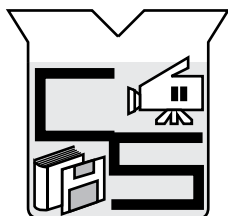
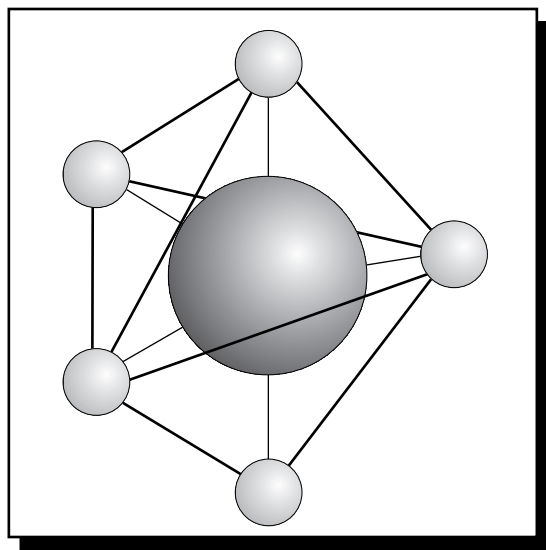


# A SourceBook Module

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*ChemSource Project Principal Investigator:  
Mary Virginia Orna, OSU  
Department of Chemistry  
College of New Rochelle  
New Rochelle, NY 10805  
Phone: (914) 654-5302  
FAX: (914) 654-5387*

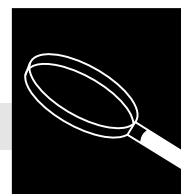


ChemSource

*Instructional Resources for Preservice and  
Inservice Chemistry Teachers*

MOLECULAR GEOMETRY

# Topic Overview



## CONTENT IN A NUTSHELL

One outstanding accomplishment of quantum mechanical theory is its success in the treatment of molecular geometry. The theory allows prediction of the directional nature of covalent bonds. Although there are many ways to handle molecular stereochemistry, the one discussed in this module is the simplest. It does not involve consideration of hybrid orbitals as in valence bond theory, nor molecular orbitals as in molecular orbital theory. The key to treating molecular geometry is understanding the spatial arrangement of atoms or groups of atoms relative to the central atom(s) in a molecule or ion through bonds with a substantial degree of covalent character.

The stereochemistry of molecules refers to the three-dimensional geometric arrangement of atoms or groups around a central atom(s). The molecular shapes are named according to the geometric shapes of the solid figures defined by the bonds between the central atom and the atoms attached to it. The most common shapes are linear, bent, trigonal planar, trigonal pyramidal, square pyramidal, tetrahedral, trigonal bipyramidal, and octahedral. Experimental methods for determining structure are diffraction methods (X-ray, electron, and neutron diffraction), spectroscopic methods (infrared, microwave, visible, ultraviolet, and Raman), resonance methods (nuclear magnetic and electron paramagnetic), and physical methods such as dipole moment and magnetic susceptibility determinations. These methods will not be considered in this module.

N. Sidgwick and H. Powell, in 1940, developed the foundation for a new, simplified theory of the stereochemistry of molecules. Based upon a survey of the then known inorganic compounds, they suggested that the electron pairs in the valence shell of a polyvalent atom (capable of forming more than one covalent bond) are always arranged in a way so as to minimize the repulsions between them. This arrangement applies to both bonding pairs (shared pairs) or nonbonding pairs (unshared or lone pairs) of electrons. Thus, two electron pairs will arrange linearly, three pairs as a planar triangle, four pairs tetrahedrally, five pairs as a trigonal bipyramid, and six pairs octahedrally. This simple theory is capable of predicting the shape of all known compounds of representative elements for which the valence shell electron pairs are all bonded to identical atoms or groups. If one or more electron pairs are unshared, or if there are two or more different kinds of bonded atoms, deviations from the regular structures are expected.

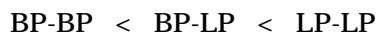
This theory of the stereochemistry of molecules is now called the Valence Shell Electron Pair Repulsion theory and is usually referred to by its acronym VSEPR. VSEPR became popular after Gillespie published an article about it in the *Journal of Chemical Education* in 1963 [Gillespie, R. J. (1963). *Journal of Chemical Education*, 40, 295]. Today it is the theory of choice in most high school chemistry texts and ranks high in college general chemistry texts. Valence bond theory, which invokes the use of hybrid orbitals, is another popular theory discussed in most textbooks.

The shape and polarity of molecules determine the type of intermolecular interaction, which, in turn, determines the properties of molecules. Generally, molecular species have low melting and boiling points, are relatively soft, may form acids or bases in solution, and are soluble or insoluble depending upon their polarity and the nature of the solvent.

Molecular geometry logically follows development of the covalent bond concept. Most chemistry teachers prefer introducing it along with or immediately after covalent bonding and polar covalent bonding. Personal preference or the organization of the student textbook may well dictate its placement. In any case, students first need to be able to write Lewis-dot structures, have an understanding of electrostatic forces, polar and nonpolar covalent bonds, and some knowledge of elementary geometric shapes.

