1. Molecular Shapes and Structures

Objective

Models will be built according to the predictions of the VSEPR theory to illustrate the regular patterns of molecular shapes.

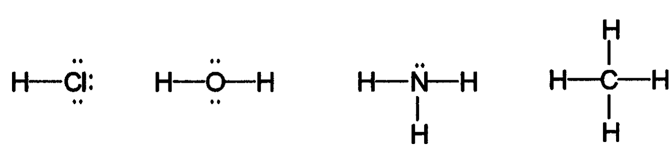
Introduction

The shapes exhibited by molecules are often very difficult for beginning chemistry students to visualize, especially since most students' training in geometry is limited to *plane* geometry. To understand the geometric shapes exhibited by molecules, a course in solid geometry, which covers the shapes of three-dimensional figures, would be more useful. In this experiment you will encounter some unfamiliar geometrical arrangements that will help you to appreciate the complexity and importance of molecular geometry.

The basic derivation and explanation of molecular shapes arises from the valence shell electron pair repulsion theory, usually known by its abbreviation, **VSEPR**. This theory considers the environment of the most central atom in a molecule and imagines first how the valence electron pairs of that central atom must be arranged in three-dimensional space around the atom to minimize repulsion among the electron pairs. The general principle is as follows: For a given number of pairs of electrons, the pairs will be oriented in three-dimensional space to be as *far away from each other as possible.* For example, if a central atom were to have only two pairs of valence electrons around it, the electron pairs would be expected to be 180° from each other.

The VSEPR theory then also considers which pairs of electron pairs around the central atom are **bonding pairs** (with atoms attached) and which are **nonbonding pairs** (lone pairs). The overall geometric shape of the molecule as a whole is determined by *how many* pairs of electrons are on the central atom and by which of those pairs are used for *bonding* to other atoms.

It is sometimes difficult for students to distinguish between the orientation of the electron pairs of the central atom of a molecule and the overall geometric shape of that molecule. A simple example that clearly makes this distinction concerns the case in which the central atom of the molecule has four valence electron pairs. Consider the Lewis structures of the following four molecules: hydrogen chloride, HCl; water, H_2O; ammonia, NH_3; and methane, CH_4.



The central atom in each of these molecules is surrounded by four pairs of valence electrons. According to the VSEPR theory, these four pairs of electrons will be oriented in three-dimensional space to be as far away from each other as possible. The four pairs of electrons point to the corners of the geometrical figure known as a **tetrahedron**. The four pairs of electrons are said to be tetrahedrally oriented, and are separated by angles of approximately 109.5°.

However, three of the molecules shown are *not* tetrahedral in *overall shape,* because some of the valence electron pairs in the HCl, H_2O, and NH_3 molecules are not *bonding* pairs. The angular position of the bonding pairs (and hence the overall shape of the molecule) is determined by the *total* number of valence electron pairs on the central atom, but the nonbonding electron pairs are *not* included in the description of the molecules' overall shape. For example, the HCl molecule could hardly be said to be tetrahedral in shape, since there are only two atoms in the molecule. HCl is linear even though the valence electron pairs of the chlorine atom are tetrahedrally oriented. Similarly the H_2O molecule cannot be tetrahedral. Water is said to be *V*-shaped (bent, or nonlinear), with the nonlinear shape a result of the tetrahedral orientation of the valence electron pairs of oxygen. Ammonia's overall shape is said to be that of a trigonal (triangular) pyramid. Of the four molecules used as examples, only methane, CH_4, has both tetrahedrally oriented valence electron pairs and an overall geometric shape that can be described as tetrahedral (since all four pairs of electrons about the central atom are bonding pairs).

During this experiment, your instructor will construct a large-scale demonstration model of each of the molecular structures to be studied. At your desk, you will construct a smaller model of the structure, measure the bond angles in the structure with a protractor, sketch the structure on paper, and suggest a real molecule that would be likely to have that structure.

SAFETY PRECAUTIONS

- **Safety glasses must be worn at all times while in the laboratory.**
- **Although this experiment does not involve any chemical substances, you should exercise normal caution while in the laboratory.**

Apparatus/Reagents Required

Demonstration molecular model kit, student model kit, protractor

Procedure

Record all data and observations directly in your notebook in ink.

Your instructor will build demonstration models of each of the shapes listed in the Table of Geometries on the next page. Examine these large-scale models; then build a similar model with the student kit.

With the protractor, measure all bond angles in your models.

Sketch a representation of the models, and indicate the measured bond angles. Your sketches do not have to be fine artwork, but the overall shape of the molecule, as well as the position of all electron pairs on the central atom (both bonding and nonbonding), must be clear.

For each structure you build and sketch, use your textbook to suggest a real molecule that would be expected to have that shape, based on its Lewis dot electron structure. (Give the Lewis dot formula for each of the molecules you suggest.)

Table of Geometries

	No. Valence pairs on central atom	*Arrangement of valence pairs*	*No. Bonding pairs on central atom*	*Molecular shape*	*Type formula*
(a)	2	linear	2	linear	AB_2
(b)	3	trigonal planar	1	linear	—
(c)	3	trigonal planar	2	bent	—
(d)	3	trigonal planar	3	trigonal planar	AB_3
(e)	4	tetrahedral	1	linear	AB
(f)	4	tetrahedral	2	bent	AB_2
(g)	4	tetrahedral	3	trigonal pyramid	AB_3
(h)	4	tetrahedral	4	tetrahedral	AB_4
(i)	5	trigonal bipyramid	1	linear	—
(j)	5	trigonal bipyramid	2	linear	AB_2
(k)	5	trigonal bipyramid	3	T-shape	AB_3
(l)	5	trigonal bipyramid	4	see-saw	AB_4
(m)	5	trigonal bipyramid	5	trigonal bipyramid	AB_5
(n)	6	octahedral	1	linear	—
(o)	6	octahedral	2	linear	—
(p)	6	octahedral	3	T-shape	—
(q)	6	octahedral	4	square planar	AB_4
(r)	6	octahedral	5	square pyramid	AB_5
(s)	6	octahedral	6	octahedral	AB_6

Note. A "—" in the *Type formula* column indicates that no simple molecules with this structure are known (or likely to be discussed in an introductory general chemistry text).

Molecular Shapes and Structures

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

Prelaboratory Questions

1. Give a short summary of the two main points of VSEPR theory.

2. Draw Lewis dot structures and predict the bond angles in the following molecules:

   PF_3

   SF_6

   ICl_5

   HBr

   H_2Se

Molecular Shapes and Structures

Date:	....	Student name:	....
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Section:	....		....
Instructor:	....		....

Results/Observations

Sketch (showing bond angles) ***Lewis dot formula***

(a)

(b)

(c)

(d)

(e)

(f)

Sketch (showing bond angles) ***Lewis dot formula***

(g)

(h)

(i)

(j)

(k)

(l)

(m)

(n)

(o)

Student name: .... Course/Section: .... Date: ....

Sketch (showing bond angles) ***Lewis dot formula***

(p)

(q)

(r)

(s)

Questions

1. The models you have built and sketched do not take into account the fact that bonding and nonbonding pairs of electrons do not repel each other to exactly the same extent; repulsion by nonbonding pairs is stronger than by bonding pairs. How will this affect the true geometric shape of the molecules you have drawn? How will the bond angles you have measured be changed by this effect? Use specific examples.

2. The models you have built also do not consider those molecules having double or triple bonds predicted for their Lewis dot structures. What effect might a second or third pair of electrons shared between two individual atoms have on the overall shape of a molecule?