1. *Molecular Architecture of Tetrahedral Molecules*

Introduction

This experiment asks you to visualize molecules in three dimensions with the help of a computer and the Internet so that you can begin to appreciate the structures and shapes of molecules (Ebbing/Gammon, Chapter 10). The Internet site is at

http://www.hmco.com/college

Purpose

You will study the molecular architecture of some tetrahedral molecules by turning and twisting their molecular models. Your goal is to locate and identify precisely some of the features that cause them to be similar and some of the features that cause them to be different.

Symmetry

The spatial relationships of the atoms in a molecule are best understood in terms of the molecule's *symmetry*. Symmetry is an exact correspondence of form on opposite sides of a dividing line or an axis. For example, each of the snowflakes in Figure 1.1 has symmetry because the left side looks like the right side, and the top looks like the bottom. Our eyes and minds pick up these symmetry elements, even if we aren't trying to process what we see.

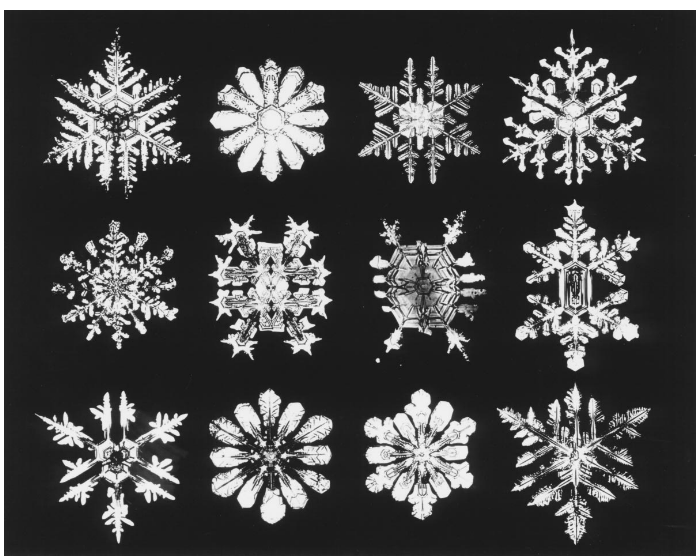


FIGURE 1.1
The symmetry of snowflakes. Photo courtesy of NOAA.

A *symmetry element* can be defined in terms of a *symmetry operation:* a rotation or reflection causing an orientation of an object (including a molecule) that is indistinguishable from its original orientation. If we had not seen the symmetry operation, we would never know that it had taken place. For example, suppose we rotate one of the snowflakes in Figure 1.1 by either 60°, 120°, 180°, 240°, 300°, or 360° around an imaginary spike driven through the snowflake's center. The result of one of these rotations is shown in Figure 1.2. Because the rotation results in an orientation of the snowflake that is indistinguishable from the snowflake's original orientation, this rotation is a symmetry operation.

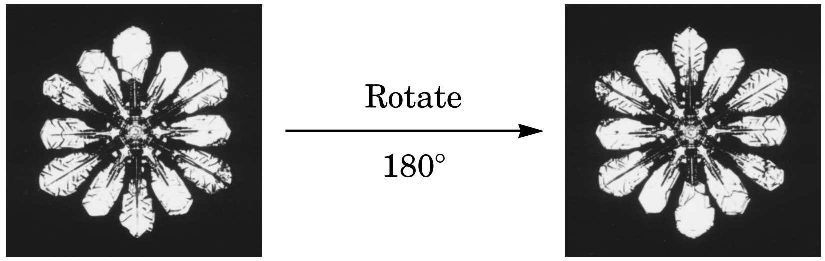


FIGURE 1.2
A rotation of 180° around an imaginary spike driven through the center of the snowflake results in an orientation of the snowflake that is indistinguishable from the snowflake's original orientation. Photo courtesy of NOAA.

Description of a tetrahedron

A *tetrahedron* is a three-dimensional solid with four identical sides, each of which is an equilateral triangle, as shown in Figure 1.3. The symmetry elements of a tetrahedron are particularly important to chemists because many molecules and parts of thousands of other molecules, including those vital to life, can be inscribed within a tetrahedron, and these molecules retain many of the symmetry elements of the tetrahedron.

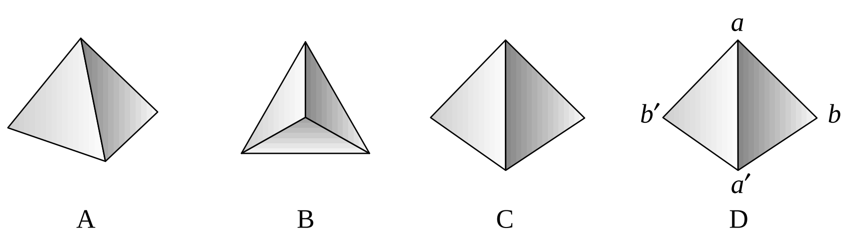


FIGURE 1.3
(A) A tetrahedron.
(B) Looking down one of the threefold axes.
(C) Looking down one of the twofold axes.
(D) A mirror plane passes through the edge marked a and a′.

