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eChem - PART I HYDROCARBONS AND ALKANES

In this activity, you will be learning how to use eChem, a piece of
educational software, to build chemical structures. Additionally, you will
learn what "alkanes" are in organic chemistry, and what their molecular
structures look like at the "microscopic" or atomic level.

What is eChem?

eChem is a chemistry software package for you to create three-
dimensional-like models of molecules, simultaneously visualize
multiple representations of the molecules, and compare properties of
the molecules. eChem includes three actions: Construct, Visualize
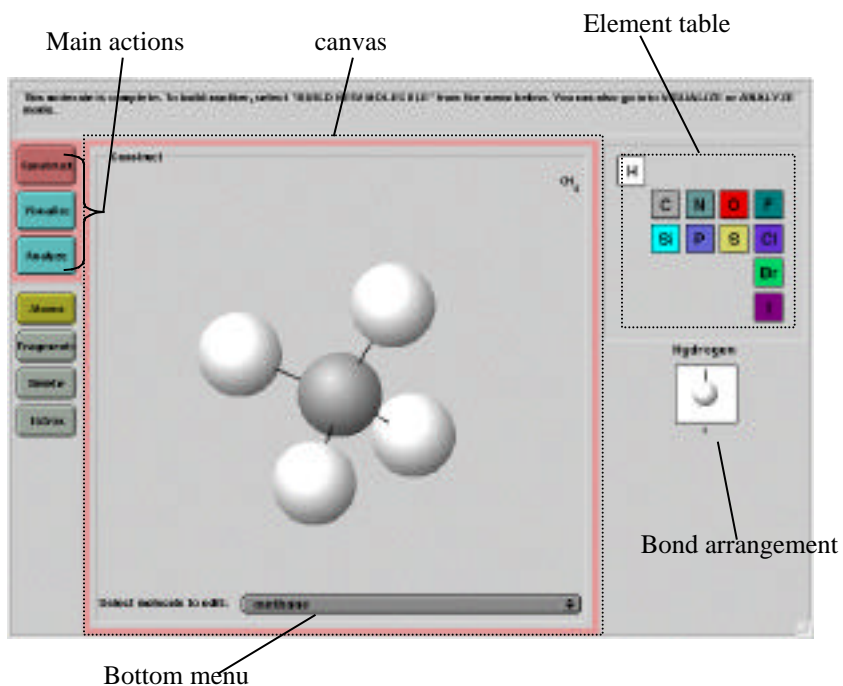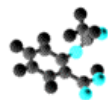and Analyze. Let's see how "construct" works for you.

Main actions   canvas   Element table

Bottom menu

Fig. 1 Construct window

Construct--creating models of covalent-bonded molecules

On the left side of the screen (Fig. 1), you have three button
"Construct", "Visualize" and "Analyze".

•   Click "Construct"

You will work with organic compounds. *Organic chemistry* is the study of
carbon compounds. Carbon is connected to other elements by bonds.
Carbon can have four bonds. (Why?) When organic compounds contain
only carbon and hydrogen, they are called *hydrocarbons*. Hydrogen is an
element that can only have one bond. (Why?) Let's begin with one family
of hydrocarbons: *Alkanes*. Alkanes are hydrocarbons with only single
bonds. This first molecule we will build is "methane." Methane is the
simplest alkane with only one carbon and hydrogens (CH_4.) Natural gas
contains 75 to 85 percent methane. Methane is a colorless, odorless gas[1]
with a boiling point of -160°C.

•   Enter the name of molecule: methane (Why do we call it
    methane? "Meth" means one and "ane" means single bonds)

•   Click "Atoms", and select "C" from the element table on the right
    side of screen.

You can see carbon has different types of bond arrangement. No matter
what kinds of bonds (single, double or triple bonds) a carbon atom has, the
total number of bonds is four. Why does carbon always have four bonds?
Why does carbon have these arrangements? Have you heard about the
"octet rule"? If alkanes are hydrocarbons with single bonds, which bond
arrangement of carbon should you choose?

