

Chemical Structures

Objectives

1. To practice with the different atoms used in Bio 111: to know the number of bonds made by each kind of atom, the structures that they form, and the charges they have.
2. To build molecular models of various bio-molecules.
3. To understand and be able to work with the different representations of molecules used in Bio 111.

Introduction

Matter is made up of approximately 100 elements. Of these, only carbon, hydrogen, oxygen, nitrogen, sulfur and about a dozen others are found in living organisms. Atoms of these elements can attach to one another by chemical bonds. There are five types of bonds important to us in Bio 111:

1. covalent bonds
2. hydrogen bonds
3. ionic bonds
4. Hydrophobic interaction
5. van der Waals interaction

Today, we will focus on **covalent bonds**, which are the result of a sharing of electrons between two or more atoms. In this case the electrons of the atoms forming the bond occupy the space between each others' nuclei. Molecules can be made up of atoms of different elements, such as the gas methane (CH₄), in which one atom of carbon shares electrons with four atoms of hydrogen, or the molecule can be made up of atoms of the same element (O₂). Carbon atoms are unusual in that they will bond together to form long chains of carbons (-C-C-C-C-) thus making possible very elaborate molecules with carbon "backbones".

Part 0: Notebook Review

To be sure that you have all the information you need for this lab, with your lab partners, go over the notes you took while doing the SPOC and from lecture and be sure you have the information listed below. You should fill in any gaps in your notes so everyone in your group has all they need. You can check these items off as you go.

- How many covalent bonds does each of the following atoms make (HONCSP)?
- Which atoms are charged and under which circumstances?
- Which atoms have lone pairs, how many, and under which circumstances?
- How can I build a molecule that fits a particular formula?
- What are isomers and how can I tell if two molecules are isomers or identical?

You will then discuss these with your TA as a class to clarify any issues that remain.

Part I: Structures on paper and in 3-d

Using the model kits

The molecular model kits have five different types of atoms. Carbon (black), Oxygen (red), Nitrogen (light blue), Chlorine (green), and Hydrogen (white). Each of these represents an atom, composed of its nucleus and the surrounding electrons. These atoms can be connected to each other by inserting the white rods into the holes. It will become apparent to you that different atoms have different capacities for bonding with other atoms. The holes in the plastic "atoms" indicate the number of electrons that the atom is able to share with another atom.

Note that there are two types of blue "nitrogen" atoms. One type has 3 holes - you should use these ones. Others have 2 holes; don't use them since the geometry will be wrong. A reminder of the number of bonds each atom makes and the corresponding charge:

Element	Number of Bonds					
	0	1	2	3	4	5
H	+	neutral				
O		-	neutral			
N				neutral	+	
C					neutral	
S			neutral			
P						neutral

A simple mnemonic is "HONC" - H makes 1 bond, O makes 2, N makes 3, and C makes 4.

Also a reminder of the relative electronegativities of a few relevant elements:

Low: C, S, P, and H

High: N, O, and Cl

These properties can all be explained in terms of the electronic structures of the elements involved. You may want to take time to discuss this as a class. See periodic table at the end of this section for details.

The short rods are used to indicate the covalent bond involving hydrogen, since hydrogen, being the smallest atom, has a smaller distance between it and a carbon atom. Similarly, the curved rods are used to show double and triple bonds and have the effect of bringing the atoms closer together, which reflects the true situation. The nuclei of carbon atoms in a C=C bond are closer together than in an C-C, but not so close as in a C≡C bond.

Working in groups of three, build these molecules using the stick models and have your TA check them off.

1) Simple hydrocarbons

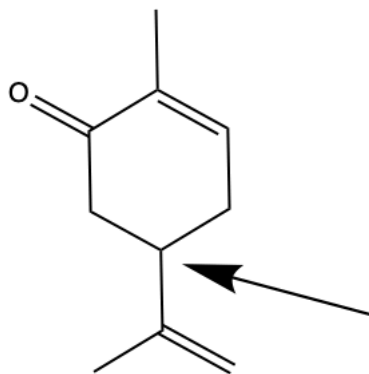
methane CH₄

2) Alcohols

butanol C₄H₉-O-H

Note: there are 5 isomers of butanol. Three are structural isomers. Two are enantiomers - that is, they are mirror-image isomers (Wikipedia has a good entry on isomers and enantiomers). Build models of all five forms.

3) Chirality is a very important feature of biological molecules because their exact 3-dimensional shape determines their function. An interesting example of this are the two forms of the molecule carvone:



Although it looks like there would only be one way to make this molecule, it turns out that there are two very similar but importantly different versions of this molecule – the two versions are mirror-image isomers, or enantiomers.

The carbon atom indicated by the arrow has four things attached to it: two of the bonds go to the ring, one goes to a hydrogen atom, and the last goes to the 3-carbon branch. Because there are two ways to arrange these four items, this carbon is called a “chiral center”.

