Structure in Organic Compounds: Use of Molecular Models. I

BACKGROUND

The study of organic chemistry usually involves molecules that contain carbon. Thus a convenient definition of organic chemistry is the chemistry of carbon compounds.

There are several characteristics of organic compounds that make their study interesting:

1. Carbon forms strong bonds to itself as well as to other elements; the most common elements found in organic compounds, other than carbon, are hydrogen, oxygen, and nitrogen.

2. Carbon atoms are generally tetravalent. This means that carbon atoms in most organic compounds are bound by four covalent bonds to adjacent atoms.

3. Organic molecules are three-dimensional and occupy space. The covalent bonds that carbon makes to adjacent atoms are at discrete angles to each other. Depending on the type of organic compound, the angle may be 180°, 120°, or 109.5°. These angles correspond to compounds that have triple bonds (1), double bonds (2), and single bonds (3), respectively.

\[
\begin{align*}
-\text{C}=\text{C} & \quad & \text{C} &= \text{C} \quad & \text{C} &= \text{C} \\
\text{(1)} & \quad & \text{(2)} & \quad & \text{(3)}
\end{align*}
\]

4. Organic compounds can have a limitless variety in composition, shape, and structure.

Thus, while a molecular formula tells the number and type of atoms present in a compound, it tells nothing about the structure. The structural formula is a two-dimensional representation of a molecule and shows the sequence in which the atoms are connected and the bond type. For example, the molecular formula, C₄H₁₀, can be represented by two different structures: butane (4) and 2-methylpropane (isobutane) (5).
Consider also the molecular formula, $\text{C}_2\text{H}_6\text{O}$. Two structures correspond to this formula: dimethyl ether (6) and ethanol (ethyl alcohol) (7).

In the pairs above, each structural formula represents a different compound. Each compound has its own unique set of physical and chemical properties. Compounds with the same molecular formula but with different structural formulas are called isomers.

The three-dimensional character of molecules is expressed by its stereochemistry. By looking at the stereochemistry of a molecule, the spatial relationships between atoms on one carbon and the atoms on an adjacent carbon can be examined. Because rotation can occur around carbon–carbon single bonds in open chain molecules, the atoms on adjacent carbons can assume different spatial relationships with respect to each other. The different arrangements that atoms can assume as a result of a rotation about a single bond are called conformations. A specific conformation is called a conformation. Whereas individual isomers can be isolated, conformers cannot because interconversion, by rotation, is too rapid.

Conformers may be represented by projections through the use of two conventions, as shown in Figure 21.1. These projections attempt to show on a flat surface how three-dimensional objects, in this case organic molecules, might look in three-dimensional space.

The sawhorse projection views the carbon–carbon bond at an angle and, by showing all the bonds and atoms, shows their spatial arrangements. The Newman projection provides a view along a carbon–carbon bond by sighting directly along the carbon–carbon bond. The near carbon is represented by a circle, and bonds attached to it are represented by lines going to the center of the circle. The carbon behind is not visible (it is blocked by the near carbon), but the bonds attached to it are partially visible and are represented by lines going to the edge of the circle. With Newman projections, rotations show the spatial relationships of atoms on adjacent carbons easily. Two conformers that represent extremes are shown in Figure 21.2.
The *eclipsed* conformation has the bonds (and the atoms) on the adjacent carbons as close as possible. The *staggered* conformation has the bonds (and the atoms) on adjacent carbons as far as possible. One conformation can interconvert into the other by rotation around the carbon–carbon bond axis.

The three-dimensional character of molecular structure is shown through molecular model building. With molecular models, the number and types of bonds between atoms and the spatial arrangements of the atoms can be visualized for the molecules. This allows comparison of isomers and of conformers for a given set of compounds. The models also will let you see what is meant by *chemical equivalence*. Here *equivalence* relates to those positions or to those hydrogens on carbon(s) in an organic molecule that are equal in terms of chemical reactivity. In the case of hydrogen, replacement of any one of the equivalent hydrogens in a molecule by a substituent (any atom or group of atoms, for example, Cl or OH, respectively) leads to the identical substituted molecule.

