Unsaturated & Aromatic Hydrocarbons

Lec. Dr. Haider Abdulkareem AlMashhadani

Lecture 7

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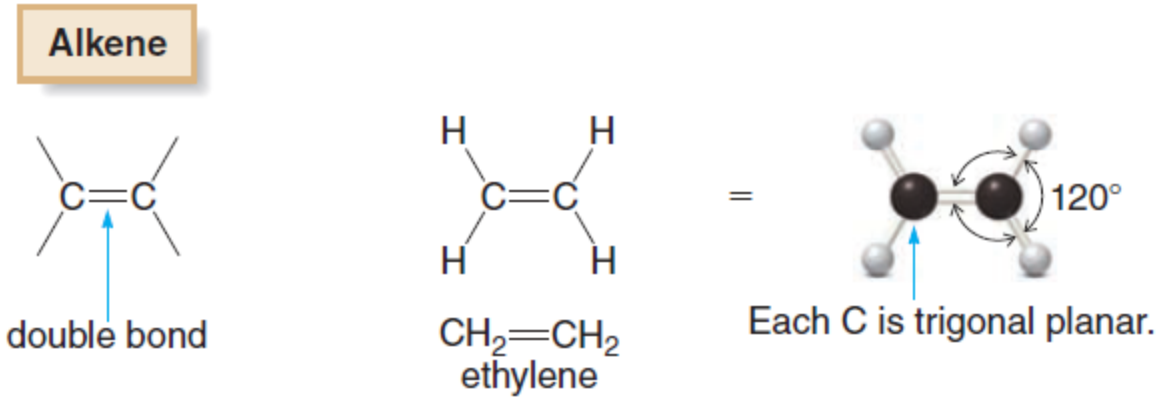
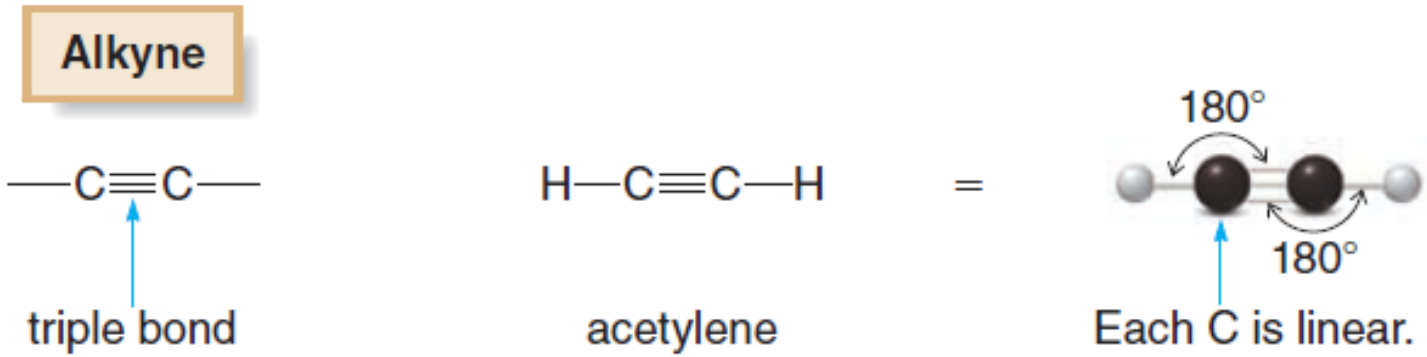
1. Unsaturated H.C

- **Alkanes** are called saturated hydrocarbons, because they contain the maximum number of hydrogen atoms per carbon. In contrast, **alkenes and alkynes** are called unsaturated hydrocarbons.
- **Unsaturated hydrocarbons** are compounds that contain fewer than the maximum number of hydrogen atoms per carbon (or contain double or triple bond).
- **Alkenes and alkynes** are two families of organic molecules that contain multiple bonds.
- **Alkenes** are compounds that contain a carbon–carbon double bond.
- The general molecular formula of an alkene is C_nH_{2n}, so an alkene has **two fewer** hydrogens than an alkane.



- **Alkynes** are compounds that contain a carbon–carbon triple bond.
- The general molecular formula for an alkyne is C_nH_{2n-2}, so an alkyne has **four fewer** hydrogens than an acyclic alkane.



- Because alkenes and alkynes are composed of nonpolar carbon–carbon and carbon–hydrogen bonds, their physical properties are similar to other hydrocarbons. Like alkanes.

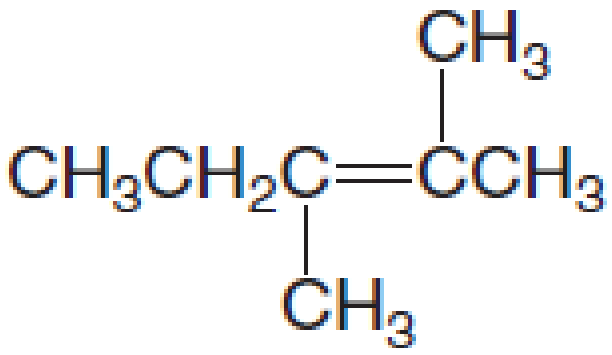
Alkenes and alkynes *have low melting points and boiling points and are insoluble in water.*

2. Nomenclature of Alkenes and Alkynes

- Whenever we encounter a new functional group, we must learn how to use the IUPAC system to name it. In the IUPAC system:
- *An alkene is identified by the suffix -ene.*
- *An alkyne is identified by the suffix -yne.*

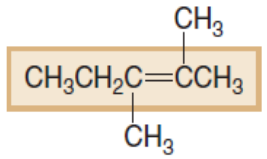
- A few simple alkenes and alkynes have names that do not follow the IUPAC system. The simplest alkene, CH2=CH2, is called ethene in the IUPAC system, but it is commonly called ethylene.
- The simplest alkyne, HC≡CH, is called ethyne in the IUPAC system, but it is commonly named acetylene. We will use these common names since they are more widely used than their systematic IUPAC names.