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[1] But why is natural gas not odorless? Well, natural gas is essentially
odorless, but we add trace amounts of unpleasant-smelling sulfur-containing
compounds such as ethanethiol to warn of any potentially dangerous leak.

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- Select "sp^3 Tetrahedron" as the hybridization of carbon and click on the canvas (the large screen in the middle.)

- You may need to rotate this carbon atom and to see all the bond sites. Just hold down the mouse button, and move the cursor.

- Let's finish methane by attaching hydrogens. Select "H" from the element table and select hybridization. (While carbon has four bonds, why does hydrogen have only one bond?)

- Add hydrogen atoms to the carbon atom by clicking on the carbon bonds.

- How can you save this methane model? Go to menu bar "file" and select "save."   Input the file name as "methane.alc" (remember to add ".alc" after the compound's name or you won't be able to open the file next time)

- Did you attach a wrong atom on carbon (like adding an oxygen atom for methane)? Select "Delete" on the left side of screen, and click the atom ball you want to erase.

1. Why does carbon have several types of bond arrangements and hydrogen have only one? Write down your explanations in the space below. (Hint: How many valence electrons does carbon have? Following the **octet rule**, how many electrons can carbons share to make a stable compound?)
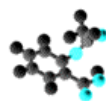
 Let's build other members of the alkane family in eChem.

- Pull down the menu on the bottom of canvas, and select "build a new molecule".

- Methane is the alkane with one carbon, so try to make a compound with two carbons and all the other spots taken up with hydrogens.

- A compound with 2 carbons and 6 hydrogens is called ethane (eth=two.) The rule for naming unbranched alkanes is to put the name of number of carbon first (prop=three, but=four, pent=five, hex=six, hept=seven, oct=eight, non=nine and dec=ten) and then add "ane" on it.

- Save your ethane model as "ethane.alc"

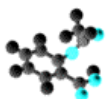**2.** On eChem create and save the following molecules:

(a) Propane:
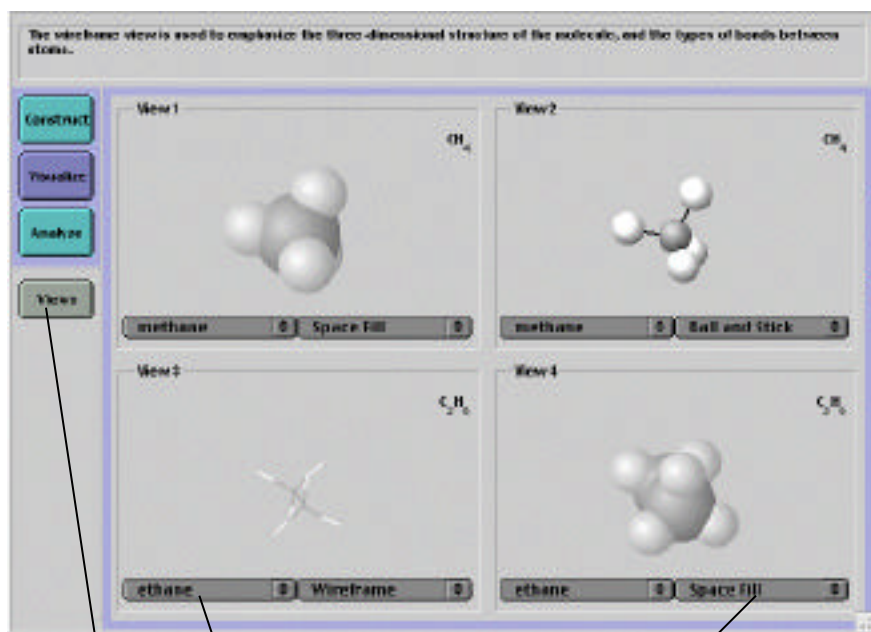
Number of Carbons_____ Number of Hydrogens_____

(b) Pentane:

Number of Carbons_____ Number of Hydrogens_____

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3. Is there a general formula of alkanes? If the number of carbons is

n for an alkane, its number of hydrogens will be _____, so

the general formula is C*n*H_____.

