Al-Rasheed University College
Department of Dentistry
1st Stage

MEDICAL CHEMISTRY

lecture 6
Hydrocarbons

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Introduction

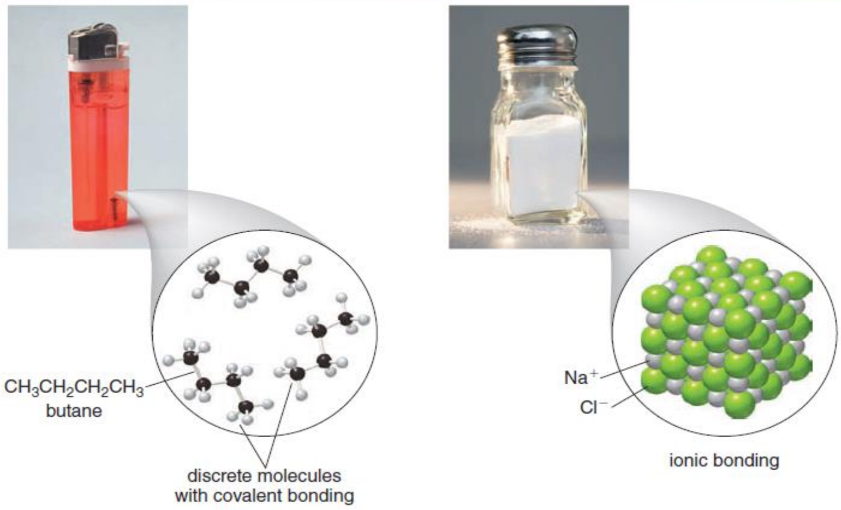
☒ *What is organic chemistry?*

Organic chemistry is the study of compounds that contain *the element carbon*.

- Clothes, foods, medicines, gasoline, refrigerants, and soaps are composed almost solely of organic compounds.
- Organic compounds exist as discrete molecules with much weaker intermolecular forces, the forces that exist between molecules, than those seen in ionic compounds, which are held together by very strong interactions of oppositely charged ions.

✓ As a result, organic compounds resemble other covalent compounds in that they have much lower melting points and boiling points than ionic compounds. While ionic compounds are generally solids at room temperature, many organic compounds are liquids and some are even gases. Table 10.1 compares these and other properties of a typical organic compound (butane, $CH_3CH_2CH_2CH_3$) and a typical ionic inorganic compound (sodium chloride, NaCl).

Table 10.1 Comparing the Properties of an Organic Compound ($CH_3CH_2CH_2CH_3$) and an Ionic Inorganic Compound (NaCl)



Property	$CH_3CH_2CH_2CH_3$ (An Organic Compound)	NaCl (An Inorganic Compound)
Bonding	Covalent	Ionic
Physical state	Gas at room temperature	Solid at room temperature
Boiling point	Low (–0.5 °C)	High (1413 °C)
Melting point	Low (–138 °C)	High (801 °C)
Solubility in water	Insoluble	Soluble
Solubility in organic solvents	Soluble	Insoluble
Flammability	Flammable	Nonflammable

? **Problem:** Which chemical formulas represent organic compounds and which represent inorganic compounds?

a. C_6H_{12} b. KI c. CH_4O d. H_2O e. $MgSO_4$ f. NaOH

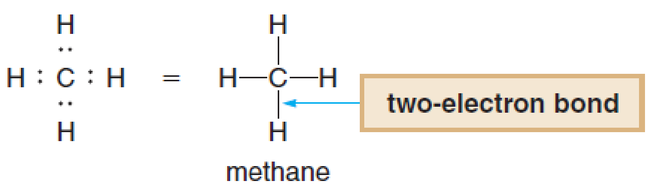
The Physical Properties of organic compounds

1. Organic compounds resemble other covalent compounds.
2. They have much lower melting points and boiling points than ionic compounds.
3. Many organic compounds are liquids and some are even gases.

