

MOLECULAR GEOMETRY WITH MOLECULAR MODELS

Discussion

Organic compounds are extremely numerous - on the order of tens of millions, and several new compounds are being discovered and synthesized each day. The chemical and physical properties of these compounds depend upon what elements are present, how many atoms of each element are present, and how these atoms are arranged in the molecule.

Molecular formulas often, permit one to distinguish between two compounds. However, there are many substances that have identical molecular formulas but are completely different compounds. Consider the molecular formula C_2H_6O . There are two compounds that correspond to the formula: ethyl alcohol and dimethyl ether. While the molecular formula gives no clue as to which compound one may be referring, examination of the structural formula immediately reveals a different arrangement of atoms for these substances.

In addition, when molecular models are used, trial and error will show that there are just two ways that two carbons, six hydrogens, and one oxygen can be arranged without violating the usual valances of the elements. Compounds that have the same molecular formula but different structural formulas are termed isomers. This difference in molecular structure results in differences in chemical and physical properties of isomers. In the case of ethyl alcohol and dimethyl ether, these differences are very pronounced. In other cases, the differences may be more subtle.

	Ethyl Alcohol	Dimethyl Ether
Structural Formula	$\begin{array}{c} \text{H} & \text{H} \\ & \\ \text{H}-\text{C}-\text{C}-\text{OH} \\ & \\ \text{H} & \text{H} \end{array}$	$\begin{array}{c} \text{H} & & \text{H} \\ & & \\ \text{H}-\text{C}-\text{O}-\text{C}-\text{H} \\ & & \\ \text{H} & & \text{H} \end{array}$
Condensed Structural Formula	$\text{CH}_3\text{CH}_2\text{OH}$	CH_3OCH_3
Molecular Formula	$\text{C}_2\text{H}_6\text{O}$	$\text{C}_2\text{H}_6\text{O}$
Boiling Point	78.5°C	-24°C
Melting Point	-117°C	-139°C
Solubility in Water	Infinite	Very Slight
Behavior towards Sodium metal	Reacts vigorously, liberating hydrogen	No reaction

A short glance at these formulas readily reveals their difference. The compounds differ in the connectivity. The atoms in ethyl alcohol are connected or bonded in a different sequence from those in dimethyl ether.

You must learn to translate these condensed formulas into three-dimensional mental structures and to translate structures represented by molecular models to condensed structural formulas.

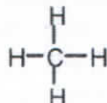
Procedure

Construct models of the molecules as directed and determine the number of isomers by trial and error as directed below. Use a black ball with four holes for carbon, a yellow ball with one hole for hydrogen, and a green ball with one hole for chlorine

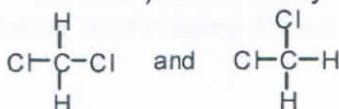
Answer the following questions on a separate sheet of paper to be submitted for grading.

A. Methane

Construct a model of methane, CH_4 . Place the model on the desk top and note the symmetry of the molecule. Note that the molecule looks the same regardless of which three hydrogens are resting on the desk. All four hydrogens are said to be equivalent. Now, grasp the top hydrogen and tilt the molecule so that only two hydrogens rest on the desk and the other two are in a plane parallel to the desk top. Now imagine pressing this methane model flat onto the desk top. The resulting imaginary projection in the plane of the desk in the conventional representation of the structural formula of methane:



Replace one of the hydrogen atoms with a chlorine atom to construct a model of chloromethane, CH_3Cl . Replace a second hydrogen atom by a chlorine atom to make dichloromethane, CH_2Cl_2 (methylene chloride). Convince yourself that the two formulas



represent the same three-dimensional structure and are not isomers. Replace another hydrogen to make CHCl_3 , trichloromethane (chloroform). Finally, make CCl_4 , tetrachloromethane (carbon tetrachloride).

1. Draw the structure of and name each of the chloromethanes (3 total).

B. Ethane

Make a model of ethane, C_2H_6 , from your model of methane by replacing one of the hydrogens by a CH_3 unit; the $-\text{CH}_3$ unit is called a methyl group. Note that the hydrogens of ethane are all equivalent. Replace one of the hydrogens in the model by a chlorine. Does it matter which hydrogen you replace? How many monochloro ethanes exist? Now examine your model of $\text{C}_2\text{H}_5\text{Cl}$ and note how many different hydrogen atoms are present. If another hydrogen is replaced by a chlorine atom to yield $\text{C}_2\text{H}_4\text{Cl}_2$, how many isomers would result? Does the formula $\text{C}_2\text{H}_4\text{Cl}_2$ distinguish the possible isomers corresponding to this formula? Draw the structural and condensed structural formulas for all possible isomers of $\text{C}_2\text{H}_4\text{Cl}_2$ and assign the IUPAC names to each.