Problem: Give the IUPAC name for the following compound.



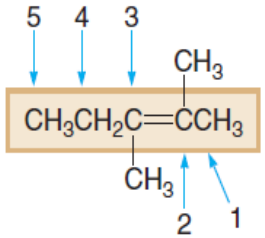
Analysis and Solution

[1] Find the longest chain containing both carbon atoms of the multiple bond.



5 C's in the longest chain ⟶ **pentene**

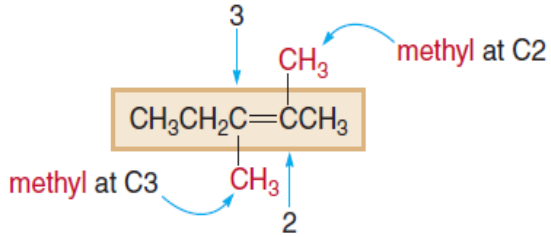
[2] Number the chain to give the double bond the lower number.



- Numbering from right to left is preferred since the double bond begins at C2 (not C3). The molecule is named as a **2-pentene.**

[3] Name and number the substituents and write the complete name.

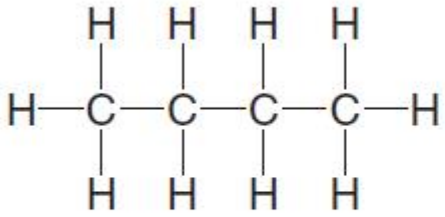
- The alkene has two methyl groups located at C2 and C3. Use the prefix di- before methyl → 2,3-**di**methyl.



Answer: 2,3-dimethyl-2-pentene

3. Isomerism and Stereoisomers

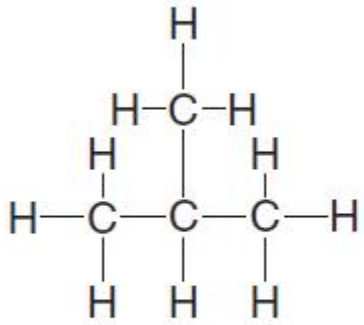
- **Isomers** are two different compounds with the same molecular formula.



butane = $CH_3CH_2CH_2CH_3$

4 C's in a row

straight-chain alkane



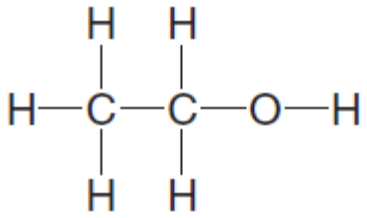
isobutane = $CH_3CH(CH_3)CH_3$

3 C's with a one-carbon branch

branched-chain alkane

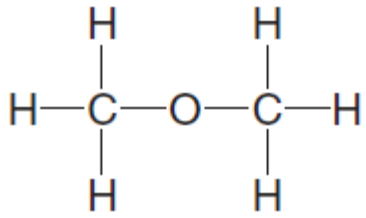
- They are two major classes of isomers:
- ✓ **Constitutional isomers**: differ in the way the atoms are connected to each other.
- ✓ **Stereoisomer**: are isomers that differ only in the 3D arrangement of atoms.

- **<u>Constitutional isomers</u>** like butane and isobutane belong to the same family of compounds: they are both alkanes.
- Ethanol (CH_3CH_2OH) and dimethyl ether (CH_3OCH_3) are constitutional isomers with different functional groups: CH_3CH_2OH is an alcohol and CH_3OCH_3 is an ether.



