Chem 191: Biochemistry
Lecture 1 – Organic Molecules: Alkanes

I. Introduction

- A. "Organic" has several different meanings.
  - 1. Chemists originally used it to mean molecules that could be extracted from living systems.
  - 2. It is now used to mean the chemistry of carbon containing compounds.

II. Carbon

- A. Nearly all carbon containing molecules are derived from living systems and are classified as organic molecules.
  - 1. There are some exceptions.
    - a. CO, CO_2, CO_3^{-2} and $CN^{=}$ are considered inorganic.
- B. Organic molecules are important because
  - 1. Living systems are made primarily of water and organic molecules.
  - 2. There are more organic molecules than molecules that are not.
    - a. Reflecting this importance, al molecules are classified as either *organic* or *inorganic*.
      - i. 250,000 inorganic molecules.
      - ii. 6,000,000 organic molecules.
- C. Carbon has the unique ability of form stable covalent bonds with other carbon atoms and with atoms of many other elements.
  - 1. This is what allows for the large and diverse number of organic molecules.
  - 2. A single organic molecule can contain a few or even over a million covalently bonded carbon atoms.

III. Bonding characteristics and isomerism

- A. Carbon has four valence electrons
  - 1. It needs to gain four electrons to reach an octet.
  - 2. This is why carbon is typically found to participate in four covalent bonds.
  - 3. The electronic configuration of carbon is $1s^2$, $2s^2$,$2p^2$ or [He] $2s^2$,$2p^2$.
    - a. The valence shell electrons are therefore the electrons in the 2s and 2p atomic orbitals.

  - 4. To explain the bonding characteristics of carbon, Linus Pauling proposed that the 2*s* and 2*p* orbitals can mix to produce equivalent hybrid orbitals.
    - a. If the 2*s* and all three of the 2*p* orbitals can combine to form four equivalent orbitals.
      - i. These are called sp^3 orbitals

            ii. Each will contain a single unpaired electron and can combine with an electron from another element to forma covalent bond.
        b. We will see later that the 2*s* orbital can also combine with fewer than all three of the 2*p* orbitals to form *sp*^{2} and *sp* hybrid orbitals.
            i. These are used to form double and triple bonds.
    5.

IV. Functional Groups

A. Functional groups are groups of atoms that are attached to carbon atoms in organic molecules
    1. They usually contain other nonmetalic elements such as oxygen, nitrogen,sulfur, phosphorous and the halides (F, Cl, Br and I).
    2. They are called functional groups because they strongly influence the chemical and physical properties of organic molecules.
    3. For this reason, organic molecules are classified according the functional groups they contain.

Table 11.2 – Classes and Functional Groups of Organic Compounds

V. Alkane Structure

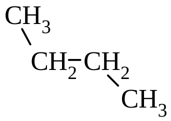
A. Hydrocarbons are the simplest organic molecules
B. Alkanes are *saturated hydrocarbons*, which contain only single bonds between carbon atoms.
    1. If a hydrogen carbon contains at least one double or triple carbon-carbon bond, it is said to be unsaturated.
        a. Unsaturated hydrocarbons include the alkenes, alkynes and aromatic hydrocarbons.

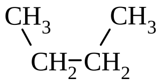
Figure 11.7 – Classification of Hydrocarbons

C. Methane
D. Ethane
E. Propane
F. Butane
    1. Structural isomers are possible
G. Alkanes containing *n* Carbon atoms, will contain 2*n* + 2 hydrogen atoms.

VI. Conformations of Alkanes

A. Conformation *versus* isomer (configuration)
    1. Single bonds can rotate freely
        a. This leads to different conformations for some organic molecules
    2. Do not be fooled by how a structure is drawn on paper
        a. Some may look different but are actually different conformations of the same molecule.
        b. For example:



and


are identical molecules

VII. Alkane Nomenclature

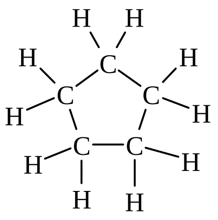
A. Prefix + Root + ending
  1. Ending tells what family a particular compound is a member of.
    a. These are based on what functional group the molecule contains
    b. Alkanes are the family that contain no functional groups.
    c. The ending used for alkanes is *–ane*.
  2. The root part of the name tells how many carbons the molecule contains.
  3. For alkanes with four or more carbons, the prefix is used to describe the branching pattern
    a. Straight chain or normal, *n-*
    b. Branched at the second to last carbon in a chain, *iso-*
  4. For larger more complicate molecules a more systematic method is needed.
    a. The root part of the name tells how many carbons are in the longest continuous unbranched chain of carbons within the molecule.
    b. A prefix is used to denote the identity, number and location of groups attached to the longest chain
      i. Names of alkyl groups:

