Chem 101: General Chemistry
Lecture 10 - Organic Compounds: Alkanes

I. Carbon: The element of organic molecules

A. Organic compounds are compounds that contain the element carbon
   1. There are a few exceptions
      a. CO_2
      b. CO
      c. CN^-
      d. CO_3^{2-}
   2. These molecules are grouped with the inorganic, which are all moleucles that do not contain carbon.

B. It was early recognized that organic molecules are derived from living systems.

C. Most of the matter that we come in contact with in our environment is composed of organic compounds.

Exercise:	Look around the room you are now sitting in and identify three items made of organic compounds and three items made of inorganic compounds.

II. Organic and inorganic compounds compared

A. Organic compounds
   1. There are many more known organic compounds than inorganic molecules
      a. Over 6,000,000 organic compounds *versus* 250,000 inorganic molecules.
      b. Carbon is able to make so many molecules because it is able to make stable covalent bonds with itself and with other elements.
         i. Carbon is able to form long chains of covalently bonded carbons.

Demo:	Show this with the modeling kit.

1. These can contain up to a million carbon atoms in a single molecule.
2. This is the primary reason there are so many organic compounds.

B. In organic compounds
   1. Usually held together by ionic bonds instead of covalent bonds.
   2. This causes them to have different physical properties than organic molecules

Figure:	Table 11.1: Properties of typical organic and inorganic compounds

Exercise 11.5 (p354)

11.5 Classify each of the following compounds as organic or inorganic:

a. KBr

b. H_2O

c. H-C≡C-H

d. Li

e. CH_3-NH_3

Exercise 11.9 (p354)

11.9 Devise a test, based on the general properties in Table 11.1, that you could use to quickly distinguish between the substances in each of the following pairs:

a. Gasoline (liquid, organic) and water (liquid, inorganic)

b. Naphthalene (solid, organic) and sodium chloride (solid, inorganic)

c. Methane (gaseous, organic) and hyrogen chloride (gaseous, inorganic)

III. Bonding characteristics and isomerism

A. Hybrid valence orbitals

1. Carbon has four *valence electrons*
    - a. It needs to gain four electrons to reach the stable octet (8) configuration.
        - i. (Look back at Chapter 3 if you have forgotten this.)
    - b. This is why carbon typically forms four covalent bonds with other atoms.
    - c. The electron configuration for carbon is $1s^2$, $2s^2$, $2p^2$ or [He] $2s^2$, $2p^2$.
        - i. The valence shell electrons are therefore the electrons in the *2s* and *2p* orbitals.
            1. Two electrons in the *2s* orbital plus one electron each in two of the three *2p* orbitals.
            2. As such, carbon has only two half-filled orbitals that are available to form covalent bonds.
2. To explain the bonding characteristics of carbon, Linus Pauling proposed that the *2s* and *2p* orbitals mix to produce four equivalent **hybrid orbitals**.
    - a. These four hybrid orbitals are called sp^3 to indicate that they are made by mixing one *s* orbital with three parts *p* orbitals.
    - **b.** Each contain a single unpaired electron, therefore, there are now four half-filled orbitals that are available to form a covalent bonds.

Figure 11.3 Mixing *2s* and *2p* orbitals to form $2sp^3$ orbitals.

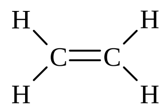
3. In methane (CH_4), each of the carbons four sp^3 orbitals overlaps with a hydrogen's half-filled *1s* orbital to produce a σ (sigma) covalent bond, which contains 2 shared electrons.
4. The four sp^3 orbitals point away from each other to form a tetrahedron.

a. This is the geometry that positions the shared electrons as far apart from one another as possible.

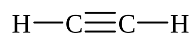
Figure 11.5 Directional characteristics of *sp*^{3} orbitals

Figure 11.9 Structural representations of methane, CH_4.

5. Carbon can also form single covalent bonds with up to 4 other carbon atoms.
   a. This allows carbon to form long chain molecules, which can be branched.
6. Carbon can also share more than one pair of electrons to form double and triple bonds.