CH_3CH_2OH

ethanol



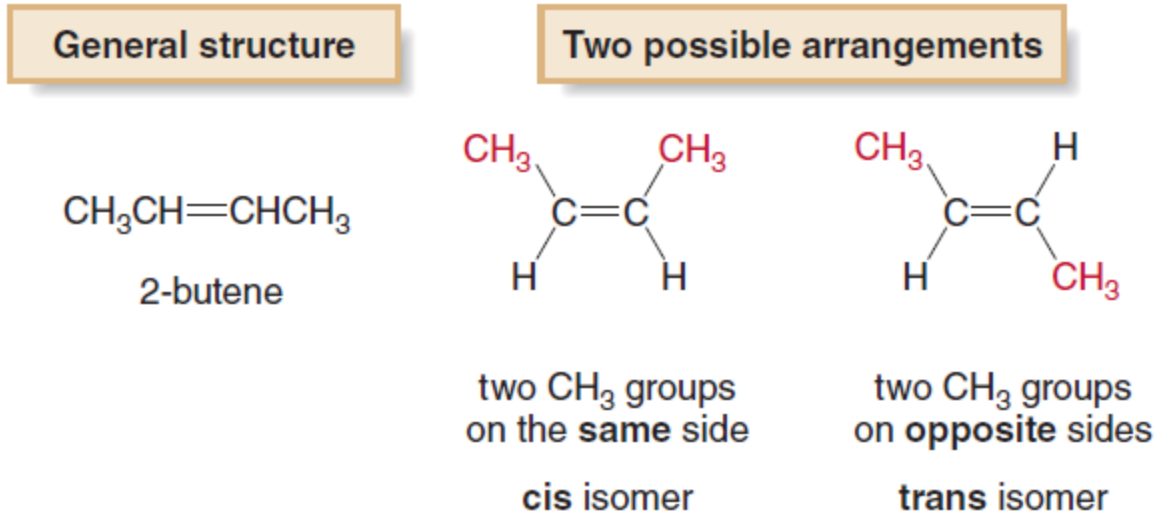
CH_3OCH_3

dimethyl ether

❑Stereoisomers:

- 2-Butene illustrates another important aspect about alkenes. There is restricted rotation around the carbon atoms of a double bond. As a result, the groups on one side of the double bond cannot rotate to the other side.
- With 2-butene, there are two ways to arrange the atoms on the double bond. The two CH_3 groups can be on the same side of the double bond or they can be on opposite sides of the double bond. These molecules are different compounds with the same molecular formula; that is, they are isomers.

- When the two CH_3 groups are on the same side of the double bond, the compound is called the ***cis isomer***.
- When the two CH_3 groups are on opposite sides of the double bond, the compound is called the ***trans isomer***.



SAMPLE PROBLEM 11.3

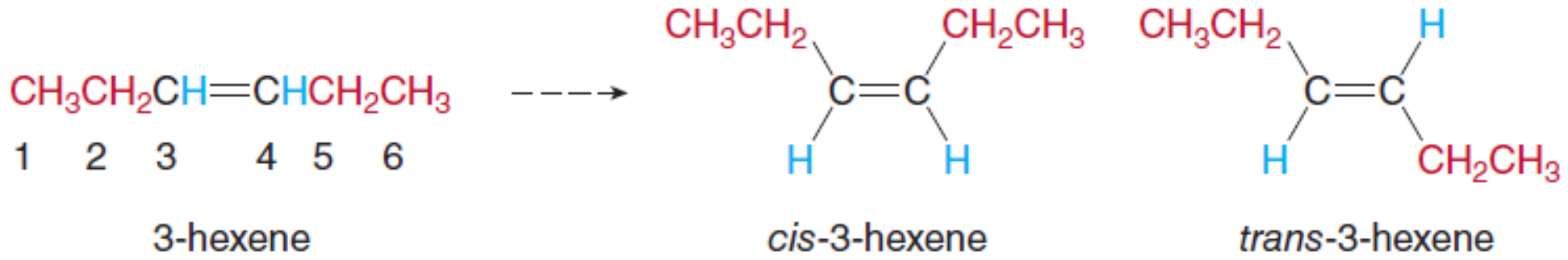
Draw *cis*- and *trans*-3-hexene.

Analysis

First, use the parent name to draw the carbon skeleton, and place the double bond at the correct carbon; 3-hexene indicates a 6 C chain with the double bond beginning at C3. Then use the definitions of cis and trans to draw the isomers.

Solution

Each C of the double bond is bonded to a CH_3CH_2 group and a hydrogen. A cis isomer has the CH_3CH_2 groups bonded to the same side of the double bond. A trans isomer has the two CH_3CH_2 groups bonded to the opposite sides of the double bond.

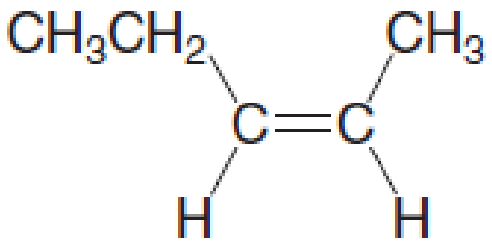
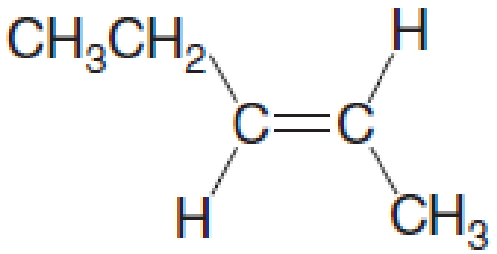


3-hexene *cis*-3-hexene *trans*-3-hexene

PROBLEM

Label each pair of alkenes as constitutional isomers or stereoisomers.