The Characteristic Features of organic compounds

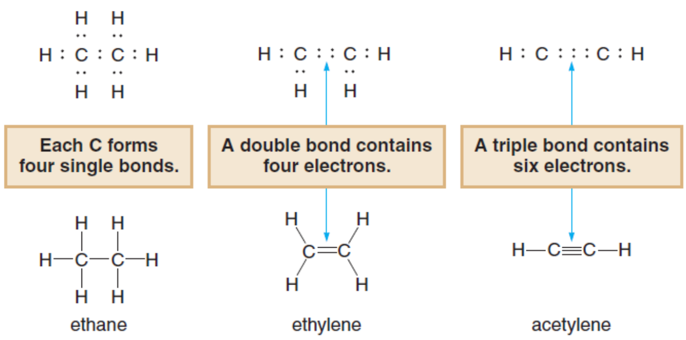
1. All organic compounds contain carbon atoms and most contain hydrogen atoms. Carbon always forms four covalent bonds, and hydrogen forms one covalent bond.

   Carbon is located in group 4A of the periodic table, so a carbon atom has four valence electrons available for bonding (Section 3.7). Since hydrogen has a single valence electron, methane (CH_4) consists of four single bonds, each formed from one electron from a hydrogen atom and one electron from carbon.



2. Carbon forms single, double, and triple bonds to other carbon atoms.

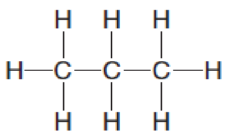
   When a compound contains two or more carbon atoms, the type of bonding is determined by the number of atoms around carbon. Consider the three compounds drawn below:



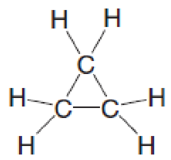
- *A C atom surrounded by four atoms forms four single bonds.* In ethane (C_2H_6), each carbon atom is bonded to three hydrogen atoms and one carbon atom. All bonds are single bonds.
- *A C atom surrounded by three atoms forms one double bond.* In ethylene (C_2H_4), each carbon atom is surrounded by three atoms (two hydrogens and one carbon); thus, each C forms a single bond to each hydrogen atom and a double bond to carbon.
- *A C atom surrounded by two atoms generally forms one triple bond.* In acetylene (C_2H_2), each carbon atom is surrounded by two atoms (one hydrogen and one carbon); thus, each C forms a single bond to hydrogen and a triple bond to carbon.

3. Some compounds have chains of atoms and some compounds have rings.

   For example, three carbon atoms can bond in a row to form propane, or form a ring called cyclopropane. Propane is the fuel burned in gas grills, and cyclopropane is an anesthetic.



propane
C_3H_8



cyclopropane
C_3H_6

4. Organic compounds may also contain elements other than carbon and hydrogen. **Any atom that is not carbon or hydrogen is called a heteroatom**.

   The most common heteroatoms are nitrogen, oxygen, and the halogens (F, Cl, Br, and I).

   • Each heteroatom forms a characteristic number of bonds, determined by its location in the periodic table.

   • The common heteroatoms also have nonbonding, lone pairs of electrons, so that each atom is surrounded by eight electrons.

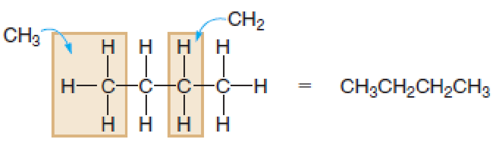
Drawing Organic Molecules

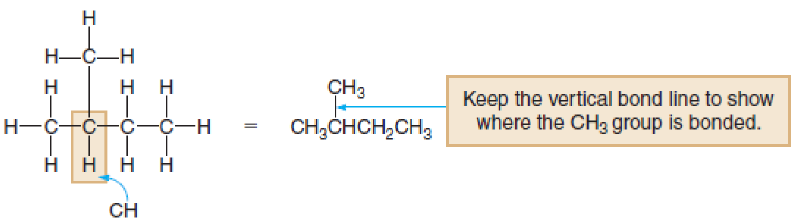
Because organic molecules often contain many atoms, we need shorthand methods to simplify their structures. The two main types of shorthand representations used for organic compounds are ***condensed structures*** and ***skeletal structures***.