**OBJECTIVES**

1. To use models to visualize structure in organic molecules.
2. To build and compare isomers having a given molecular formula.
3. To explore the three-dimensional character of organic molecules.
4. To demonstrate equivalence of hydrogens in organic molecules.
PROCEDURE

Obtain a set of ball-and-stick molecular models from the laboratory instructor. The set contains the following parts (other colored spheres may be substituted as available):

- 2 Black spheres representing Carbon; this tetracovalent element has four holes
- 6 Yellow spheres representing Hydrogen; this monovalent element has one hole
- 2 Colored spheres representing the halogen Chlorine; this monovalent element has one hole
- 1 Blue sphere representing Oxygen; this divalent element has two holes
- 8 Sticks to represent bonds

1. With your models, construct the molecule methane. Methane is a simple hydrocarbon consisting of one carbon and four hydrogens. After you put the model together, answer the questions below in the appropriate space on the Report Sheet.

   a. With the model resting so that three hydrogens are on the desk, examine the structure. Move the structure so that a different set of three hydrogens are on the desk each time. Is there any difference between the way that the two structures look (1a)?

   b. Does the term equivalent adequately describe the four hydrogens of methane (1b)?

   c. Tilt the model so that only two hydrogens are in contact with the desk and imagine pressing the model flat onto the desktop. Draw the way in which the methane molecule would look in two-dimensional space (1c). This is the usual way that three-dimensional structures are written.

   d. Using a protractor, measure the angle H—C—H on the model (1d).

2. Replace one of the hydrogens of the methane model with a colored sphere, which represents the halogen chlorine. The new model is chloromethane (methyl chloride), CH$_3$Cl. Position the model so that the three hydrogens are on the desk.

   a. Grasp the atom representing chlorine and tilt it to the right, keeping two hydrogens on the desk. Write the structure of the projection on the Report Sheet (2a).

   b. Return the model to its original position and then tilt as before, but this time to the left. Write this projection on the Report Sheet (2b).

   c. While the projection of the molecule changes, does the structure of chloromethane change (2c)?

3. Now replace a second hydrogen with another chlorine sphere. The new molecule is dichloromethane, CH$_2$Cl$_2$.

   a. Examine the model as you twist and turn it in space. Are the projections given below isomers of the molecule CH$_2$Cl$_2$ or
representations of the same structure only seen differently in three dimensions (3a)?

\[
\begin{align*}
\text{H} & \quad \text{Cl} \\
\text{Cl} \quad \text{C} \quad \text{H} & \quad \text{Cl} \quad \text{C} \quad \text{Cl} \\
\text{Cl} & \quad \text{Cl} \\
\text{H} & \quad \text{H} \\
\text{Cl} & \quad \text{Cl}
\end{align*}
\]

4. Construct the molecule ethane, C\(_2\)H\(_6\). Note that you can make ethane from the methane model by removing a hydrogen and replacing the hydrogen with a methyl group, —CH\(_3\).
   a. Write the structural formula for ethane (4a).
   b. Are all the hydrogens attached to the carbon atoms equivalent (4b)?
   d. Replace any hydrogen in your model with chlorine. Write the structure of the molecule chloroethane (ethyl chloride), C\(_2\)H\(_5\)Cl (4d).
   e. Twist and turn your model. Draw two Newman projections of the chloroethane molecule (4e).
   f. Do the projections that you drew represent different isomers or conformers of the same compound (4f)?

5. Dichloroethane, C\(_2\)H\(_4\)Cl\(_2\)
   a. In your molecule of chloroethane, if you choose to remove another hydrogen note that you now have a choice among the hydrogens. You can either remove a hydrogen from the carbon to which the chlorine is attached, or you can remove a hydrogen from the carbon that has only hydrogens attached. First, remove the hydrogen from the carbon that has the chlorine attached and replace it with a second chlorine. Write its structure on the Report Sheet (5a).
   b. Compare this structure to the model that would result from removal of a hydrogen from the other carbon and its replacement by chlorine. Write its structure (5b) and compare it to the previous example. One isomer is 1,1-dichloroethane; the other is 1,2-dichloroethane. Label the structures drawn on the Report Sheet with the correct name.
   c. From what you did in a and b, above, you can make some conclusions about the hydrogens that are equivalent to each other in chloroethane. Draw the structure of chloroethane and label the hydrogens that are equivalent to each other (for example, as H\(_a\)). Are all the hydrogens of chloroethane equivalent? Are some of the hydrogens equivalent? How many sets of equivalent hydrogens are there?