a. $CH_3CH{=}CHCH_2CH_3$ and $CH_2{=}CHCH_2CH_2CH_3$

b.  and 

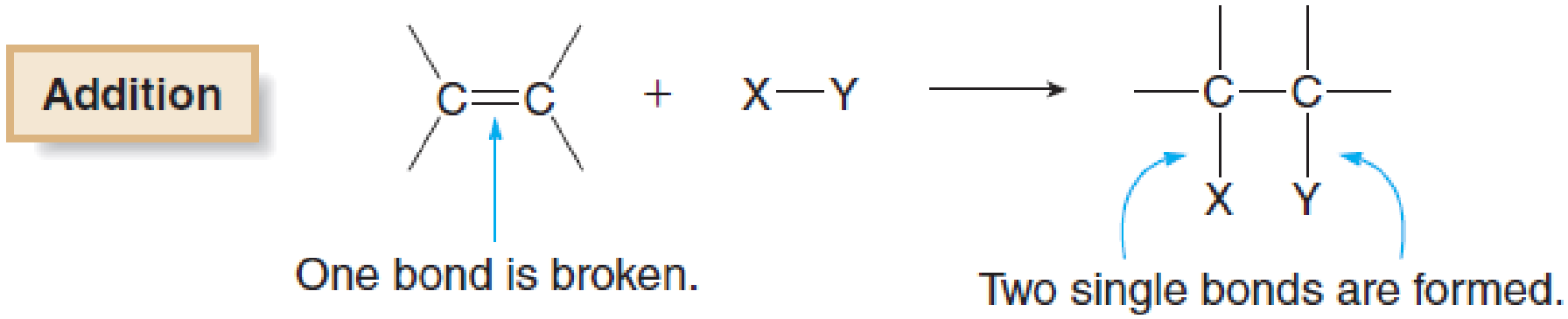
4. Reactions of Alkenes

- Most families of organic compounds undergo a characteristic type of reaction. Alkenes undergo addition reactions. In an **addition reaction**, new groups X and Y are added to a starting material. One bond of the double bond is broken and two new single bonds are formed.

- Addition reaction is a reaction in which elements are added to a compound.

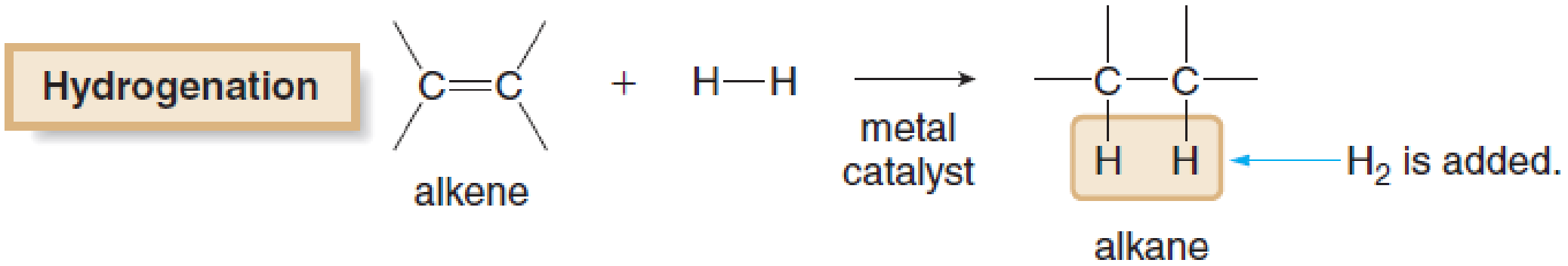
- **Why does addition occur?**

- A double bond is composed of one strong bond and one weak bond. In an addition reaction, the weak bond is broken and two new strong single bonds are formed.



4.1. Addition of Hydrogen—Hydrogenation

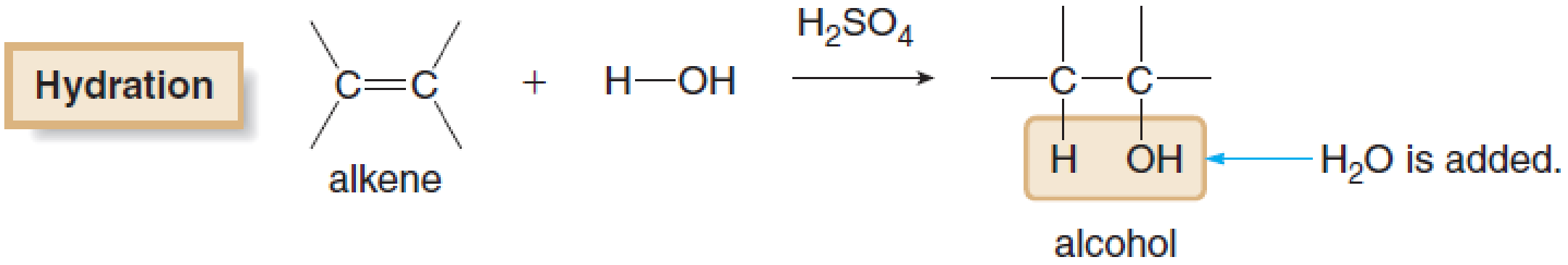
- Hydrogenation is the addition of hydrogen (H_2) to an alkene. Two bonds are broken: one bond of the carbon–carbon double bond and the H-H bond—and two new C-H bonds are formed.



- The addition of H_2 occurs only in the presence of a metal catalyst such as palladium (Pd). The metal provides a surface that binds both the alkene and H_2, and this speed up the rate of reaction. Hydrogenation of an alkene forms an ***alkane*** since the product has only C-C single bonds.