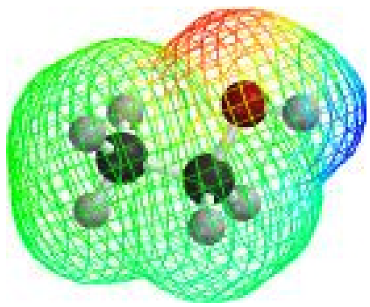
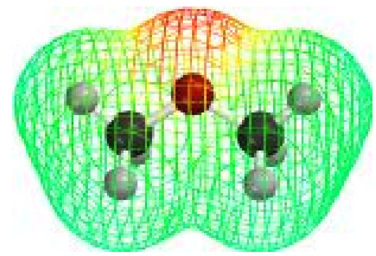
double bond



triple bond

7. The large variety in the arrangement of carbons in organic molecules is what leads to an incredibly large number of possible molecules.
   a. The different arrangements produce different molecules with distinguishing physical and chemical properties.
8. When different molecules share the same **chemical formula**, they are called **isomers** of one another.
   a. If the difference is due to the arrangement of the atoms the isomers are called **structural isomers**.
   b. There are 366,319 different structural isomers for the chemical formula $C_{20}H_{42}$.

Figure: Models of ethanol and dimethylether. Both these molecules have the same chemical formula (C_2H_6O), but a different arrangement of the atoms (CH_3CH_2OH *versus* CH_3-O-CH_3). They also have different physical properties: ethanol is a liquid at room temperature, while dimethylether is a gas

	
Ethanol (CH_3CH_2OH) **Liquid at room temperature**	**Dimethylether (CH_3-O-CH_3)** **Gas at room temperature**

B. Typical number of bonds for Oxygen, Nitrogen, Halogens

1. The number of bonds that the non-metals like to form can be determined by applying the **octet rule**: determine the number of electrons that each needs to fill their valence shell.
   a. *Carbon* is a group IV element and has 4 valence electrons, it therefore likes to form 4 bonds in order to obtain 8 electrons in its valence shell.
   b. *Nitrogen* is a group V element and has 5 valence electrons, it therefore likes to form 3 bonds in order to obtain 8 electrons in its valence shell.
   c. *Oxygen* is a group VI element and has 6 valence electrons, it therefore likes to form 2 bonds in order to obtain 8 electrons in its valence shell.
   d. The halogens, *fluorine*, *chlorine*, *bromine* and *iodine*, are group VII elements and have 6 valence electrons, they therefore like to form 1 bond in order to obtain 8 electrons in their valence shell.
   e. *Hydrogen* represents an exception to the octet rule. It only need 2 electrons to fill its valence shell. It has 1 electron in its valence shell, it therefore likes to form 1 bond in order to fill its valence shell.

Element	Symbol	Group	Number of bonds formed
Carbon	**C**	IV	4
Nitrogen	**N**	V	3
Oxygen	**O**	VI	2
Halogens	**F**, **Cl**, **Br** & **I**	VII	1
Hydrogen	**H**	I or VII	1

Exercise 11.15 (p354)

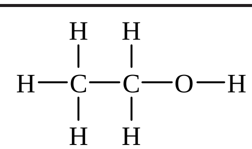
11.15 Use Example 11.1 and Tables 11.6 and 11.2 to determine the number of covalent bonds formed by atoms of the following elements: carbon, hydrogen, oxygen, nitrogen, and bromine.

IV. Functional groups: The organization of organic chemistry

A. The study of organic chemistry is usually organized according to functional group.
   1. A functional group is a group of covalent bonded atoms that often contain elements other than carbon and hydrogen, which have distinctive chemical and physical properties.
   2. They are called *functional groups* because their presence in an organic molecule greatly influences the chemical and physical properties displayed by that molecule.

