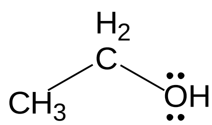
Experiment 10: Molecular Models

Modeling the shape of small organic molecules

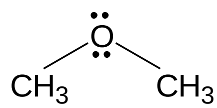
Background

Modeling the shape of small organic molecules

Previously we have considered molecules and ions for which one chemical formula corresponded to one chemical compound only. Not all chemical compounds are like that. For example, consider the formula C_2H_6O. It turns out that there is more than one compound with that chemical formula:



ethanol

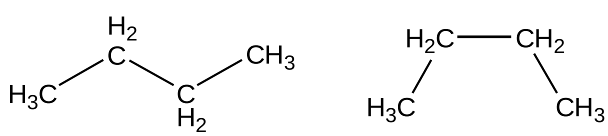


dimethyl ether

***Structural* isomerism**

These two molecules have completely different chemical and physical properties. They are called *structural isomers.* They have the same chemical formula with different bonding between atoms. Another example would be the compounds that correspond to butane, with the chemical formula C_4H_{10}. There are two structural isomers of butane.

Using your model kit, construct the structures of *n*-butane ("straight-chain" butane; see below) and answer the following questions.



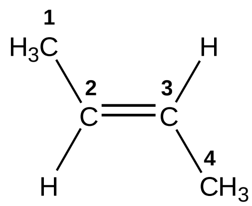
1. Explain why the two structures above are NOT considered structural isomers.

2. Construct two *structural* isomers of C_4H_{10}. Draw them below using expanded structural or line formulas. When you are finished, **compare them with the results of other students.**

Geometric isomerism

An example of a different kind of isomerism occurs when the molecules have the same bonding between the atoms but their arrangement in space is different. We say that these compounds are *geometric isomers*. A classic example involves molecules that contain double bonds.

Take the *n*-butane model you just built (the straight-chain one), remove two hydrogens and make a double bond (between carbon 2 and 3) such that you achieve the following molecule:



trans-2-butene

3. There are two other isomers of trans-2-butene. Draw them below. Compare the structures with other students.

Isomers of *trans*-2-butene

Circle the structure drawn above that contains a double bond between carbons 2 and 3. The name of this isomer is called *cis*-2-butene. The double bond between the carbon atoms does not allow the free rotation of the methyl (CH_3) groups with respect to one another, preventing the interconversion between the *trans* and *cis* isomers. Geometric isomers have different physical properties but almost identical chemical properties.

Build models of cis and trans 2-butene. Examine them and answer this question:

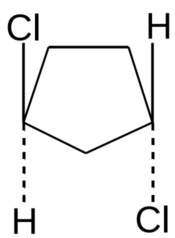
What do you think is the meaning of the prefix "***cis-***" vs "***trans-***"?

More *Geometric* isomerism

4. Here's another example of geometric isomers.

Construct cyclopentane, C_5H_{10}, which does not contain any double bonds.

Replace two hydrogens with chlorines to obtain *trans*-1,3-dichloropcyclopentane (as in the drawing below). Build the *cis*-isomer of this molecule (based on what you learned above) and draw your structure below.



trans-1,3-dichlorocyclopentane

cis-1,3-dichlorocyclopentane

(the dotted lines show these atoms are on the other side of the ring)

There is no free rotation around the C-C bonds that connect the carbons where the chlorine atoms are bound because of the rigidity of the cyclopentane molecule. Therefore, there is no interconversion between the *cis* and *trans* forms.

Thus, *cis*- and *trans*- prefixes refer to *geometrical* isomers!

We have briefly introduced the concepts of *structural* and *geometric* isomers. There is yet a third type of isomerism that we will leave out of this discussion: it is the so-called *optical* isomerism that will be covered in the organic chemistry courses.

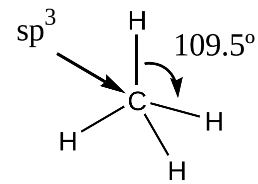
Procedure

In the following exercise construct the molecule using the model kits. Calculate the number of valence electrons for each molecule. Find the molecular geometry at ***each*** central atom (if there is more than one) according to VSEPR theory. Determine the hybridization *of* ***each*** carbon atom and the value of ***each*** dihedral angle (HCH, HCC, etc). You may wish to draw these on the Lewis structure to be clear which hybridization/angle belongs to which carbon. Sketch the molecule in the right hand box and draw the structure of all possible isomers. The first one is completed as an example.

Procedure

<table>
<tr><td>Example:

Molecule = CH_4
# of valence electrons = 8

At each carbon atom:
molecular geometry = tetrahedral
hybridization = sp^3
HCH angle = 109.5°</td><td>Lewis structure
(example)
</td></tr>
<tr><td colspan="2">Isomers (none)</td></tr>
<tr><td>Molecule = C_2H_6
# of valence electrons =

At each carbon atom:
molecular geometry =

hybridization =

HCH angle =</td><td>Lewis structure</td></tr>
<tr><td colspan="2">Isomers (none)</td></tr>
<tr><td>Molecule = $C_2H_3Cl_3$
# of valence electrons =

At each carbon atom:
molecular geometry =

hybridization =

HCH angle =</td><td>Lewis structure</td></tr>
<tr><td colspan="2">Isomers (Besides the one above, there is one more isomer—draw it in the space below):

The two isomers above are (circle one): structural geometric both structural and geometric</td></tr>
</table>