Locating a threefold symmetry axis

Locate the tetrahedron at the Internet site. Using your mouse, rotate it until you have brought each of the four sides into view. Next, orient the tetrahedron until it looks like the tetrahedron shown in Figure 1.3B. You are looking down a *rotation axis*. If an imaginary spike were driven down this axis, the rotation of the tetrahedron by 120° would lead to an orientation that cannot be distinguished from the original orientation. Because *three* successive rotations of 120° will bring the tetrahedron back to its original orientation, this symmetry axis is called a *threefold axis of symmetry*. Show that it is a threefold axis by rotating the molecule.

A tetrahedron has several of these axes. Manipulate the tetrahedron at the Internet site until you find them. How many threefold axes does a tetrahedron have? Click on the answer button to check your answer.

Locating a twofold symmetry axis

Next, orient the tetrahedron at the Internet site until it looks like the tetrahedron shown in Figure 1.3C. You are looking down a *twofold rotation axis*. If an imaginary spike were driven down this axis, a rotation of the tetrahedron by 180° would lead to an orientation that cannot be distinguished from the original orientation. Two successive rotations of 180° will bring the tetrahedron back to its original orientation. Show that it is a twofold axis by rotating the molecule.

A tetrahedron has several of these axes. Manipulate the tetrahedron at the Internet site until you find them. How many twofold axes does a tetrahedron have? Click on the answer button to check your answer.

Locating a mirror plane of symmetry

Imagine that you place an upright two-sided mirror on the edge of the tetrahedron shown in Figure 1.3D. This edge is marked a and a′. As you look into the right side of the mirror, you will see that the reflection of the corner marked b is exactly where the corner b′ would appear if the mirror were not in the way. The same thing happens on the other side of the mirror. This is a *mirror plane of symmetry*. A tetrahedron has several of these planes. Manipulate the tetrahedron at the Internet site until you find them. How many of these planes does a tetrahedron have? Click on the answer button to check your answer.

Molecules can retain some tetrahedral symmetry elements

Certain molecules can be inscribed within a tetrahedron. Three examples are shown in Figure 1.4. Molecules such as these retain many of the symmetry elements of a tetrahedron. Go to the Procedure section of this experiment, search for symmetry in some molecules that can be inscribed within a tetrahedron, record your results, and then return here for additional information about symmetry.

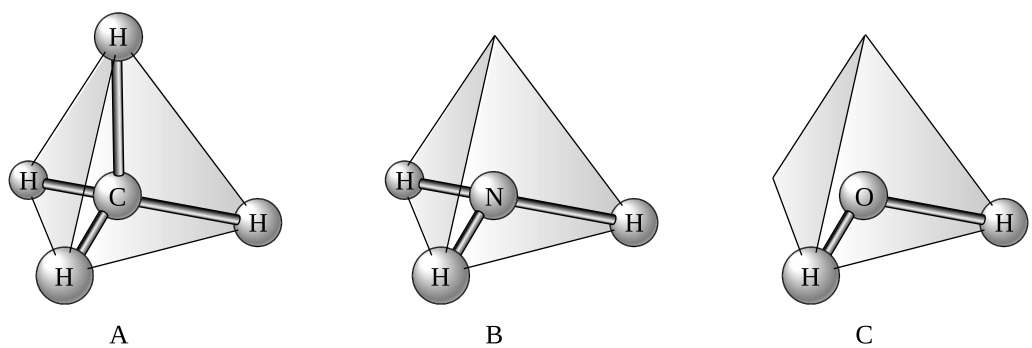
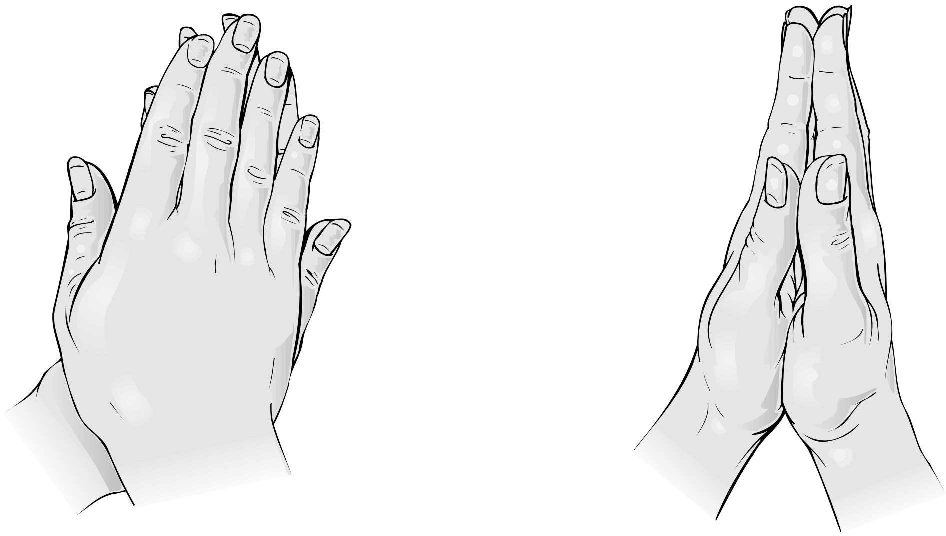


FIGURE 1.4
Tetrahedra containing molecules of (A) CH_4, (B) NH_3, and (C) H_2O.

