# EXPERIMENT 5

# Isomerism in Alkanes, Alcohols, and Alkenes using Molecular Models

**Materials Needed**

Molecular model kit

**Relevant Textbook Reading**

Smith, Chapter 10.1-10.6, 11.1-11.3, 12.1-12.2

**Background**

Carbon almost always forms four bonds, nitrogen forms three, oxygen two, hydrogen one, and the halogens all form only one bond. The bonds formed can include double and triple as well as single bonds. This leads to myriad different bonding patterns (i.e., **"molecular structures"**) for all but the smallest sets of atoms (i.e., **"molecular formula"**). Different molecular structures represent different compounds with different properties. **Different molecules with the same molecular formula are called isomers.**

The main purpose of this experiment is to acquaint you with the phenomenon of isomerism and help you learn how to determine when two molecules are the same and when they are different.

There are two broad categories of isomerism: **constitutional isomerism** and **stereoisomerism**:

**Constitutional isomers have their atoms connected in different ways.** Constitutional isomerism includes such types as ***positional isomerism*** (for example, 2-methylpentane and 3-methylpentane both of which have molecular formula $C_6H_{14}$), and ***functional group isomerism*** (for example, ethyl alcohol ($CH_3CH_2OH$) and dimethyl ether ($CH_3OCH_3$), both of which have molecular formula $C_2H_6O$).

**Stereoisomers have their atoms connected in the same way.** However, the three-dimensional arrangement of the atoms (i.e., the shape) is different. The category of stereoisomers includes ***cis-trans isomerism*** (*cis*-2-butene vs. *trans*-2-butene, both of which are $C_4H_8$), and ***optical isomerism*** [(+)-lactic acid vs. (-)-lactic acid, both of which are $C_3H_6O_3$].

Determining whether two structural drawings represent the same or different compounds is not always easy. It would be easier if we could actually see the molecules. We would simply ask, "Are the two molecules ***superimposable***?" If the answer is yes then the two drawings are identical and they represent the same compound. Conversely, if two molecules cannot be superimposed without breaking bonds, then they are different compounds. If two molecules are superimposable but we must rotate around single bonds in order to superimpose them, they are ***conformations***, really just different forms of the same compound.

Most of the problem in determining whether two molecules are the same or not arises because we have to visualize them from simple drawings. Because the same molecule can be drawn in many ways, we need to be able to tell **whether or not two drawings that look different actually represent different molecules.** A good way to determine whether two drawings represent the same or different molecules is to make models of the two molecules and see if they are superimposable. If the models are superimposable, then the drawings they represent must be the same molecule.

# PRE-LABORATORY QUESTIONS

## EXPERIMENT 4

## Isomerism in Alkanes, Alcohols, and Alkenes using Molecular Models

Name ____________________________________________ Section ____________ Date ____________

1. Draw structural formulas of (a) *n*-hexane (b) 1-hexene (c) cyclohexane (d) cyclohexene.

2. Which if any of the above are isomers of each other? Explain your answer fully.

PROCEDURE AND REPORT SHEET

EXPERIMENT 4

# Isomerism in Alkanes, Alcohols, and Alkenes using Molecular Models

Name ______________________________________________ Section ____________ Date ____________

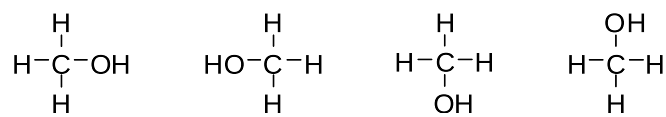
Partners_____________________________________________ Instructor ___________________________

I. **Constitutional Isomerism**

1. **<u>Positional Isomerism of Alkanes and Alcohols</u>**.

A. **<u>Methanol and methanediol</u>**.

Make a model for each of the following structures:

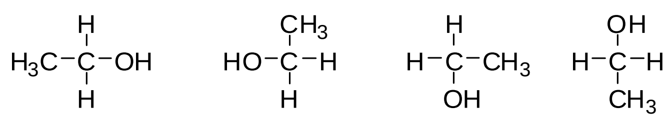


Are all four of the above superimposable on each other? ______

Do the four formulas represent different molecules? ______

B. **<u>Ethanol</u>**. Prepare models of each of the molecules shown below..

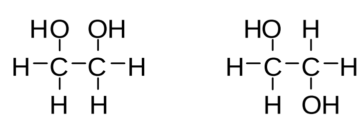
Now make a model for each of the following structural formulas:



Are all four of the models superimposable on each other? ______

Do the four formulas represent different molecules? ______

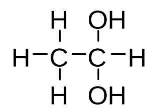
C. **<u>Ethanediol.</u>** Prepare a model of each of the molecules shown below



Are the two models superimposable? Remember that rotation of the C-C bond easily occurs. ______

Are the two molecules isomers or the same compound? ______

Now rearrange one of the models to form the molecule shown below.



Is the new model superimposable on the one you did nothing to? __________

You now have models of two molecules that are isomers of each other: they are different compounds (with different names) that have the same molecular formula ($C_2H_6O_2$). Furthermore, because the only difference in their structures is the position of a substituent (the hydroxyl) these isomers can be considered to be ***positional isomers*** of each other.

C. **Propane and Propanol**. Prepare a model of propane, $C_3H_8$. Can the three carbons and eight hydrogens be arranged to form more than one different molecular structure? ____________

Now replace any one hydrogen attached to an end carbon on the molecule with an OH group. Draw the structural formula for the molecule in the space below, and label it with its IUPAC name.