You can see this if you build a model of the molecule, lay it on the table, and have the oxygen atom at the left (as shown), there are two ways to arrange the hydrogen atom and the 3-carbon branch – these are the two enantiomers:

- If you build it with the **hydrogen atom pointing up** from the table and the 3-carbon branch pointing down into the table, this is “(-) carvone”, which smells like spearmint.
- If you build the mirror-image, with the **hydrogen atom pointing down** into the table and the 3-carbon branch pointing up, this is “(+) carvone”, which smells like caraway seeds (rye bread).

Your TA will give you samples of the two carvones to smell. Notice that their similar structures lead to similar smells, but there is a difference due to the slight difference in shape.

Part II: Molecules on the computer

Objectives

- To look at the structures of some important biological molecules and get a feel for their three-dimensional structure.
- To familiarize yourself with the representations of molecules used by the Jmol program, which we will use extensively in future labs.

Background

Jmol is a molecular viewing application. It lets you rotate, highlight, zoom in on, etc. a two-dimensional image of a three-dimensional molecule. It shows molecules in a simplified format, specifically:

- all covalent bonds are shown as a single rod, whether the bond is single, double, or triple
- atoms are shown as colored spheres; the colors identify each type of atom

Procedure

You will follow the exercise on the course web site for this lab and fill in the worksheet described below. You should work in groups of three; your worksheet will be a group effort for a group grade.

- 1) Go back to the dock at the bottom of the screen.
- 2) Click on the "Safari" icon.
- 3) Safari will start up and go to the Biology 111/112 home page.
- 5) Click on the link to the "OLLM" ("On-Line Lab Manual")
- 6) Click on the link to "Chemical Structures Exercises" for this lab.
- 7) Follow the exercise there and fill in the worksheet on pages 9 and 10 of this section of the lab manual.

Briefly, you will:

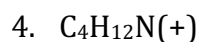
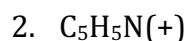
- (1) Based on the image on the computer, draw the structures of two sugars, glucose and fructose as well as an amino acid. These images have hydrogen atoms included as a warm-up. You will be asked to find the differences between the sugar structures and identify the amino acid.

Part III: Possible and Impossible Formulas

Objective: to get more practice with the bonding rules.

Background: While there are many molecules with the formula $C_4H_{10}O$, there are no molecules with the formula CH_5 – since carbon only makes 4 covalent bonds and hydrogen only makes one, there is no molecule that satisfies the rules and has this formula. Learning to figure out which are possible and which are not is a great way to practice with the bonding rules.

Challenges: For each of the following formulae, draw a molecule with that formula or determine that it is not possible. If it is possible, try to come up with as many different molecule with that formula as you can. Try also to write them in complete and abbreviated forms.



6. Make up some of your own.

Preparing for the Take Home Exam

Take Home Exam 1 will be, in part, based on this lab. You should look at the exam on Blackboard before you leave lab today. You may want to use some of the remaining time in lab to prepare for the exam.

Bio 111 Small Molecules Worksheet

Name _____ TA & Sect. _____

Name _____

This is a
group effort
for a group
grade.

Name _____ Score _____/20

This is due at the end of lab today.

The numbers of these questions correspond to the numbers on the web site.

1) Using the image from the web site, draw the structure of the linear form of glucose. You need not indicate the chiral parts of the molecule. (4 pts)

2) Using the image from the web site, draw the structure of the linear form of fructose. You need not indicate the chiral parts of the molecule. (4 pts)

3) On the structure in question (2), indicate the differences between glucose and fructose. (2 pts)

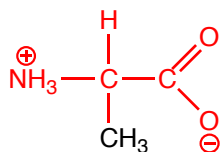
4) Using the image from the web site, draw the structure of the circular form of glucose. You need not indicate the chiral parts of the molecule. (4 pts)

5) On the structure in question (1), make a drawing that shows which parts of the molecule have been linked to form ring structure. (2 pts)

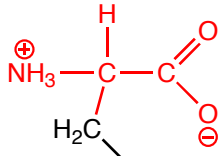
6) Using the image from the web site, draw the structure of the amino acid for part (6). You need not indicate the chiral parts of the molecule. (2 pts)

7) Using the chart of amino acid structures in the lab manual, identify the amino acid you drew in question (6). (2 pts)

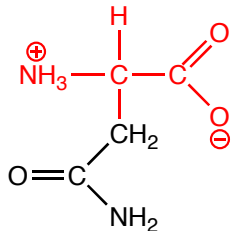
Structures of Amino Acids



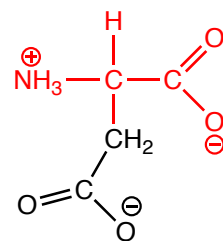
Alanine (Ala)



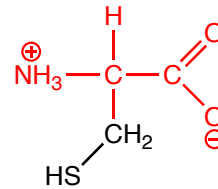
Arginine (Arg)



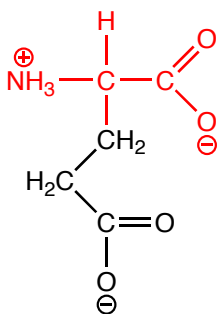
Asparagine (Asn)