Molecule = $C_2H_2Cl_2$ # of valence electrons = *At each carbon atom:* molecular geometry = hybridization = HCH angle =	Lewis structure
Isomers (two others) The isomers above are (circle one): structural geometric both structural and geometric	
Molecule = $C_3H_6Cl_2$ # of valence electrons = *At each carbon atom:* molecular geometry = hybridization = HCH angle =	Lewis structure
Isomers (three others) The isomers above are (circle one): structural geometric both structural and geometric	
Molecule = $C_3H_5Cl_3$ # of valence electrons = *At each carbon atom:* molecular geometry = hybridization = HCH angle =	Lewis structure
Isomers (four others) The isomers above are (circle one): structural geometric both structural and geometric	

Molecule = C_5H_{10} # of valence electrons = *At each carbon atom:* molecular geometry = hybridization = HCH angle =	Lewis structure
Isomers (a total of 6 cyclic isomers and 6 acyclic isomers, including the one above) Hint: Geometric isomers! The isomers above are (circle one): structural geometric both structural and geometric	
Molecule = $C_5H_8Cl_2$ # of valence electrons = *At each carbon atom:* molecular geometry = hybridization = HCH angle =	Lewis structure
Isomers: O*nly work with cyclopentanes (no double bonds, etc…)* The isomers above are (circle one): structural geometric both structural and geometric	

Name________________________ Section______

Follow-up Questions

1. In the first few pages you learned about structural isomers and geometric isomers. Define these terms below:

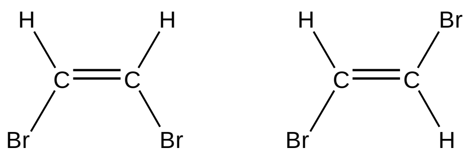
Structural isomer ____

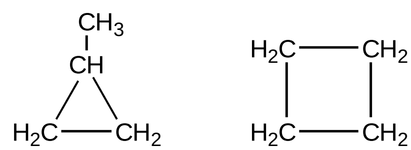
____

Geometric isomer ____

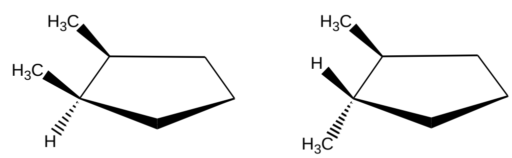
____

2. Identify whether the following pairs of compounds are structural isomers, geometric isomers, or identical molecules.

a) 

b) 

c) $(CH_3)_2CHCH_2CH_3$ $CH_3(CH_2)_3CH_3$

d) 

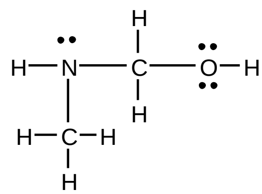
e) 

f) 

3. What relationship did you find between *molecular geometry*, *hybridization*, and *bond angle*? Create a chart that summarizes all the geometries and their hybridizations and bond angles.

Pre-lab Assignment—To be completed BEFORE lab!

1. The chemical composition of a compound is usually given by its chemical formula. There are different ways to express information about the structure of a compound. An expanded structural formula shows all the bonds. Sometimes this is shortened into a condensed structural formula.



expanded structural formula

$CH_3(NH)CH_2OH$

condensed structural formula

Questions:

a) Do the two formulas above match in the number and type of atoms they contain? ________

b) Examining the structure above for patterns, how many bonds does:

hydrogen tend to form? _____ oxygen? _____ nitrogen? _____ carbon?_____

(These are numbers are called "valences")

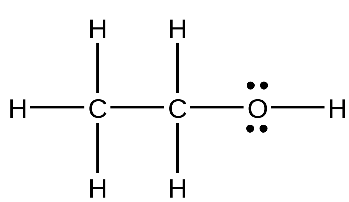
Convert the following into an expanded structural formula:

c) $(CH_3)_2CHCH_2CH_3$

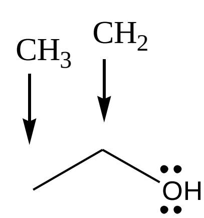
d) $CH_3CH(OH)CH_2CH_3$

e) $Br(CH_2)_3CH_3$

2. Skeletal structures are another way to draw structures.



expanded structural formula of C_2H_5OH



skeletal structure of C_2H_5OH

Note: In the skeletal structure above, carbons and hydrogens are implied.

Do the two formulas above match in the number and type of atoms they contain? ________

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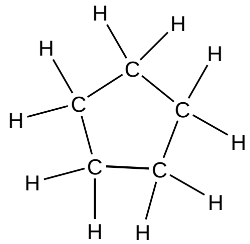
Convert the following structural formulas into skeletal structures:

a)



b) $(CH_3)_2CHCH_2CH_3$

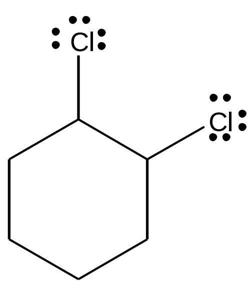
c) $CH_3CH(OH)CH_2CH_3$

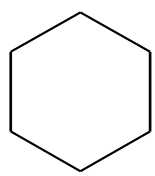
d) $Br(CH_2)_3CH_3$

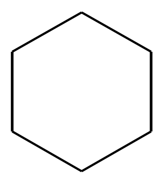
3. Structural isomers have the same chemical formula but different structures in terms of how the atoms are connected. Below is a skeletal drawing of 1,2-dichlorocyclohexane.

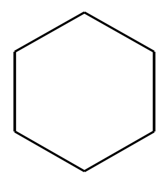
a) What is the chemical formula of this compound? _______________

b) Draw three other ***structural*** isomers of this compound. Use the skeletal templates below.









c) Would you expect these isomers to have different physical properties? Explain.

d) Can you think of any acyclic (no ring) structural isomer of 1,2-dichlorocyclohexane? **Draw at least three below** (even though one can easily draw over fifty of these isomers in no time…!)