Visualize--seeing multiple views of the molecules

left menu for selecting molecules

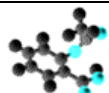views   right menu for selecting models

Fig. 2 Visualize window

• Select "visualize" button.

• Pull down the right menu on the canvas, and select "wireframe" or "space fill." You can get other models of your alkanes.

• To view different molecules or different representations at the same time, try "views".

• Select 2 or 4 views. Fig.2 is showing what the visualize window looks like if you choose 4 views.

• Pull down the left menu of each view to select molecules and the right menu to select models.

4. How do the wireframe and space-fill models differ from the stick-and-ball one? What information about bonds, atoms and structures does each of these models provide?

Let's view these alkanes in another way:

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Structures and properties

Why do we need to know chemical structures? What information can we get from molecular structures? Here is a case: chemical structures of alkanes and their boiling points. You will learn how you use structures to predict boiling points in this activity, and eChem provides "analyze" to help you visualize structures and compare their properties. Let's see how it works.

**Analyze**--make a connection between structures and properties

Menu of properties

Fig. 3 Analyze window

- First, construct the alkanes the you will compare: C_2H_6 (ethane), C_4H_{10} (butane), C_5H_{12} (pentane), C_6H_{14} (hexane). If you have files of these molecules, you can just open them.

Hint: To attach all hydrogen atoms with one click, select "extras" feature in the "construct" window. Click "fill in hydrogens."

- Click "Analyze" button. You can select "all molecules" to compare boiling points of all molecules or select "some molecules" to analyze molecules you want.

- Pull down the menu of properties, and choose "boiling point" and "carbon count" of these alkanes

5. Draw a graph of boiling points and carbon count.
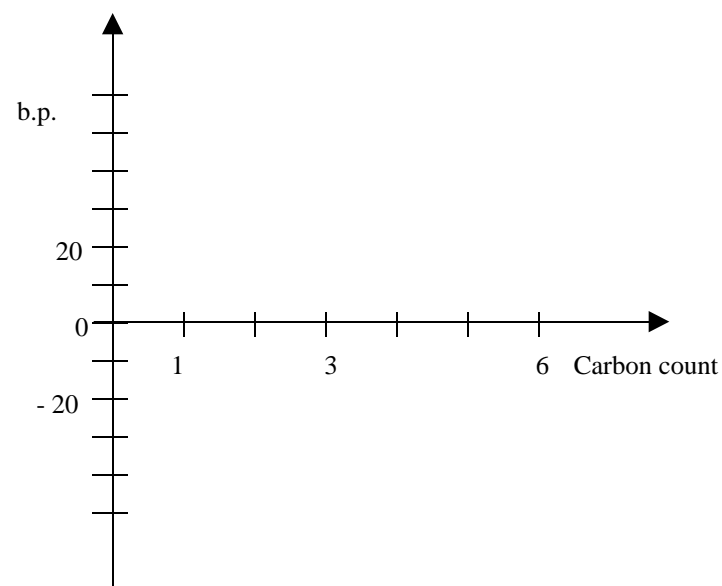
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6. What pattern do you see in the graph of question **5**? How does carbon count (number of carbons) influence boiling point (b.p.)?

9. Based on the boiling point of pentane, is it a gas, liquid or solid at room temperature (20^0C)? What other alkanes would be in the same physical state at room temperature? Explain your answer.

7. Following the pattern you found, predict the boiling points of propane and heptane.

8. Go to "analyze" to find the theoretical boiling points of propane and heptane. Compare your predictions with theoretical values. Were your predicted values higher, lower or the same as the theoretical values? Explain why.