6. Butane
   a. Butane has the formula C\(_4\)H\(_{10}\). With help from a partner, construct a model of butane by connecting the four carbons in a series (C—C—C—C) and then adding the needed hydrogens. First,
orient the model in such a way that the carbons appear as a straight line. Next, tilt the model so that the carbons appear as a zig-zag line. Then, twist around any of the C—C bonds so that a part of the chain is at an angle to the remainder. Draw each of these structures in the space on the Report Sheet (6a). Note that the structures you draw are for the same molecule but represent a different orientation and projection.

b. Sight along the carbon–carbon bond of C₂ and C₃ on the butane chain. CH₂—CH₂—CH₂—CH₃. Draw a staggered Newman projection. Rotate the C₂ carbon clockwise by 60°; draw the eclipsed Newman projection. Again, rotate the C₂ carbon clockwise by 60°; draw the Newman projection. Is the last projection staggered or eclipsed (6b)? Continue rotation of the C₂ carbon clockwise by 60° increments and observe the changes that take place.

c. Examine the structure of butane for equivalent hydrogens. In the space on the Report Sheet (6c), redraw the structure of butane and label the hydrogens that are equivalent to each other. On the basis of this examination, predict how many monochlorobutane isomers (C₄H₉Cl) could be obtained from the structure you drew in 6c (6d). Test your prediction by replacement of hydrogen by chlorine on the models. Draw the structures of these isomers (6e).

d. Reconstruct the butane system. First, form a three-carbon chain, then connect the fourth carbon to the center carbon of the three-carbon chain. Add the necessary hydrogens. Draw the structure of 2-methylpropane (isobutane) (6f). Can any manipulation of the model, by twisting or turning of the model or by rotation of any of the bonds, give you the butane system? If these two, butane and 2-methylpropane (isobutane), are isomers, then how may we recognize that any two structures are isomers (6g)?

e. Examine the structure of 2-methylpropane for equivalent hydrogens. In the space on the Report Sheet (6h), redraw the structure of 2-methylpropane and label the equivalent hydrogens. Predict how many monochloroisomers of 2-methylpropane could be formed (6i) and test your prediction by replacement of hydrogen by chlorine on the model. Draw the structures of these isomers (6j).

7. C₂H₆O

a. There are two isomers with the molecular formula C₂H₆O: ethanol (ethyl alcohol) and dimethyl ether. With your partner, construct both of these isomers. Draw these isomers on the Report Sheet (7a) and name each one.

b. Manipulate each model. Can either be turned into the other by a simple twist or turn (7b)?

c. For each compound, label the hydrogens that are equivalent. How many sets of equivalent hydrogens are there in ethanol (ethyl alcohol) and dimethyl ether (7c)?
8. Optional: Butenes
   a. If springs are available for the construction of double bonds (Figure 21.3), construct 2-butene, \( \text{CH}_3-\text{CH}=\text{CH}-\text{CH}_3 \). There are two isomers for compounds of this formulation: the isomer with the two \(-\text{CH}_3\) groups on the same side of the double bond, cis-2-butene; and the isomer with the two \(-\text{CH}_3\) groups on opposite sides of the double bond, trans-2-butene. Draw these two structures on the Report Sheet (8a).
   b. Can you twist, turn, or rotate one model into the other? Explain (8b).
   c. How many bonds are connected to any single carbon of these structures (8c)?
   d. With the protractor, measure the \( \text{C}-\text{C}=\text{C} \) angle (8d).
   e. Construct methylpropene, \( \text{CH}_3-\text{C}=\text{CH}_2 \).

   \[
   \begin{align*}
   &| \\
   \text{CH}_3 \\
   \end{align*}
   \]

   Can you have a cis or a trans isomer in this system (8e)?