Prepare another propane molecule and then replace any one hydrogen attached to the middle carbon with an OH group. Draw its structural formula, and label it with its IUPAC name.

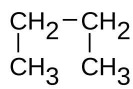
Are the two molecules that you have just prepared superimposable? __________

Are they isomers? _________ If so, what type of isomerism do they exhibit? ________________

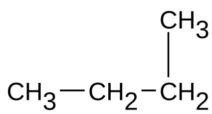
D. **Butane and Butanol**. Replace the OH groups in your two propanol molecules with methyl ($CH_3$) groups. Draw structural formulas for the two positional isomers of butane you have just prepared, and give IUPAC names for them.

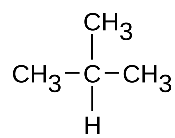
Note that one of the isomers contains an unbranched carbon chain while the other has a branch in the middle. The unbranched isomer is commonly called *n*-butane while the branched molecule is called isobutane.

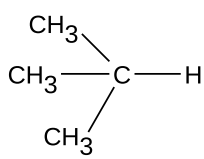
For each of the structures below, indicate whether it is *n*-butane, isobutane, or neither.

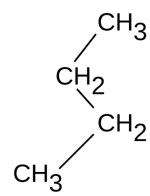
 ________

$CH_3CH_2CH_2CH_3$ ________

 ________

 ________

 ________

 ________

Post lab assignment #1: Give structures for *n*-pentane, and its two isomers. Note that one of the isomers contains a quaternary (4°) carbon atom. Name all three isomers.

names: ____________________ ______________________ ____________________

Post-lab assignment #2: Using a chemical handbook or internet reference to fill out the following table illustrating the different physical properties of the three pentane isomers drawn and named above.

| Pentane Isomer | Literature boiling point (°C) | Literature melting point (°C) |
|---|---|---|
| | | |
| | | |
| | | |

Reference used ________________________________________________________________

1. ***Cis-Trans*** **Isomerism of Alkenes**

(1) **Ethene**. Prepare two models of ethene, $C_2H_4$.

Is ethene an isomer of ethane? ____________

Can you rotate the molecule around the double bond? ____________

(2) **Propene**. Now substitute a methyl group for one of the hydrogen atoms in each of the ethene models to form a model of propene.

Are the two models superimposable? ____________

Does it matter which hydrogen in ethene you replace with the methyl group? (Is there any way to make a propene model that is not superimposable on the first one?) ____________

What is the C-C-C bond angle approximately? ____________

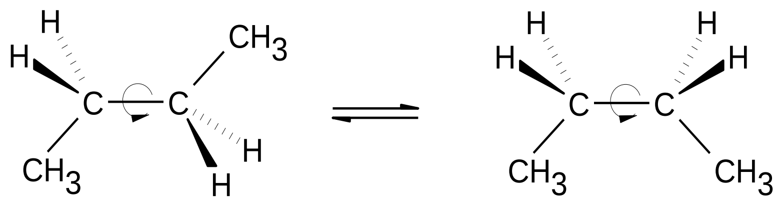
Give a structure for propene that shows the C-C-C bond angle.

(3) Butenes. There are four butene isomers, $C_4H_8$. You can come up with a model of each by in turn replacing different hydrogens on propene with a methyl group.

Prepare the four isomers of butene, give their structures (show C-C-C bond angles realistically please), and name them by IUPAC rules.

| structural formula | IUPAC name |
|---|---|
| 1. | ________________________ |
| 2. | ________________________ |
| 3. | ________________________ |
| 4. | ________________________ |

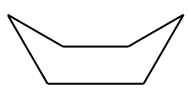
Notice that there are two isomers that have a double bond between the second and third carbon atoms of a chain. The compound with both methyl groups on the same side of the double bond is *cis*-2-butene (*cis* = on this side), and the one with the methyl groups on opposite sides of the double bond is *trans*-2-butene (*trans* = across). These are different compounds due to the fact that ***rotation around carbon-carbon double bonds is difficult and does not ordinarily occur***, a fact accurately depicted by your models. Isomers of this type are called **cis/trans isomers**. (Remember, though that the structures shown below, which would be alkanes analogous to *cis*- and *trans*-2-butene, ***are <u>not</u> isomers*** but are the ***same molecule*** due to the fact that ***rotation <u>can</u> occur around carbon-carbon <u>single bonds</u>***.)



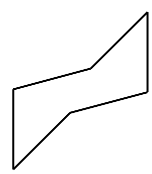

. **<u>Cycloalkanes</u>**

(1) **<u>Cyclohexane</u>**. Make a ring of six carbon atoms using single bonds. Fill in the remaining positions with hydrogen. This molecule is cyclohexane.

Cyclohexane can exist in the two non-planar forms shown below.



boat form



chair form

Change your model back and forth between the chair and boat forms. This process occurs very rapidly at room temperature.

What is the relationship between the chair and the boat form of cyclohexane?
A. stereoisomers B. structural isomers C. different conformations of the same moleucle

The chair conformation is much more stable than the boat. Thus, cyclohexane mainly exists in the chair conformation. Answer the following questions by looking at your model of the chair conformation.

What are the bond angles around the carbon atoms? __________

What is the preferred bond angle for these carbon atoms as predicted by VSEPR theory? ________

Is cyclohexane a stable molecule? __________

(2) **<u>Cyclopropane</u>**. Make a ring of three carbon atoms using single bonds. Fill in the remaining positions with hydrogen. This molecule is cyclopropane.

What are the C-C-C bond angles in cyclopropane? ___________

What is the preferred bond angle for these carbon atoms as predicted by VSEPR theory? ________

Is cyclopropane a stable molecule? __________