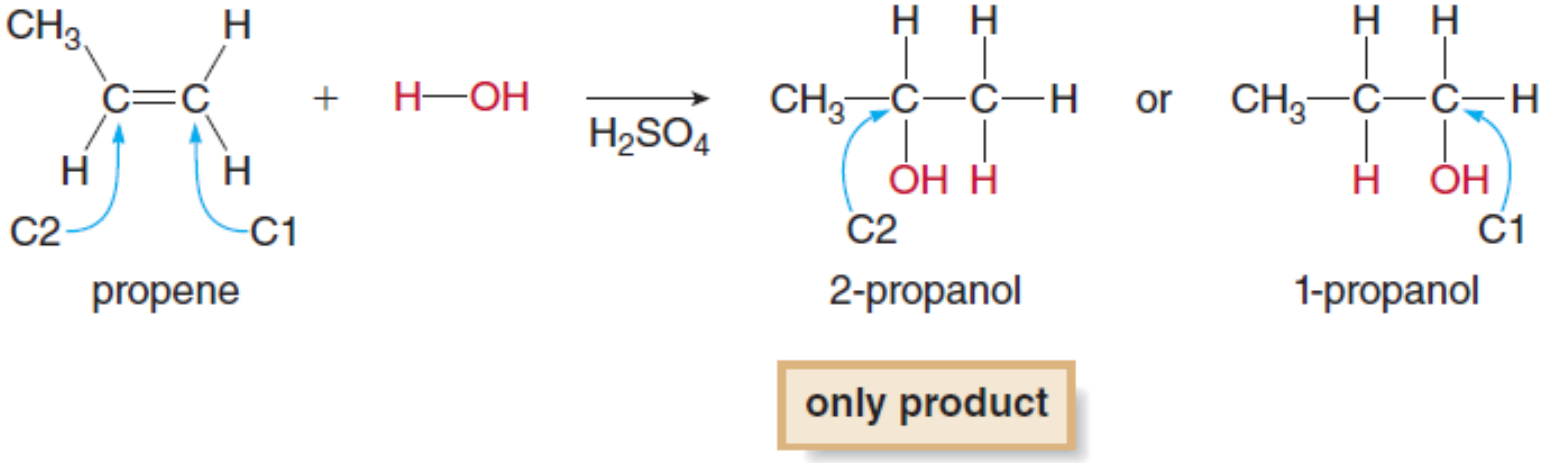
4.2. Addition of Water—Hydration

- Hydration is the addition of water to an alkene. Two bonds are broken—one bond of the carbon–carbon double bond and the H-OH bond—and new C-H and C-OH bonds are formed.



- **Hydration** occurs only if a **strong acid** such as **H_2SO_4** is added to the reaction mixture. The product of hydration is an ***alcohol***.

- There is one important difference in this addition reaction compared to the addition of H_2. In this case, addition puts different groups-H and OH-on the two carbons of the double bond. As a result, *H_2O can add to the double bond to give two **constitutional isomers** when an **unsymmetrical alkene** is used as starting material.*

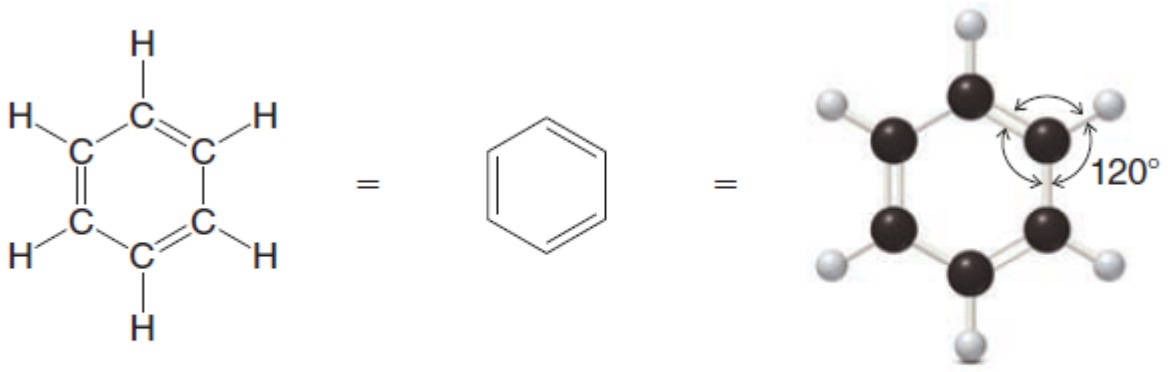


- This is specific example of a general trend called **Markovnikov's rule**

➢In the addition of H_2O to an unsymmetrical alkene, the H atom bonds to the less substituted carbon atom—that is, the carbon that has more H's to begin with.

