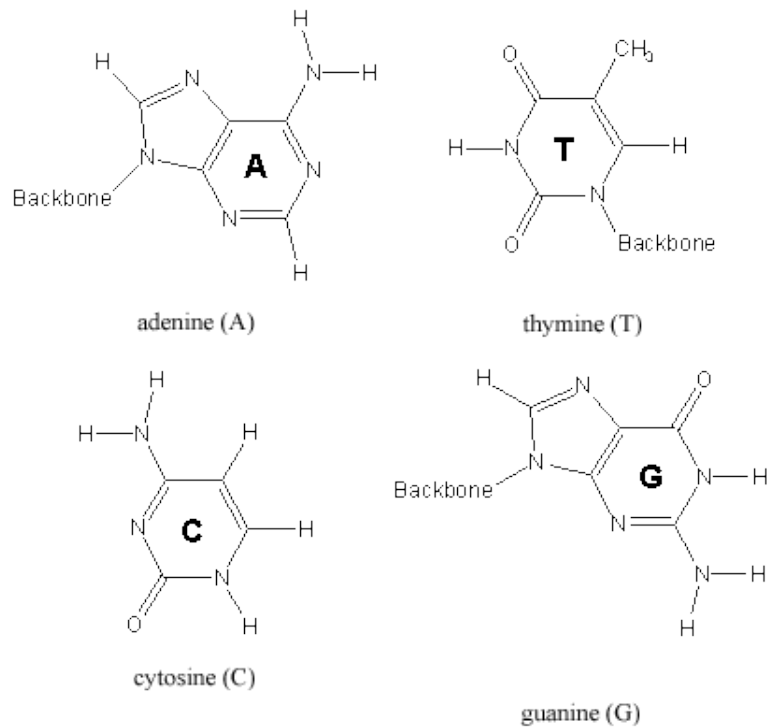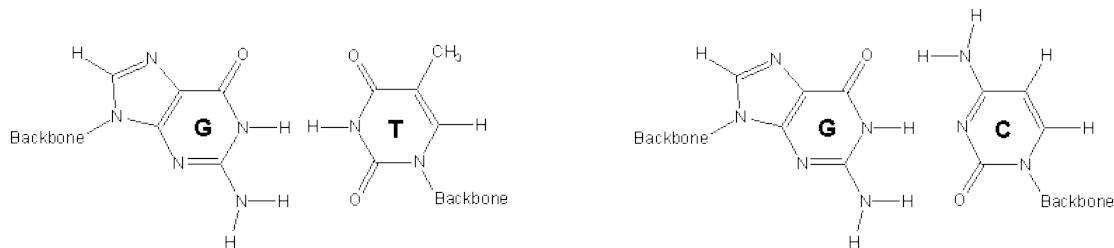
cytosine (C)

guanine (G)

Figure 13.44

The above bases can be combined into two base pairs due to the strong hydrogen bonding that can exist between the members of each pair.
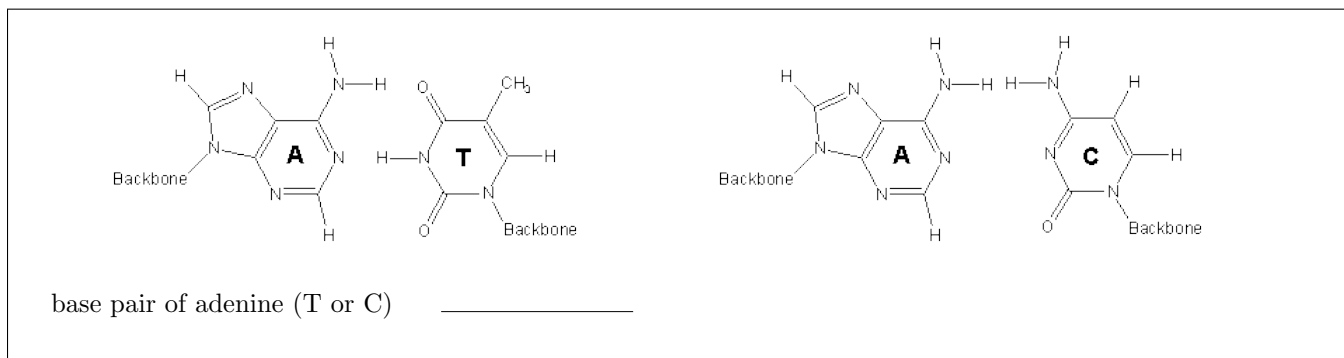
13.6-11. Determining Base-Pairs Exercise