Table 11.2 (p330) Classes and functional groups of organic compounds

B. Expanded and condensed structural formulas
   1. Unlike **chemical formulas**, which give only the identity and numbers of each element in the molecule of a compound, **structural formulas** give the bonding arrangement with in the molecule.
   2. **Expanded structural formulas** explicitly shows all of the bonds with the molecule



ethanol
expanded structural formula

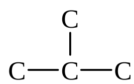
   3. **Condensed structural formulas** show only some of the bonds
      a. The other bonds are implied, for example, the hydrogens that are attached to carbon atoms are just indicated by writing the chemical symbol for hydrogen next to the carbon and using a subscript to indicate the number of hydrogens.
         i. It is understood that each hydrogen is attached to the carbon by a single bond.

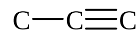
$CH_3{-}CH_2{-}OH$

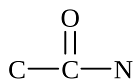
ethanol
condensed structural formula

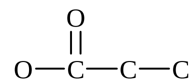
Exercise 11.17 (p355)

11.17 Complete the following structures by adding hydrogen atoms where needed

a. 

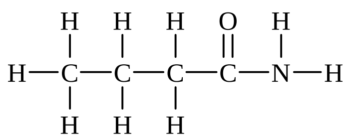
b. 

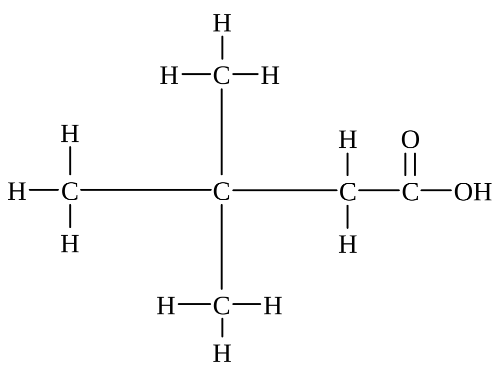
c. 

d. 

Exercise 11.23 (p356)

11.23 Write a condensed structural formula for the following compouds:

a. 

b. 

V. Alkane structures

A. **Hydrocarbons** are the simplest of organic compounds
   1. Hydrocarbons contain only the elements hydrogen and carbon
   2. If only they contain only single bonds between carbons they are called **saturated hydrocarbons** or **alkanes**.
   3. If they contain any double or triple bonds they are called **unsaturated hydrocarbons.**
      a. The unsaturated hydrocarbons include the **alkenes**, **alynes**, and **aromatics**.

Figure 11.7 Classification of hydrocarbons

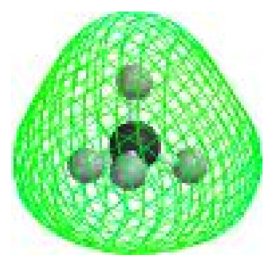
B. Most biochemical reactions involve the functional groups.
   1. Since alkanes have no functional groups they are rarely found in living systems.

C. Hydrocarbons, however, form the core of most organic molecules
   1. The functional groups hang off of this core.

2. For this reason we need to understand a little bit about the structure. chemical and physical properties of hydrocarbons.

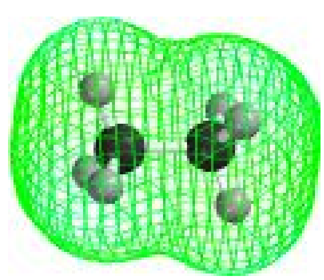
D. The chemical formulas for alkanes has the form $C_nH_{2n\_2}$, where *n* is the number of carbon atoms.

E. Methane
1. Has only one carbon.
2. Methane is the primary component of natural gas
3. The carbon is sp^3 hybridized and has a tetrahedral geometry.
   a. The bond angles between the C-H bonds is 109.5°



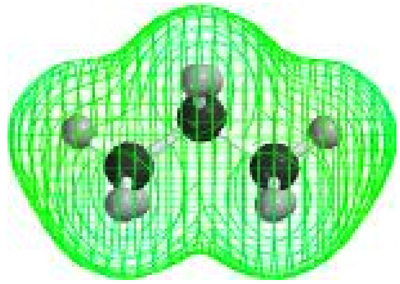
Methane (CH_4)