1. Condensed Structures

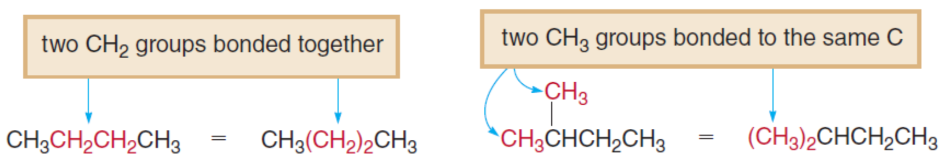
- Condensed structures are most often used for a compound having a chain of atoms bonded together, rather than a ring. The following conventions are used.

- *All of the atoms are drawn in, but the two-electron bond lines are generally omitted.*
- *Lone pairs on heteroatoms are omitted.*
- To interpret a condensed formula, it is usually best to start at the left side of the molecule and remember that the carbon atoms must have four bonds.

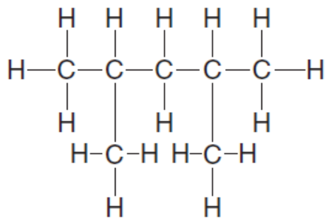


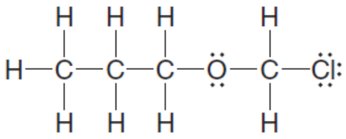


☒ Sometimes these structures are further simplified by using parentheses around like groups. Two CH_2 groups bonded together become $(CH_2)_2$. Two CH_3 groups bonded to the same carbon become $(CH_3)_2C$.



Problem: Convert each compound into a condensed structure.

a. 

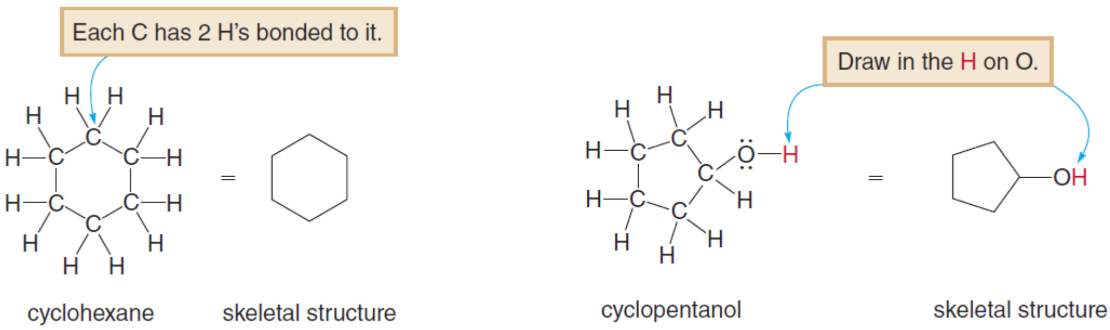
b. 

2. Skeletal Structures

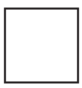
Skeletal structures are used for organic compounds containing both rings and chains of atoms.

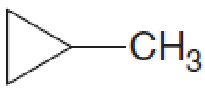
Three important rules are used in drawing them.

- Assume there is a carbon atom at the junction of any two lines or at the end of any line.
- Assume there are enough hydrogens around each carbon to give it four bonds.
- Draw in all heteroatoms and the hydrogens directly bonded to them.



Problem: Convert each skeletal structure to a complete structure with all C's and H's drawn in.

a. 

b. 

1. Hydrocarbon

<u>Hydrocarbons</u> are compounds that contain only the elements of carbon and hydrogen.

Hydrocarbon can be classification to:

i. Saturated Hydrocarbon (alkane); have only C-C single bonds and no functional group. Ethane, CH_3CH_3, is a simple alkane.
ii. Unsaturated Hydrocarbon; have a double or trible bond as their functional group. Ethylene, Acetylene.
iii. Aromatic Hydrocarbon; contain a benzene ring, a six-membered ring with three double bonds.

- ✓ All hydrocarbons other than alkanes contain multiple bonds. Alkanes, which have no functional groups and therefore no reactive sites, are notoriously unreactive except under very drastic conditions.
- ✓ For example, polyethylene is a synthetic plastic and high molecular weight alkane, consisting of long chains of $-CH_2-$ groups bonded together, hundreds or even thousands of atoms long. Because it has no reactive sites, it is a very stable compound that does not readily degrade and thus persists for years in landfills.