Table 11.5 – Common alkyl groups

Table 11.6 – Common non-alkyl groups

VIII. Cycloalkanes

A. The chain of carbon atoms in an alkane can form a ring containing 3 or more carbon atoms.
  1. These structures are called *cycloalkanes*.
  2. Often when these structures are drawn, only the bonds are shown.
    a. It is understood that the carbons are located at the angles where the bonds connect and that hydrogens are added until each carbon has four bonds to it: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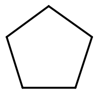

are equivalent

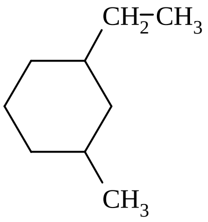
  3. When naming these compounds the prefix *cyclo-* is used.

a. For example, a cycloalkane containing three carbon atoms is called cyclopropane.

b. When groups are attached to the ring, the number of the carbon atoms in the ring begins with the carbon to which the group that comes first in the alphabet is attached,

i. Numbering then proceeds around the ring in the direction that produces the smallest numbers for the other groups

ii. For example:



is named *1-ethyl-3-methylcyclohexane.*

IX. The Shape of Cyclo alkanes

A. The closed ring gives rise to the possibility for additional structural isomers.

1. This is because the closed ring prevent free-rotation about the single bonds in the ring.

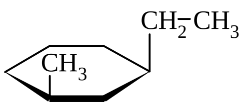
2. When two groups are are attached to the ring in different locations, they can either be on the same side of the ring or on opposite sides of the ring.

a. This produces two different molecules.

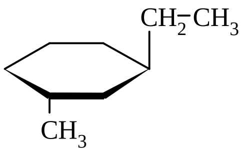
b. When the groups are on the same side of the ring the molecule is called the *cis* isomer.

c. When the groups are on the opposite sides of the ring the molecule is called the *trans* isomer.

d. Using the example shown above, there are two possible structure isomers of *1-ethyl-3-methylcyclohexane:*



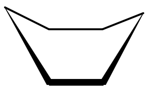
cis-1-ethyl-3-methylcyclohexane



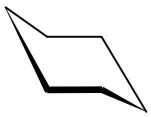
trans-1-ethyl-3-methylcyclohexane

B. Not all the carbon atoms in a cycloalkane are in the same plane.

1. In particular, cyclohexane has two conformations.



boat conformation



chair conformation

        a. These are not isomers of one another because the molecule can switch from one conformation to the other without breaking and making and bonds.
            i. Cyclohexane can switch back and forth freely from one conformation to the other.

X. Physical Properties of Alkanes

A. In Chapter 4 of your textbook the various forces that exist between atoms and molecules were discussed.
    1. The forces that hold the molecules close to one another in the liquid and sold states are weak forces that do not involve the sharing of electrons.
        a. For this reason they are called *noncovalent interactions*.
        b. When a molecule contains charged atoms these molecules can be attracted or repelled by other molecules containing charged atoms.
            i. These are called *charge/charge* interactions.
        c. When a molecule contains polar bonds, these molecules can be attracted or repelled by other molecules containing polar bonds.
            i. These are called *dipole/dipole* interactions.
        d. A molelcule containing polar bonds can also be attracted or repelled by other molecules containing charges.
            i. These are called *charge/dipole* interactions.
        e. Another important non-covalent interaction is the *hydrogen bond*.
            i. In a hydrogen bond, a hydrogen which is covalently bonded to an electronegative atom, such as oxygen or nitrogen, is attracted to another electronegative atom
            ii. Hydrogen bonding is very important for explaining the many unique properties displayed by water.
            iii. It is also very important in determining the structures of biological molecules, such as proteins and nucleic acids.

$$\text{–O–H}\cdots\text{O–}$$

            iv. Hydrogen bonds are always attractive.
        f. The weakest of the non-covalent interactions is the *London dispersion force* or *vander Waals interaction*.
            i. It is results from momentary nonsymmetric electron distributions in molelcules.
            ii. This interaction is always attractive and exists between all molecules.
    2. Hydrocarbons in general, and alkanes in particular, contain no charged atoms nor polar bonds.
        a. For this reason they cannot interact with each other through charge/charge, dipole/dipole, charge/dipole, or hydrogen bonding interactions.
        b. The only interaction left to them is the London dispersion or vander Waals interaction.

c. The strength of the this interaction increases with the size of the surface area of the molecules, therefore the interaction is stronger between larger molecules than between smaller molecules.

d. This explains the observed trends in the boiling points and melting points of alkanes.

Figure 11.9 – Boiling points of Normal Alkanes

3. Because alkanes are not polar are charges, they do not interact very favorably with water.

a. For this reason they do not mix with water: they are *immiscible*.

b. Another way to describe this is to say that they are *hydrophobic* “water-fearing” molecules.

XI. Alkane Reactions

A. We often think of akanes as being very reactive because they are very flammable.

1. When something is flammable it means it reacts readily with oxygen.

a. When alkanes react with water they produce carbon dioxide and water:

$$CH_4 + 2\,O_2 \longrightarrow CO_2 + H_2O$$

b. This reaction is called a *combustion* reaction releases a lot of energy in the form of light and heat.

2. Besides the combustion reaction, akanes are fairly unreactive.