F. Ethane
1. Has two carbon atoms
   a. Each carbon atom is sp^3 hybridized and has tetrahedral geometry



Ethane (C_2H_6)

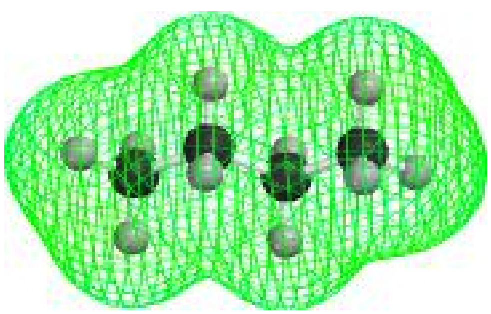
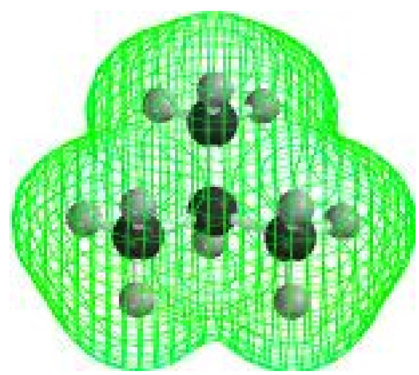
G. Propane
1. Has three carbon atoms
   a. Each carbon atom is sp^3 hybridized and has tetrahedral geometry



Propane (C_3H_8)

H. Butane

1. Has four carbon atoms
    a. Each carbon atom is sp^3 hybridized and has tetrahedral geometry
2. There a two possible arrangement of the carbon atoms in butane.
    a. This results in a pair of structural isomers
        i. The straight chain isomer is called *normal*-butane or *n*-butane.
        ii. The branched chain isomer has the common name isobutane.

	
***n*-Butane (C_4H_{10})**	**Isobutane (C_4H_{10})**

These models represent two different molecules, which are isomers of one another

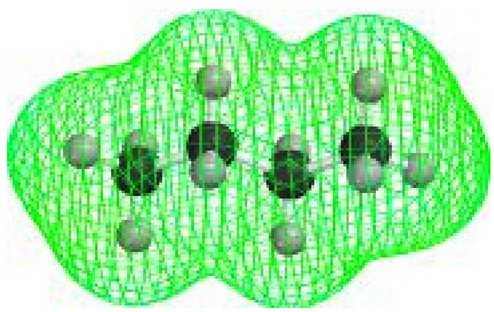
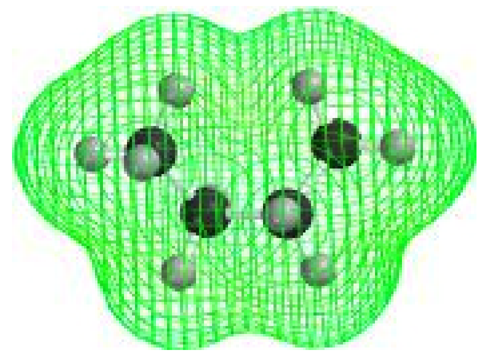
VI. Conformations of alkanes

A. In alkanes, the atoms are constantly rotating about the carbon-carbon single bonds.

1. The different arrangements that result from these rotations are called **conformations**.

2. At room temperature, any alkane with 4 or more carbon atoms can have many different conformations.

3. The different conformations are not considered isomers of each other, but different conformations of the same molecule.
   a. To switch a model from one isomer to another requires the breaking and making of covalent bonds.
   b. Switching from one conformation o another requires only rotations about carbon-carbon single bonds.

	
***n*-Butane (C_4H_{10})**	***n*-Butane (C_4H_{10})**

These models represent different conformations of the same molelcule

VII. Alkane nomenclature

A. Early on common names were given to organic compounds.
   1. However, as more and more compounds were discovered it became increasingly difficult to uniquely name them all.

B. A group called the International Union of Pure and Applied Chemistry devised a more systematic method of naming organic molecules.
   1. This naming system is referred to as the "IUPAC system" of naming.