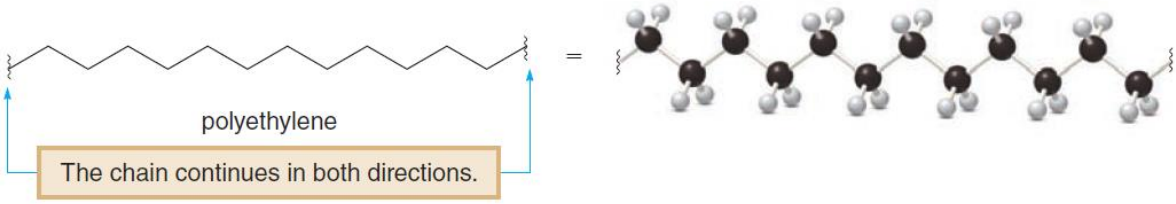
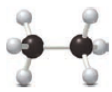
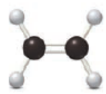
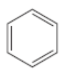
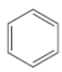
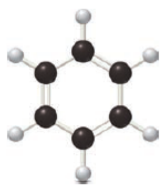


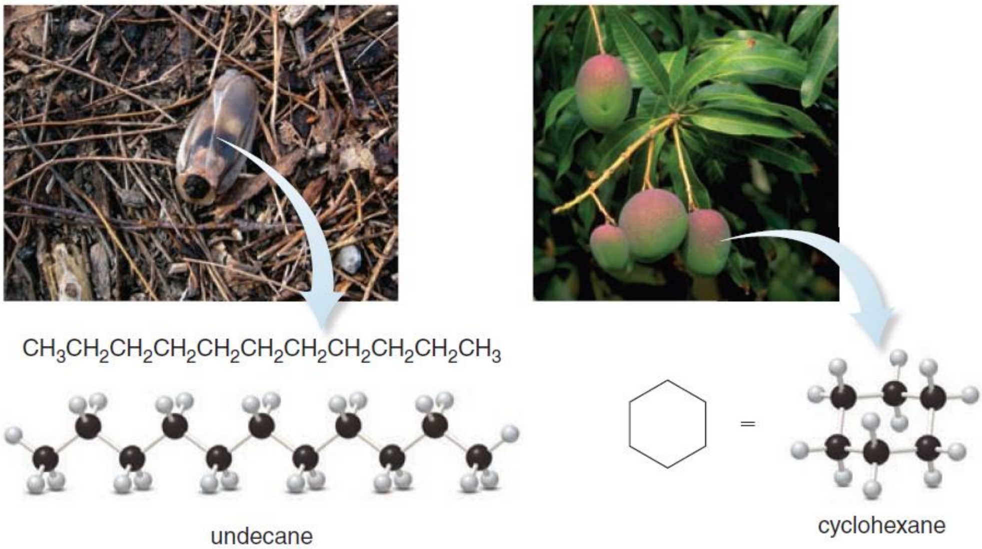
Table 10.3 Hydrocarbons

Type of Compound	General Structure	Example	3-D Structure	Functional Group
Alkane	R—H	CH_3CH_3		–
Alkene	C=C	H H C=C H H		Carbon–carbon double bond
Alkyne	—C≡C—	H—C≡C—H		Carbon–carbon triple bond
Aromatic compound				Benzene ring

2. Alkane

Alkanes are hydrocarbons having only C-C and C-H single bonds. The carbons of an alkane can be joined together to form chains or rings of atoms.

- ✓ Alkanes that contain chains of carbon atoms but no rings are called ***acyclic alkanes***. An acyclic alkane has **the molecular formula C_nH_{2n+2}**, where *n* is the number of carbons it contains. **Acyclic alkanes are also called saturated hydrocarbons because they have the maximum number of hydrogen atoms per carbon.**
- ✓ ***Cycloalkanes*** contain carbons joined in one or more rings. Since a cycloalkane has two fewer H's than an acyclic alkane with the same number of carbons, **its general formula is C_nH_{2n}.**
- ✓ Undecane and cyclohexane are examples of two naturally occurring alkanes. *Undecane* is an acyclic alkane with molecular formula $C_{11}H_{24}$.
- ✓ *Cyclohexane*, a cycloalkane with molecular formula C_6H_{12}, is one component of the mango, the most widely consumed fruit in the world.