5. Aromatic Compounds

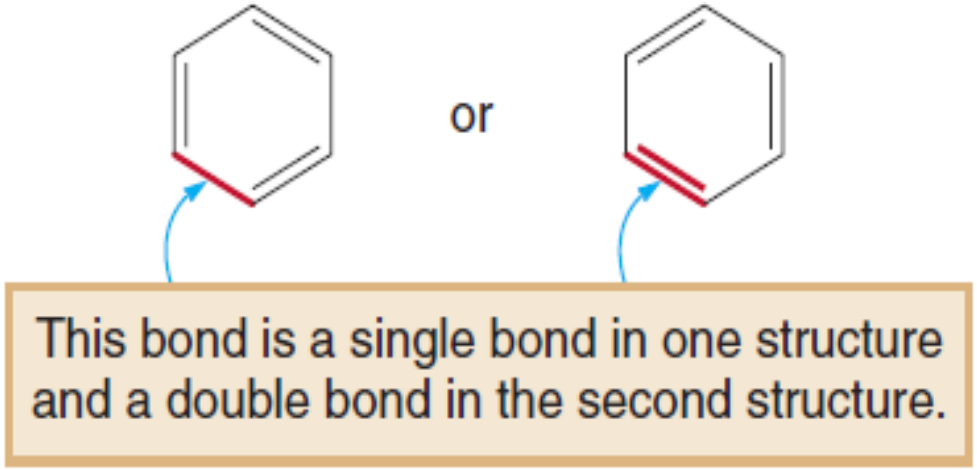
- **Aromatic compounds** represent another example of unsaturated hydrocarbons. Aromatic compounds were originally named because many simple compounds in this family have characteristic odors. Today, the word **aromatic refers to compounds that contain a benzene ring**, or **rings that react in a similar fashion to benzene**.
- **Benzene**, the simplest and most widely known aromatic compound, contains a six-membered ring and three double bonds. Since each carbon of the ring is also bonded to a hydrogen atom, the molecular formula for benzene is C_6H_6.



benzene
C_6H_6

planar molecule

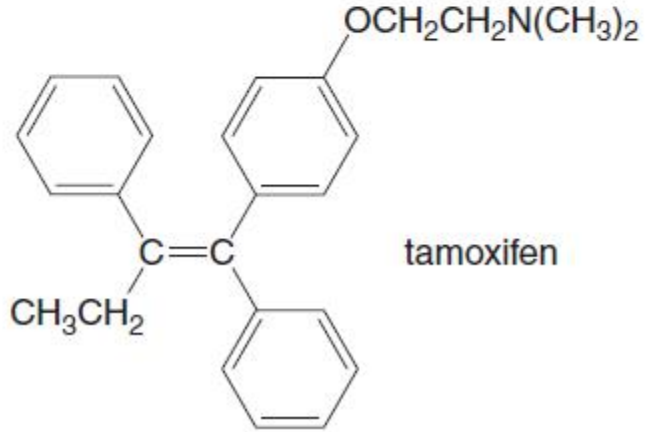
- Although benzene is drawn with a six-membered ring and three double bonds, there are two different ways to arrange the double bonds so that they alternate with single bonds around the ring. Each of these representations is equivalent.



- The physical properties of aromatic hydrocarbons are similar to other hydrocarbons—they have low melting points and boiling points and are water insoluble.

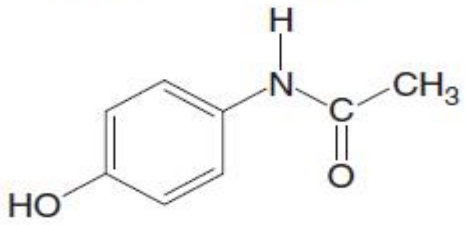
HEALTH NOTE

Tamoxifen, a potent anticancer drug sold under the trade name of Novaldex, contains three benzene rings.



tamoxifen

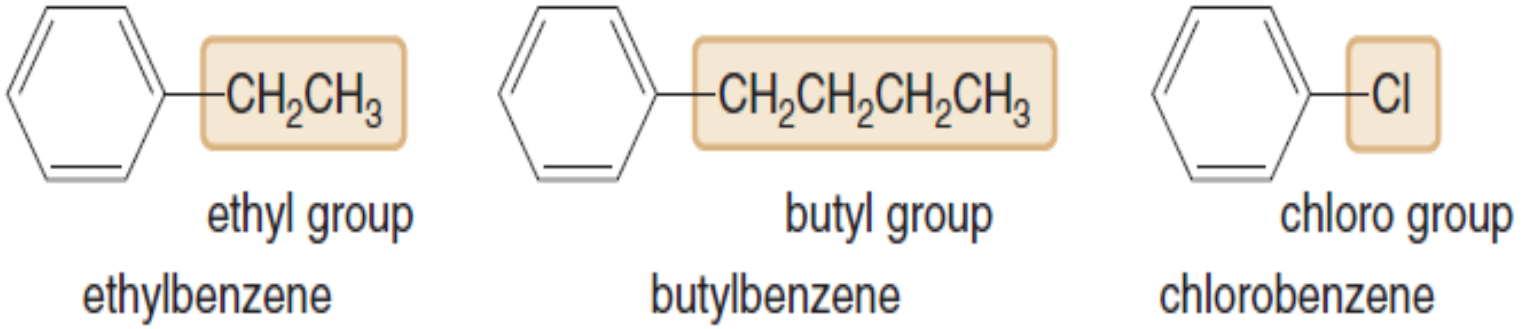
The pain reliever acetaminophen (trade name Tylenol) contains a para-disubstituted benzene ring.