C. IUPAC names
   1. Each name has three component parts

Prefix–Root–Ending

   a. The **root** part of the name gives the number of carbons in the longest continuous chain of carbons in the molecule.

i. The roots for from 1 to 10 are,

Root	**Number of Carbons**
Meth-	1
Eth-	2
Prop-	3
But-	4
Pent-	5
Hex-	6
Hept-	7
Oct-	8
Non-	9
Dec-	10

b. The **ending** part of the name gives the functional class of the primary functional group in the molecule
   i. The functional classes are given in Table 11.2
   ii. The ending used for alkanes, which do not have a functional group, is *-ane*.
c. The **prefix** part of the name gives the identity, number, and location of atoms or groups of atoms that are attached to the longest carbon chain.
   i. If there are no additional groups. then no prefix is needed.
   ii. The names used to describe saturated hydrocarbon groups are derived from the corresponding name of the corresponding alkane.
      1. The *-ane* ending is changed to *-yl*.
      2. These groups are called **alkyl** groups
         a. **Table 11.5** lists the common alkyl groups

Table 11.5 - Common alkyl groups

   iii. The prefixes used for the halogens and other common groups is given in **Table 11.6**.

Table 11.6 - Common nonalkyl groups

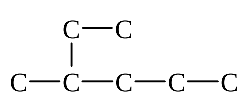
   iv. Numbers are used to indicate the location alone root chain where the group is attached

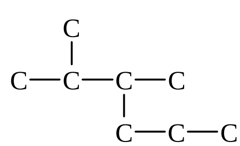
v. If more than one of the same kind of group is present, Greek prefixes are used to indicate their numbers:

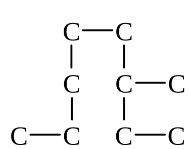
Number	Greek prefix
2	*Di-*
3	*Tri-*
4	*Tetra-*
5	*Penta-*
6	*Hexa-*
7	*Hepta-*
8	*Octa-*
9	*Nona-*
10	*Deca-*

Exercises 11.29, 11.33 & 11.35

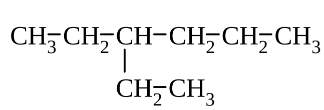
11.29 For each of the following carbon skeletons, give the number ocarbon atoms in the longest continuous chain.

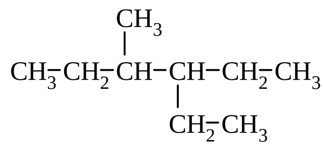
a. 

b. 

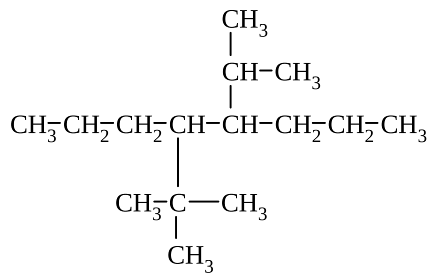
c. 

11.33 For each of the following carbon skeletons, give the number ocarbon atoms in the longest continuous chain.

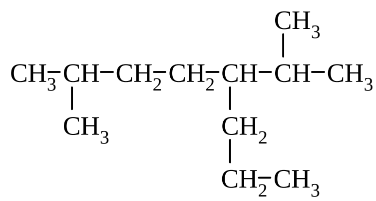
a. 



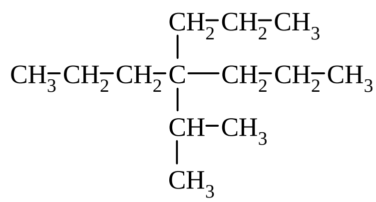
b.



c.



d.



e.