Problem: How many hydrogen atoms are present in each compound?

a. an acyclic alkane with three carbons

b. a cycloalkane with four carbons

c. a cycloalkane with nine carbons

d. an acyclic alkane with seven carbons

The Physical Properties of Alkane

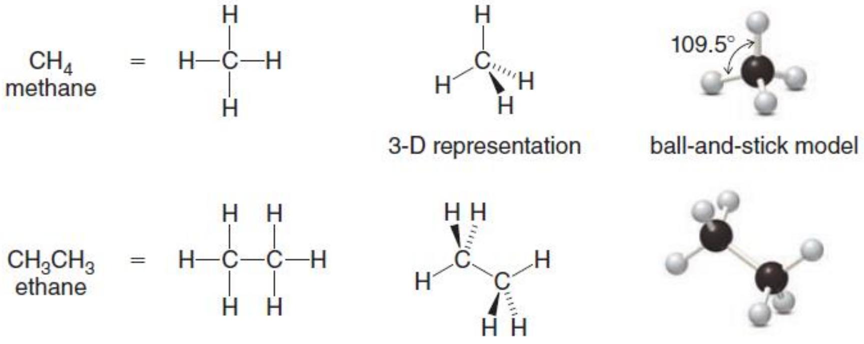
1. Alkanes have low melting points and boiling points.
2. The melting points and boiling points of alkanes increase as the number of carbons increases.
3. Low molecular weight alkanes are gases at room temperature, and alkanes used in gasoline are all liquids.
4. Increased surface area increases the force of attraction between molecules, thus raising the boiling point and melting point.
5. Alkanes are insoluble in water; because nonpolar alkanes.
6. Less dense than water

a. Acyclic Alkanes Having Fewer Than Five Carbons

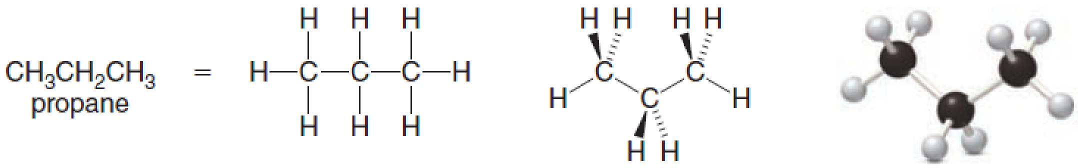
The structures for the two simplest acyclic alkanes were given in The Characteristic Features of organic compounds.

- ✓ Methane, CH_4, has a single carbon atom surrounded by four hydrogens to give it four bonds.
- ✓ Ethane, CH_3CH_3, has two carbon atoms joined together by a single bond. Each carbon is also bonded to three hydrogens to give it four bonds total.

The shape around atoms in organic molecules is determined by counting groups using the principles of VSEPR theory. Since each carbon in an alkane is surrounded by four atoms, each carbon is tetrahedral, and all bond angles are 109.5°.

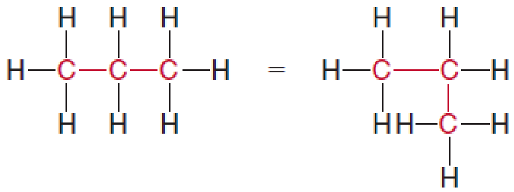


To draw a three-carbon alkane, draw three carbons joined together with single bonds and add enough hydrogens to give each carbon four bonds. This forms propane, $CH_3CH_2CH_3$.



3-D representation   ball-and-stick model

- The carbon skeleton in propane and other alkanes can be drawn in a variety of different ways and still represent the same molecule. For example, the three carbons of propane can be drawn in a horizontal row or with a bend. These representations are equivalent. If you follow the carbon chain from one end to the other, you move across the same three carbon atoms in both representations.