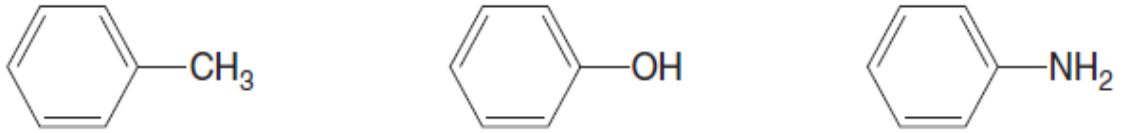
acetaminophen
(Trade name: Tylenol)

Nomenclature of Benzene Derivatives

- Many organic molecules contain a benzene ring with one or more substituents, so we must learn how to name them.
- To name a benzene ring with one substituent, name the substituent and add the word benzene. Carbon substituents are named as alkyl groups. When a halogen is a substituent, name the halogen by changing the -ine ending of the name of the halogen to the suffix -o; for example, chlorine → chloro.

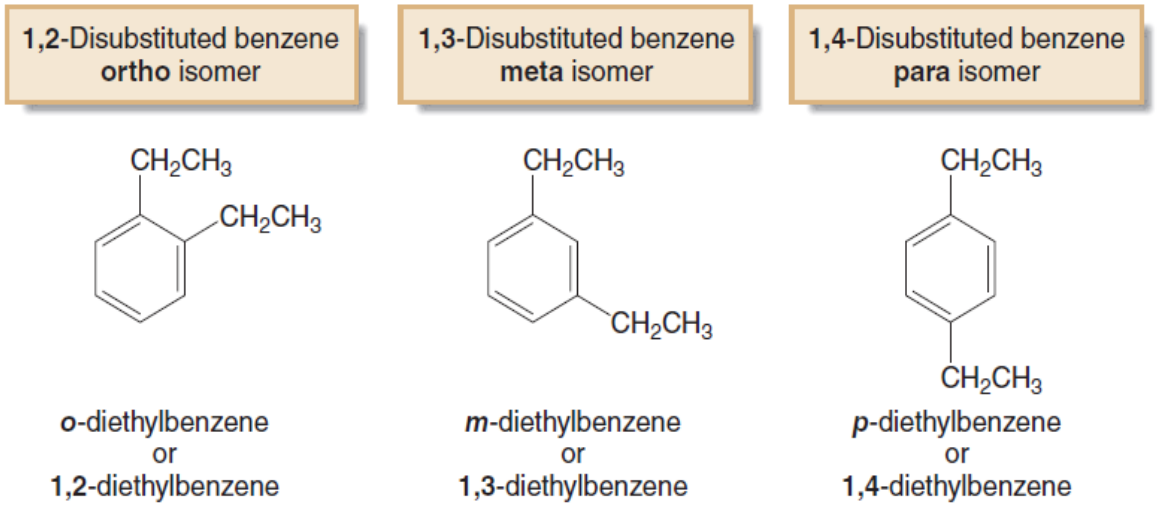


Many monosubstituted benzenes, such as those with methyl (CH_3–), hydroxyl (–OH), and amino (–NH_2) groups, have common names that you must learn, too.



toluene (methylbenzene) | phenol (hydroxybenzene) | aniline (aminobenzene)

To name a benzene ring with two substituent, there are three different ways that two groups can be attached to a benzene ring, so a prefix— ***ortho***, ***meta***, or ***para***—is used to designate the relative position of the two substituents. Ortho, meta, and para are generally abbreviated as ***o***, ***m***, and ***p***, respectively.

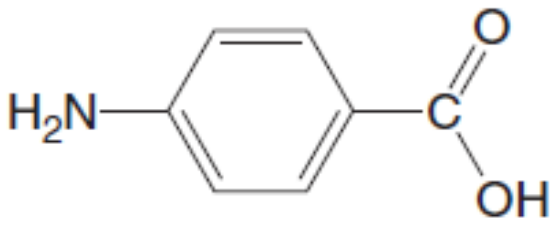


o-diethylbenzene or 1,2-diethylbenzene | *m*-diethylbenzene or 1,3-diethylbenzene | *p*-diethylbenzene or 1,4-diethylbenzene

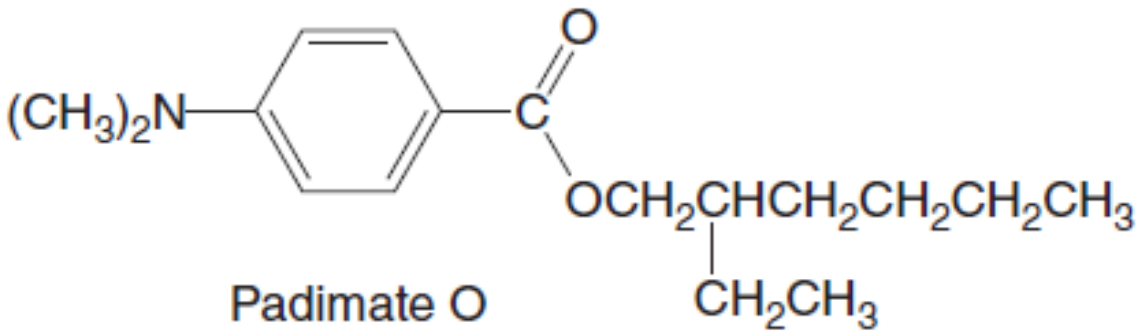
5.1. Sunscreens

(FOCUS ON HEALTH & MEDICINE)