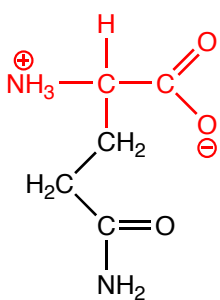
Aspartic Acid (Asp)



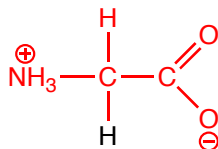
Cysteine (Cys)



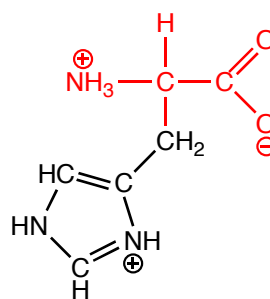
Glutamic Acid (Glu)



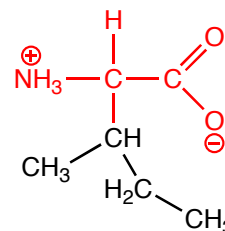
Glutamine (Gln)



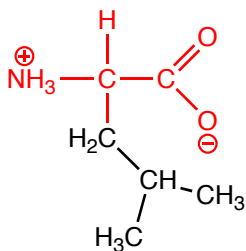
Glycine (Gly)



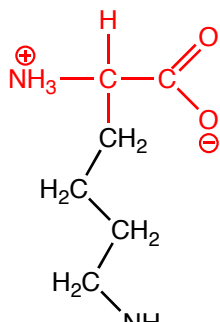
Histidine (His)



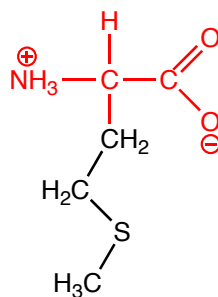
Isoleucine (Ile)



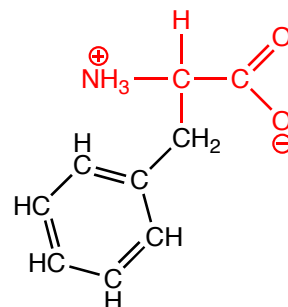
Leucine (Leu)



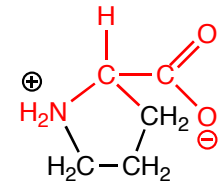
Lysine (Lys)



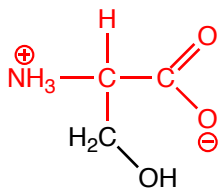
Methionine (Met)



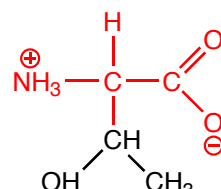
Phenylalanine (Phe)



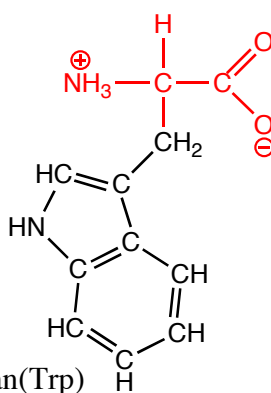
Proline (Pro)



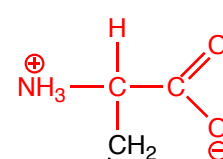
Serine (Ser)



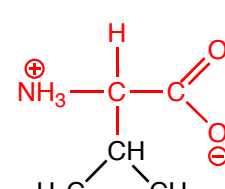
Threonine (Thr)



Tryptophan (Trp)



Tyrosine (Tyr)



Valine (Val)

Partial Periodic Table

H Hydrogen $1p^+ 0n^0$ $1e^-$ 1(1 open) $E_n = 2.1$							He Helium $2p^+ 2n^0$ $2e^-$ 2 (full) $E_n =$ none
Li Lithium $3p^+ 4n^0$ $3e^-$ 2 (full) 1 (7 open) $E_n = 1.0$	Be Beryllium $4p^+ 5n^0$ $4e^-$ 2 (full) 2 (6 open) $E_n = 1.5$	B Boron $5p^+ 6n^0$ $5e^-$ 2 (full) 3 (5 open) $E_n = 2.0$	C Carbon $6p^+ 6n^0$ $6e^-$ 2 (full) 4 (4 open) $E_n = 2.5$	N Nitrogen $7p^+ 7n^0$ $7e^-$ 2 (full) 5 (3 open) $E_n = 3.0$	O Oxygen $8p^+ 8n^0$ $8e^-$ 2 (full) 6 (2 open) $E_n = 3.5$	F Fluorine $9p^+ 10n^0$ $9e^-$ 2 (full) 7 (1 open) $E_n = 4.0$	Ne Neon $10p^+$ $10n^0$ $10e^-$ 2 (full) 8 (full) $E_n =$ none
					P Phosphorus $15p^+ 16n^0$ $15e^-$ 2 (full) 8 (full) 5 (3 open) $E_n = 2.1$	S Sulfur $16p^+$ $16n^0$ $16e^-$ 2 (full) 8 (full) 6 (2 open) $E_n = 2.5$	Elements in this column do not form any covalent bonds (at least, not in Bio 111)