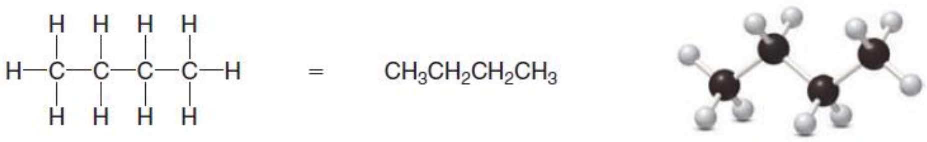


3 C's in a row   3 C's with a bend

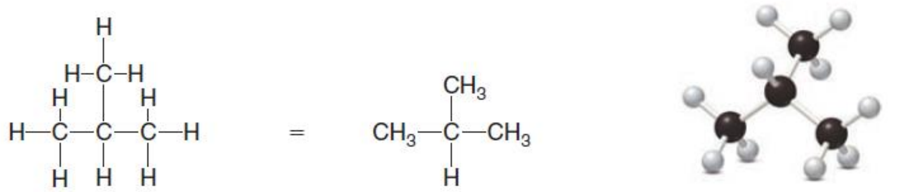
✓ The bends in a carbon chain don't matter when it comes to identifying different compounds.

There are two different ways to arrange four carbons, giving two compounds with molecular formula C_4H_{10}.

1. **Butane, $CH_3CH_2CH_2CH_3$**, has four carbon atoms in a row. Butane is a straight-chain alkane, an alkane that has all of its carbons in one continuous chain.
2. **Isobutane, $(CH_3)_3CH$**, has three carbon atoms in a row and one carbon bonded to the middle carbon. Isobutane is a branched-chain alkane, an alkane that contains one or more carbon branches bonded to a carbon chain.



butane   4 C's in a row   straight-chain alkane

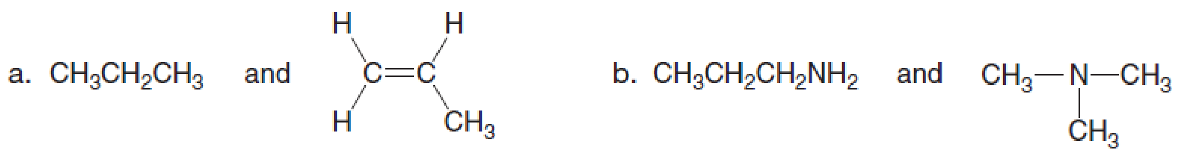


isobutane   3 C's with a one-carbon branch   branched-chain alkane

- ✓ **Butane** and **isobutane** are *isomers*, two different compounds with the same molecular formula. They belong to one of the two major classes of isomers called constitutional isomers.

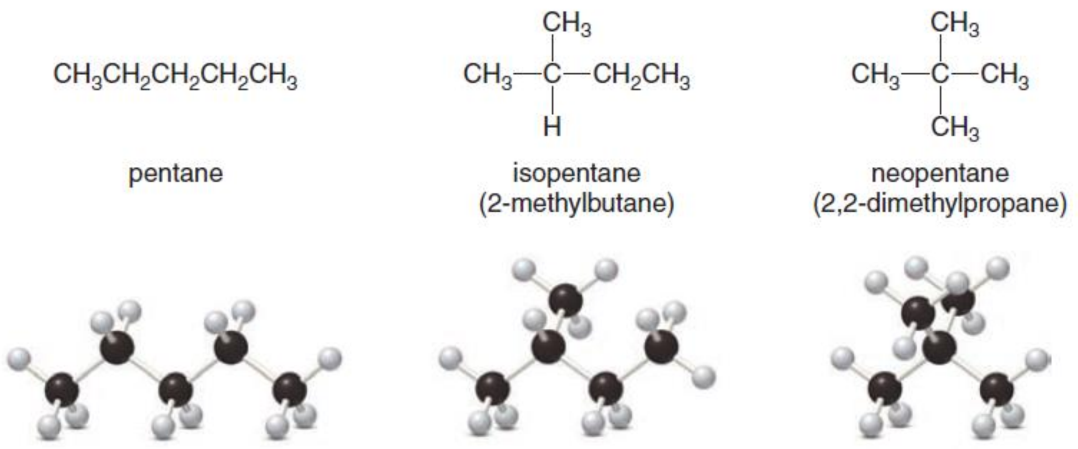
- **<u>Constitutional isomers</u>** differ in the way the atoms are connected to each other.