- All commercially available sunscreens contain a benzene ring. A sunscreen absorbs ultraviolet radiation and thus shields the skin for a time from its harmful effects. Two sunscreens that have been used for this purpose are **p-aminobenzoic acid (PABA)** and **Padimate O**.



p-aminobenzoic acid (PABA)



Padimate O

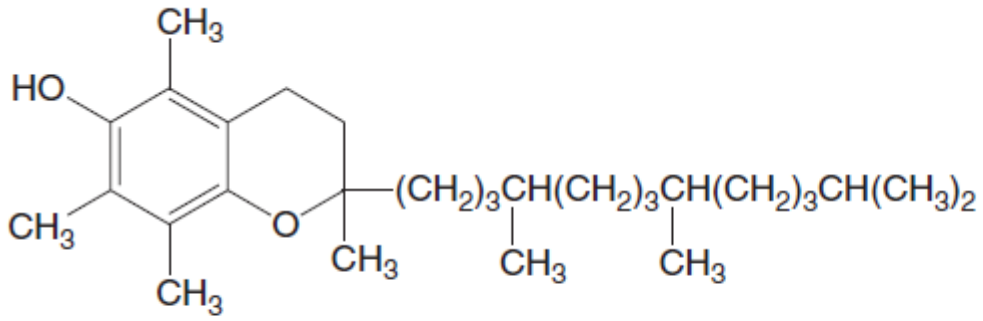
HEALTH NOTE

Commercial sunscreens are given an **SPF** rating (sun protection factor), according to the amount of sunscreen present. The higher the number, the greater the protection.

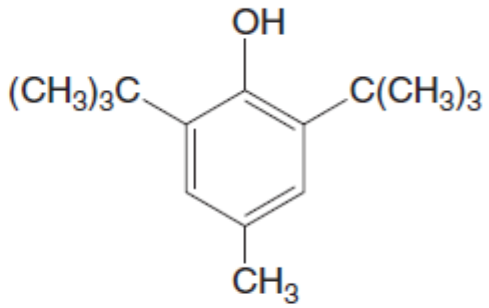
5.2. Phenols as Antioxidants

(FOCUS ON HEALTH & MEDICINE)

- A wide variety of **phenols**, compounds that contain a **hydroxyl group** bonded to a **benzene ring**, occur in nature. **Vanillin** from the vanilla bean is a phenol, as is **curcumin**, a yellow pigment isolated from turmeric.
- Many **phenols are antioxidants**, compounds that prevent unwanted oxidation reactions from occurring. Two examples are naturally occurring **vitamin E** and **synthetic BHT**. The OH group on the benzene ring is the key functional group that prevents oxidation reactions from taking place.

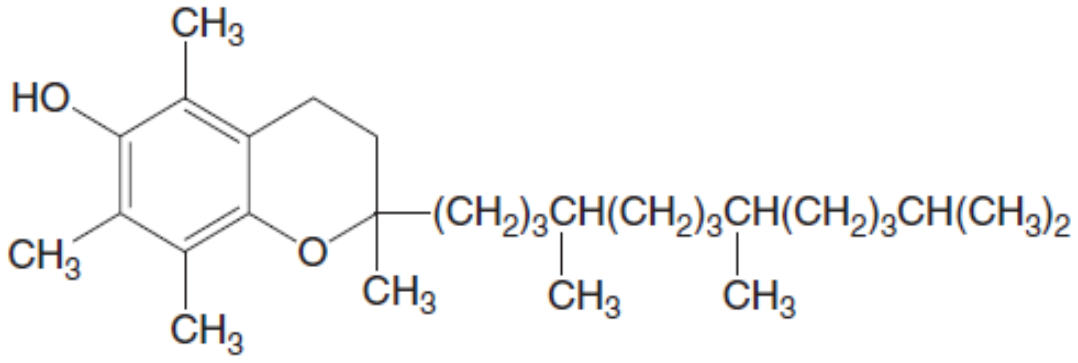


vitamin E

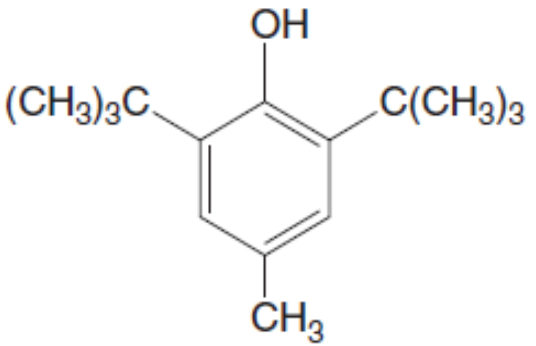


BHT
(butylated hydroxy toluene)

- Vitamin E is a natural antioxidant found in fish oil, peanut oil, wheat germ, and leafy greens. Although the molecular details of its function remain obscure, it is thought that vitamin E prevents the unwanted oxidation of unsaturated fatty acid residues in cell membranes. In this way, vitamin E helps retard the aging process.
- Synthetic antioxidants such as BHT—butylated hydroxy toluene—are added to packaged and prepared foods to prevent oxidation and spoilage. BHT is a common additive in breakfast cereals.



vitamin E



BHT
(butylated hydroxy toluene)

End