11.35 Draw a condensed structural formula for each of the following compounds:

a. 2,2,4-trimethylpentane

b. 4-isopropyloctane

c. 3,3-diethylhexane

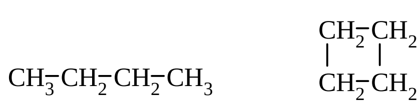
d. 5-t-butyl-2-methylnonane

VIII. Cycloalkanes

A. Alkanes with 3 or more carbon atoms can form rings.
   1. These are called **cycloalkanes**.

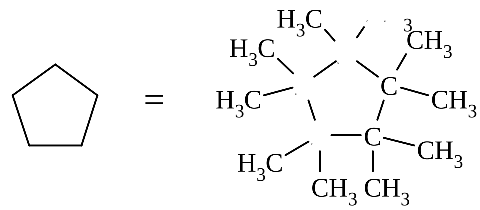
B. The chemical formula for cycloalkanes is C_nH_{2n}, where *n* is the number of carbon atoms.

C. The IUPAC name for cycloalkanes places the prefix *cyclo-* in front of the corresponding alkane name.
   1. Fore example



n-butane *cyclobutane*

D. When drawing the condensed structures of cycloalkanes, the carbon and hydrogen symbols are often omitted.
   1. It is understood that the vertices of the geometric figure give the location of the carbon atoms, and that if a carbon does not have four bonds shown to it, the remain bonds are carbon/hydrogen bonds.



E. When a single group is attached to cycloalkane, its number is assumed to be 1.

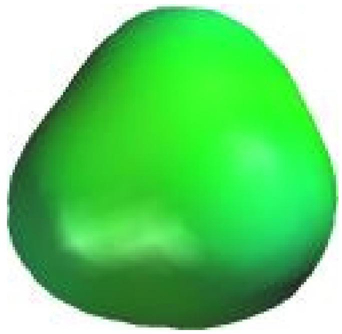
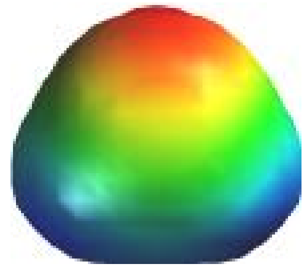
F. When more than one group is attached to a cycloalkane, the ring numbering starts from one of the groups, usually the one coming first in the alphabet.

IX. The shape of cycloalkanes

A. Even though the carbons in a cycloalkane are *sp*^{3} hybridized, there bond angles often deviate from the ideal 109.5° for a tetrahedron.
   1. Only for the 6-membered rings is the ideal angle observed.
   2. The smaller rings with 5, 4 and 3 carbons are progressively less stable because of greater strain from the ideal bond angle.

X. Physical properties of alkanes

A. Hydrocarbons, including alkanes, are non polar
   1. Below are models that compare the electrostatic charge on the surface of methane compared to water
      a. Blue signifies regions of positive charge, red signifies regions of negative charge and green signifies no charge.
      b. The methane molecule is green everywhere, indicating that it is a **nonpolar molecule**
      c. The water molecule is blue at one end and red at the other.
         i. Its net charge is 0, but the charge is not evenly distributed on the molecule; this makes it a **polar molecule**

	
Methane (CH_4)	**Water (H_2O)**

2. In Chem101 you learned that non polar molecules can only interact with one another using weak **dispersion forces.**
    a. Refer to Chapter 4, Section 4.11 (pp120-124) for a discussion of interparticle forces.
    b. This interaction is attractive, but weak
        i. This is why nonpolar molecules, such as hydrocarbons, have low melting and boiling points.

Table 11.8 Physical properties of some normal alkanes

Figure 11.19 Normal alkane boiling points depend on chain length

B. Homologous series
  1. The melting and boiling points of normal alkanes increases with the size (length) of the molecule.
      a. This is because the surface area of the molecules increases, which allows them to interact more extensively

XI. Alkane reactions

A. Alkanes are the least reactive of any organic molecules
  1. This is because they have no functional groups.

B. The most important reaction that they undergo is combustion, *i.e.* reacting with molecular oxygen

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \ \ (212.8 \text{ kcal/mol})$$

  1. If there is insufficient oxygen there can be incomplete combustion, which produces the deadly gas carbon monoxide (CO) or elemental carbon (soot)

$$2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O$$

$$CH_4 + O_2 \rightarrow C + 2H_2O$$