Problem: Are the compounds in each pair constitutional isomers or are they not isomers of each other?



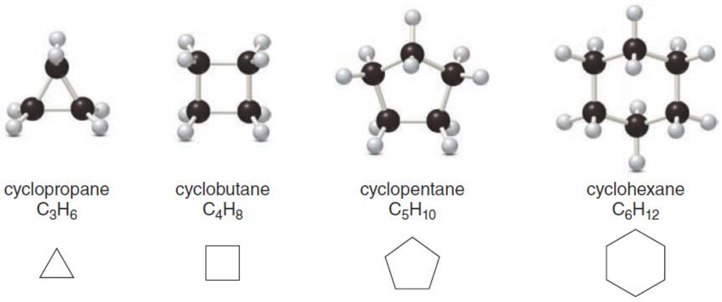
b. Acyclic Alkanes Having Five or More Carbons

As the number of carbon atoms in an alkane increases, so does the number of isomers. There are three constitutional isomers for the five-carbon alkane, each having molecular formula C_5H_{12}: pentane, isopentane (or 2-methylbutane), and neopentane (or 2,2-dimethylpropane).

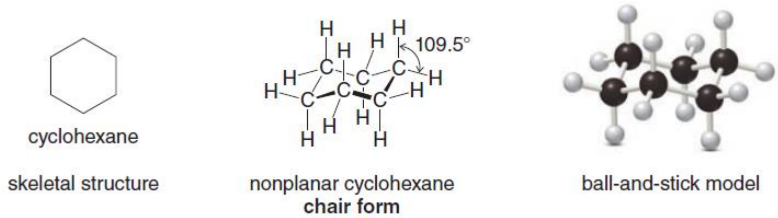


3. Cycloalkanes

- **Cycloalkanes** contain carbon atoms arranged in a ring. Think of a cycloalkane as being formed by removing two H's from the end carbons of a chain, and then bonding the two carbons together.
- Simple cycloalkanes are named by adding the prefix cyclo- to the name of the acyclic alkane having the same number of carbons. Cycloalkanes having three to six carbon atoms are shown in the accompanying figure.
- Each corner of the polygon has a carbon atom with two hydrogen atoms to give it four bonds.

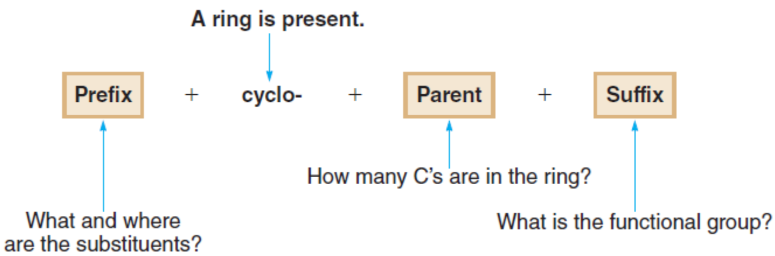


➢ Although we draw cycloalkanes as flat polygons, in reality cycloalkanes with more than three carbons are not planar molecules. Cyclohexane, for example, adopts a puckered arrangement called the chair form, in which all bond angles are 109.5°.



a. Naming Cycloalkanes

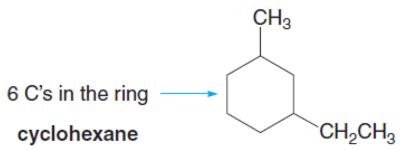
Cycloalkanes are named using the rules in Section 10.6, but the prefix cyclo- immediately precedes the name of the parent.



b. Name a Cycloalkane Using the IUPAC System

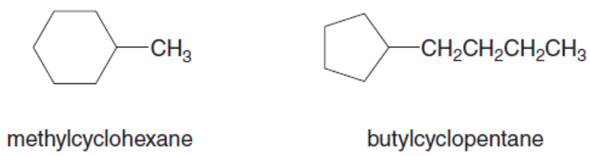
Step [1] Find the parent cycloalkane.

Count the number of carbon atoms in the ring and use the parent name for that number of carbons. Add the prefix cyclo- and the suffix -ane to the parent name.