EXERCISE 13.11:

Adenine and guanine do not interact favorably, so they are not base pairs. Determine the base pair of each (T or C) based on how well each interacts with one of the other base pairs.

base pair of guanine (T or C)   _____

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base pair of adenine (T or C) _____

13.6-12. Base Pairs

Hydrogen bonding between base pairs results in the double helix structure of DNA.

There are favorable interactions in only two pairs of bases, which are called base pairs.

1 adenine (A) - thymine (T)

2 guanine (G) - cytosine (C)

In Figure 13.45, adenine and guanine are covalently bound to strand 1, and thymine and cytosine are covalently bound to strand 2. Hydrogen bonding of the adenine on strand 1 with the thymine on strand 2 and the guanine on strand 1 with the cytosine on strand 2 hold the two strands of DNA in this portion in a **double helix**.
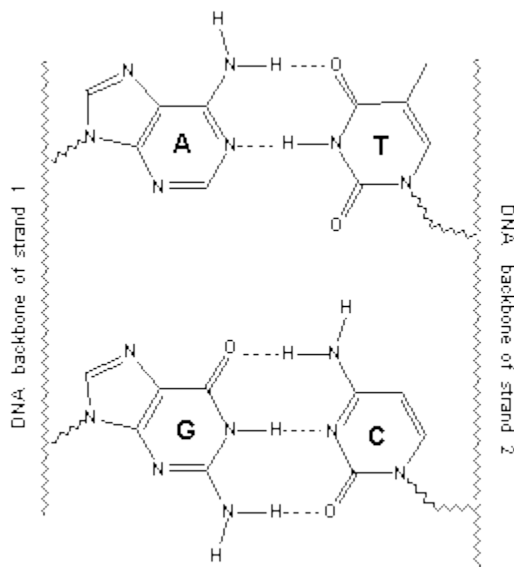

Figure 13.45: Base Pairs in DNA

13.6-13. Double Helix and Function of DNA

The structural unit of DNA is called the **double helix**. The double helix is a consequence of hydrogen bonding between base pairs on different strands. It is the sequence of the base pairs in the double helix that forms the genetic code. Thus, your genetic code requires only four different chemical letters: A, T, C, and G. However, the human cell contains about three billion base pairs.
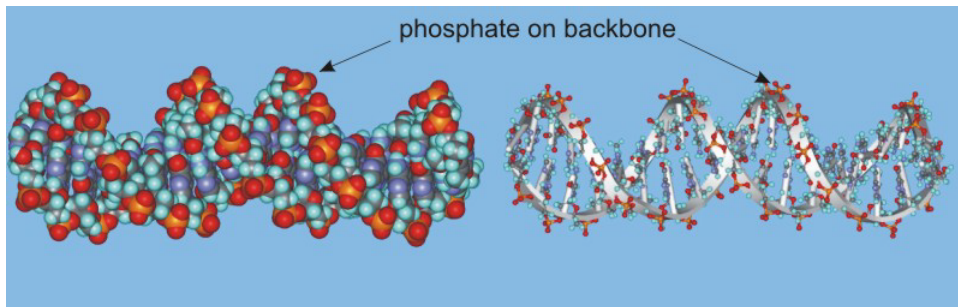
Figure 13.49: Double Helix of DNA

13.7 Exercises and Solutions

Links to view either the end-of-chapter exercises or the solutions to the odd exercises are available in the HTML version of the chapter.