9. Optional: Butynes
   a. If springs are available for the construction of triple bonds, construct 2-butyne, \( \text{CH}_3-\text{C}=\text{C}-\text{C} \). Can you have a cis or a trans isomer in this system (9a)?
   b. With the protractor, measure the \( \text{C}-\text{C}=\text{C} \) angle (9b).
   c. Construct a second butyne with your molecular models and springs. How does this isomer differ from the one in (a) above (9c)?

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**CHEMICALS AND EQUIPMENT**

1. Molecular models (you may substitute other available colors for the spheres):
   - 2 Black spheres
   - 6 Yellow spheres
   - 2 Colored spheres (e.g., green)
   - 1 Blue sphere
   - 8 Sticks

2. Protractor

3. Optional: 3 springs
Pre-Lab Questions

1. How do organic compounds differ from inorganic compounds?

2. Below are the structures of two organic compounds. What makes them different?

\[
\begin{align*}
\text{CH}_3 - \text{CH} - \text{CH}_3 & \\
\text{Cl} & \\
\text{CH}_3 - \text{CH}_2 - \text{CH}_2 - \text{Cl}
\end{align*}
\]

3. Match the bond angle on carbon with the bond type shown below: (a) 109.5°, (b) 120°, (c) 180°.

\[
\begin{align*}
\equiv & \\
\equiv & \\
\equiv & 
\end{align*}
\]

4. Below are two structures of propane, \(\text{CH}_3 - \text{CH}_2 - \text{CH}_3\). How do the two structures differ?

\[
\begin{align*}
\text{CH}_3 - \text{CH}_2 & \\
\text{CH}_3 \\
\text{CH}_3 & \\
\text{CH}_3 \\
\text{CH}_3 & \\
\text{CH}_3
\end{align*}
\]

5. Use Newman projections to show ethane in the eclipsed conformation and in the staggered conformation. Correctly label each. How can you convert one into the other?
EXPERIMENT 21

Report Sheet

1. Methane
   a. 
   b. 
   c. 
   d. 

2. Chloromethane (methyl chloride)
   a. 
   b. 
   c. 

3. Dichloromethane
   a. 

4. Ethane and chloroethane (ethyl chloride)
   a. 
   b. 
   c. 
   d. 
   e. 
   f.
5. Dichloroethane
   a.
   b.
   c.

6. Butane
   a.
   b.
   c.
   d.
   e.
   f.
   g.
   h.
   i.
   j.

7. \( \text{C}_2\text{H}_4\text{O} \)
   a.
   b.
   c. Ethanol (ethyl alcohol) has \( \underline{\quad} \) set(s) of equivalent hydrogens.
   Dimethyl ether has \( \underline{\quad} \) set(s) of equivalent hydrogens.

8. Butenes
   a.
   b.
c.

d. C—C=C angle

e.

9. Butynes

a.

b.

c.
Post-Lab Questions

1. Write the structural formulas for the two (2) chloro-isomers that can be formed from 2-methylpropane (isobutene). How many sets of equivalent hydrogen are there in the compound 2-methylpropane?

2. Given the molecular formula C₃H₇Br, draw all the structural isomers that are possible.

3. Using the Newman projection, draw a staggered conformer and an eclipsed conformer for 1-chloropropane, Cl—CH₂—CH₂—CH₃, along the bond indicated by (*). Why can these conformers be interconverted?

4. What structural feature prevents the conversion of cis-2-butene into trans-2-butene by a simple rotation?

5. Below are structures for three carbon compounds. What is the common characteristic for each of the carbons identified by (*)?

\[
\text{CH}_3^-\text{CH}_2^-\text{CH}_3 \quad \text{CH}_3^-\text{CH} \equiv \text{CH}_2 \quad \text{CH}_3^-\text{C} \equiv \text{CH}
\]