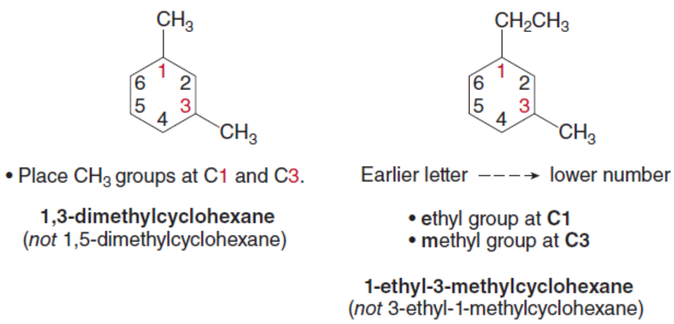


Step [2] Name and number the substituents.

• No number is needed to indicate the location of a single substituent.



• For rings with more than one substituent, begin numbering at one substituent, and then give the second substituent the lower number. With two different substituents, number the ring to assign the lower number to the substituents alphabetically.

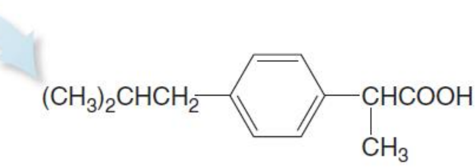


FOCUS ON HEALTH & MEDICINE
Naming New Drugs

- Naming organic compounds has become big business for drug companies. The IUPAC name of an organic compound can be long and complex. As a result, most drugs have three names:
- **Systematic:** The systematic name follows the accepted rules of nomenclature; this is the IUPAC name.
- **Generic:** The generic name is the official, internationally approved name for the drug.

- **Trade:** The trade name for a drug is assigned by the company that manufactures it. Trade names are often "**catchy**" and easy to remember. Companies hope that the public will continue to purchase a drug with an easily recalled trade name long after a cheaper generic version becomes available.

- Consider the world of over-the-counter anti-inflammatory agents. The compound a chemist calls 2-[4-(2-methylpropyl)phenyl]propanoic acid has the generic name ibuprofen. It is marketed under a variety of trade names, including Motrin and Advil.



Systematic name:	2-[4-(2-methylpropyl)phenyl]propanoic acid
Generic name:	ibuprofen
Trade name:	Motrin or Advil

4. *Combustion of Alkanes*

- **Alkanes** are the only family of organic molecules that has <u>no functional group</u>.

- so alkanes undergo few reactions. In this chapter, we consider only one reaction of alkanes—**combustion**—

- Alkanes burn in the presence of oxygen to form **carbon dioxide** (CO_2) and **water**. This is a practical example of oxidation. Every C-H and C-C bond in the starting material is converted to a C-O bond in the product.

$$2(CH_3)_3CCH_2CH(CH_3)_2 + 25O_2 \xrightarrow{\text{Flame}} 16CO_2 + 18H_2O + \text{energy}$$

Isooctane

- ✓ Note that the products, **CO_2 + H_2O,** are the same regardless of the identity of the starting material.

- ✓ **Combustion of alkanes** in the form of natural gas, gasoline, or heating oil releases energy for heating homes, powering vehicles, and cooking food.

When there is not enough oxygen available to completely burn a hydrocarbon, **incomplete combustion** may occur and **carbon monoxide** (CO) is formed instead of carbon dioxide (CO_2).

Incomplete combustion

$$\underset{\text{methane}}{2\,CH_4} + 3\,O_2 \xrightarrow{\text{flame}} \underset{\text{carbon monoxide}}{2\,CO} + 4\,H_2O + \text{energy}$$

Carbon monoxide is a poisonous gas that binds to hemoglobin in the blood, thus reducing the amount of oxygen that can be transported through the bloodstream to cells. CO can be formed whenever hydrocarbons burn. When an automobile engine burns gasoline, unwanted carbon monoxide can be produced.

Problem

a) What products are formed when the ethane (CH_3CH_3) in natural gas undergoes combustion in the presence of a flame?
b) Write a balanced equation for the incomplete combustion of ethane (CH_3CH_3) to form carbon monoxide as one product.