Finding chiral objects

Put your right hand over your left hand with the back of each hand facing your eyes. Notice that your right hand is *not* superimposed on your left hand (Figure 1.5A). The word *superimposed* means merged in space so that any point on one object coincides with an identical point on another object. Clearly, the fingers of one hand are oriented differently from those of your other hand. No amount of twisting or turning will allow you to superimpose your hands.



A B

FIGURE 1.5
(A) Our hands cannot be superimposed, but (B) one of them is the mirror image of the other.

Next we need to consider another aspect of your hands. Put the palms of your hands together so that the fingers of one hand coincide with the corresponding fingers of the other hand, as shown in Figure 1.5B. One hand is the *mirror image* of the other hand. An object that has a nonsuperimposable mirror image is said to be *chiral* (pronounced ki′-ral). Thus your hands are chiral.

Consider the chair, the shoe, and the ear shown as at the Internet site. Which, if any, of these objects are chiral?

Molecules can also be chiral. If a molecule is chiral, another molecule that is the nonsuperimposable mirror image of the original molecule must consist of exactly the same atoms. However, no amount of twisting or turning will convert one of these molecules into the other molecule because they are different molecules. They are said to be *isomers*, molecules with the same molecular formula but with different arrangements of the atoms. Their chiral nature leads to a special description. Because of the way in which they interact with a polarized light, they are called *optical isomers* (Ebbing/Gammon, Section 23.5). How they interact with polarized light is not important for our purposes, but you can read about it in the textbook.

Although chiral molecules are often prepared by chemists in laboratories, many different molecules that occur in nature are also chiral. For example, amino acids, the building blocks of proteins, are chiral. Even though a pair of chiral molecules contains the same atoms, they may taste or smell differently. For example, one optical isomer of the amino acid, isoleucine, tastes sweet, but the other isomer is bitter. These differences occur because the molecules of the living system that detect them are chiral themselves.

Procedure

Getting started

1. Return to the Internet site.

Searching for symmetry in molecules

1. Consider the molecular models of CH_4, CH_3Cl, CH_2Cl_2, CH_2BrCl, $CHCl_3$, CCl_4, and CHBrClF that are shown at the Internet site. Manipulate them

using your mouse and answer the following questions. Record your answers in the table provided at the Internet site.

2. How many threefold axes, if any, does each molecule have? Record your answer.
3. How many twofold axes, if any, does each molecule have? Record your answer.
4. How many mirror planes of symmetry, if any, does each molecule have? Record your answer.
5. Even molecular models of NH_3 and H_2O can be inscribed within a tetrahedron, as shown in Figure 1.4. You will also find pictures of each of these models at the Internet site. Manipulate them using your mouse and answer the following questions.
6. How many threefold axes, if any, does each molecule have? Record your answer.
7. How many twofold axes, if any, does each molecule have? Record your answer.
8. How many mirror planes of symmetry, if any, does each molecule have? Record your answer.

Searching for chiral molecules

1. Look at the models of CH_4, CH_3Cl, CH_2Cl_2, CH_2BrCl, $CHCl_3$, CCl_4, and CHBrClF again. For each of these models you will find an image that is fixed and another one that you can manipulate.
2. Using the mouse, rotate that image until it is the mirror image of the other one. Which molecule, if any, is chiral? Record your answers in the table provided at the Internet site.

Molecular Architecture of Tetrahedral Molecules

Date:	....	Student name:	....
Course:	....	Team members:	....
Section:	....		....
Instructor:	....		....

Prelaboratory assignment

1. What is the object of this experiment?

2. Define the following terms:

   a. Symmetry

   b. Symmetry operation

   c. Tetrahedron

   d. Threefold rotation axis

e. Twofold rotation axis

f. Mirror plane of symmetry

g. Chiral

h. Isomers

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Questions

1. How are the symmetries of the following molecules similar to the symmetry of CH_4? How do they differ?

   a. CH_3Cl

   b. CH_2Cl_2

   c. CH_2BrCl

   d. $CHCl_3$

   e. CCl_4

   f. CHBrClF

2. Based on your results, what is the condition for chirality in a tetrahedral molecule?

3. Platinum often forms square-planar molecules. If four different types of atoms were bonded to the platinum atom, would the molecule be chiral? Why or why not?

4. When four different atoms are bonded to a nitrogen atom, the molecule is chiral. What do you think the structure is? Explain.