2. Draw the structures for $\text{C}_2\text{H}_5\text{Cl}$ and $\text{C}_2\text{H}_4\text{Cl}_2$ and name each compound.

C. Propane

From your model of ethane, construct a model of propane, C_3H_8 , by replacing one of the hydrogen atoms by a methyl group. Examine your model of propane and determine how many different and distinct hydrogen atoms are present in propane. If one of the hydrogens of propane is replaced with chlorine, how many isomers of $\text{C}_3\text{H}_7\text{Cl}$ are possible? Write them and give their names. How many isomers are there corresponding to the formula $\text{C}_3\text{H}_6\text{Cl}_2$? Write their formulas and name them. Convince yourself that there are five isomers with the formula $\text{C}_3\text{H}_5\text{Cl}_3$. Write both the structural and condensed structural formula and IUPAC names for these isomers. By this stage, you should realize that a systematic approach is most useful in determining the number of isomers for a given formula.

3. Draw the structural formulas name all isomers of monochloropropane, C_3H_7Cl , and dichloropropane, $C_3H_6Cl_2$.

4. Draw the structural formulas and name all the isomers of trichloropropane, $C_3H_3Cl_3$.

D. Butane

The formula for butane is C_4H_{10} . From you model of propane, construct all possible isomers of butane by replacing a hydrogen with a methyl group. How many isomers of butane are there? Give their structural formula and IUPAC names. There are four isomers corresponding to the formula C_4H_9Cl . Write their structural formulas and name them. How many isomers of $C_4H_8Cl_2$ are there? Use your model to help answer the question. Draw their formula and name all the isomers of $C_4H_8Cl_2$.

5. Draw the structural formulas and names for all the isomers of butane.

6. Draw the structural formulas and names for all the isomers of:

a. C_4H_8Cl

b. $C_4H_8Cl_2$

E. Pentane

Use your models in a systematic manner to determine how many isomers there are for the formula C_5H_{12} . Draw their structural formulas and name them. Draw and name all of the isomers of $C_5H_{11}Cl$. Give the pure IUPAC name and the name using IUPAC reserved names for certain substituents.

7. Draw the structural formulas and names for all the isomers of C_5H_{12} .

8. Draw the structural formula and names for all the isomers of $C_5H_{11}Cl$.

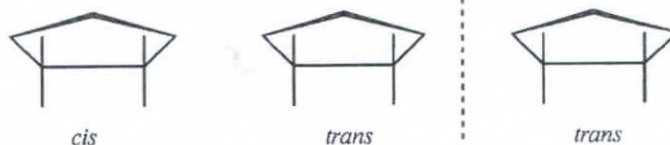
F. Cycloalkanes

Cycloalkanes corresponding to the formula C_nH_{2n} exist. Using springs for single bonds, construct models of cyclopropane, C_3H_6 ; cyclobutane, C_4H_8 . Although cyclopropane and cyclobutane exist, would you anticipate these to be highly stable molecules?

Now, using wooden pegs for bonds, carefully construct models for cyclopentane, C_5H_{10} ; and cyclohexane, C_6H_{12} – not all of the atoms will lie in the same plane.

How many isomers of 1,2-dichlorocyclopentane are there? The answer may not be obvious, but there are three. If you cannot convince yourself that there are three, check with your laboratory instructor. Two of the three will be mirror images of each other. This is another aspect of isomerization that is most significant in organic chemistry, and will be addressed in the study of stereochemistry.

9. Using the following format for the structure of cyclopentane, give the structure for all three isomers of 1,2-dichlorocyclopentane.



G. Alkenes

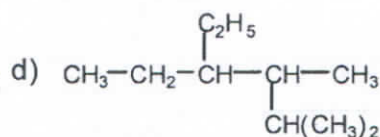
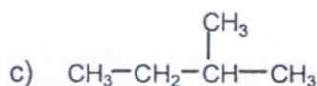
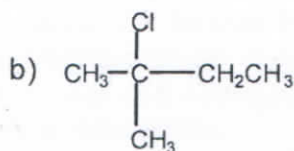
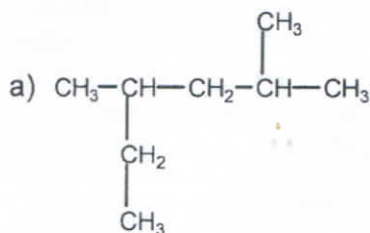
Using two springs to represent a double-bond, construct a model of ethene (ethylene), C_2H_4 . Note the rigidity of the molecule; note that there is no rotation about the carbon-carbon double-bond as there is for a carbon-carbon single-bond, such as in ethane or propane. How many isomers are there corresponding to the formulas C_2H_3Cl ? $C_2H_2Cl_2$? Draw the formulas and name them.

10. Give the structures and names of all isomers of $C_2H_2Cl_2$.

Additional Questions

1. Draw and name all isomers of the alkane C_6H_{14} .

2. Give the correct IUPAC name for each of the four compounds:



3. Draw the structural formulas for the following:

a. 2-chloropentane

b. 3-chloro-3-methylpentane

c. 2,2,3-trimethylhexane

d. 4-ethyl-2,2-dimethylhexane