## PLACE IN THE CURRICULUM

1. The geometric shape of a molecule can be predicted by focusing attention on the structure's central atom(s) and the mutually repulsive valence shell electron pairs surrounding it. This approach is known as the valence shell electron pair repulsion (VSEPR) approach.
2. Two kinds of valence electron pairs may populate the central atom(s) of a molecule—bonding pairs and nonbonding pairs (lone pairs). Repulsions between adjacent pairs of electrons vary in strength depending upon whether they are bond pair-bond pair (BP-BP), bond pair-lone pair (BP-LP), or lone pair-lone pair (LP-LP). The repulsion order is considered to be:



This concept helps explain the spatial distribution of electron pairs; lone pairs spontaneously arrange themselves to be as far apart as possible, bond pair-lone pairs are next, and bond pair-bond pairs are found to be the closest.

3. In the VSEPR approach, electron pairs on the central atom(s) are viewed as assuming positions around that atom that minimize electron pair-electron pair repulsions. The resulting electron pair geometry about the central atom determines the placement of the atoms bonded to the central atom(s). The resulting arrangement of bonded atoms determines the molecular geometry.
4. Molecular geometries may be classified according to the number of lone pairs and bonding pairs of electrons surrounding the central atom—*e.g.*, two bonding pairs = linear; three bonding pairs = trigonal planar; two bonding pairs and one lone pair = angular (bent); and so forth.
5. Molecules containing one or more polar covalent bonds may either be polar or nonpolar, based on the extent of the bond polarities and molecular geometry.
6. The shape and polarity (or lack of polarity) of a given molecule help determine the general properties of the substance composed of these molecules.

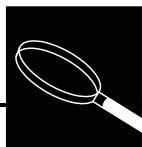
## CENTRAL CONCEPTS

Electrostatic attraction and repulsion form the basis for the bonding considered in this module; therefore, students should know that like charges repel, unlike charges attract, and electrostatic forces decrease as the inverse of the square of the separating distance.

## RELATED CONCEPTS

1. Students should be proficient at writing Lewis-dot structures of simple molecules. Check to determine whether students have retained this skill. Reteach if students are not proficient at writing Lewis-dot formulas for the kinds of molecules that are used here.
2. To visualize molecular shapes, it is necessary to be able to create three-dimensional “pictures in the mind.” Molecular models help immeasurably with this skill and should be liberally used by both student and teacher.

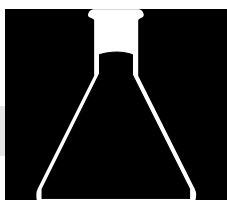
## RELATED SKILLS



## **PERFORMANCE OBJECTIVES**

After completing their study of molecular geometry, students should be able to:

1. use appropriate materials to build adequate models of simple molecules and polyatomic ions representing the shapes of these species.
2. recognize the utility of using VSEPR theory as a predictive device and use it to predict shapes of simple molecules and polyatomic ions.
3. recognize that names given to shapes of molecular and polyatomic ionic species reflect geometric shapes of polygons that would contain the species when the edge lengths are appropriate.
4. appreciate the beauty and symmetry inherent in molecular shapes.
5. use a knowledge of molecular geometry to help link topics in chemistry, related fields, societal needs and problems.
6. predict the polarity of a molecule given its shape and types of bonds.



# Concept/Skills Development

## Activity 1: Building Molecular Models

### Introduction

Most molecules in this activity obey the octet rule. Their Lewis-dot structures are straightforward. Recall that to draw the Lewis-dot structure of a molecule obeying the octet rule, eight electrons on each atom (except hydrogen and a few others) are arranged in four pairs. Each pair either participates in a covalent bond or is present as a lone pair. Some molecules may have an odd number of valence electrons or may have more than four pairs on the central atom. If any of these are encountered, your teacher will provide the necessary information.

According to the electron pair repulsion rule, the regions of high electron density (two, three, or four electron pairs) around an atom move as far apart as possible without leaving the atom. Double and triple covalent bonds are treated as a single electron pair or region of high electron density determining molecular shape. Lone pairs are considered when determining electron distribution, but only the geometric distribution of atoms dictates molecular shape.

When four electron pairs around a central atom form single bonds, the pairs can be arranged tetrahedrally. This arrangement assures that the electron pairs are as far apart as possible, satisfying the pair repulsion rule. Three electron pairs can be arranged to form a triangular plane, two to form a straight line, *etc.*

Molecular shape is determined by the positions of the atoms in a molecule, not the electrons. For a central atom with four tetrahedrally arranged electron pairs, bonding to four other atoms will yield a molecule with tetrahedral geometry; bonding to three other atoms results in a triangular pyramid with one lone pair, and bonding to two other atoms yields a bent shape with two lone pairs.

The following table summarizes these ideas.

Electron pairs	Bond pairs	Lone pairs	Example	Angle	Shape
4	4	0	$\text{CCl}_4$	$109.5^\circ$	Tetrahedral
4	3	1	$\text{PCl}_3$	$<109.5^\circ$	Pyramidal
4	2	2	$\text{SCl}_2$	$<109.5^\circ$	Bent
3	3	0	$\text{BCl}_3$	$120^\circ$	Triangular
3	2	1	$\text{SnCl}_2$	$<120^\circ$	Bent
2	2	0	$\text{BeCl}_2$	$180^\circ$	Linear

Remember that the “repulsive effect” of a double or triple bond is counted the same as that of a single electron pair.

Knowing the geometry of a molecule allows one to predict whether it is polar or nonpolar. A bond between unlike atoms is usually polar with a positive end and a negative end. The symmetry of the molecule determines polarity. Formal rules are available for this determination, but the easiest way for beginning chemistry students is to decide whether each polar bond is countered by another identical bond in the molecule.

## LABORATORY ACTIVITY: STUDENT VERSION





A diatomic molecule containing two different atoms is polar. Examples are HF, CO, and ICl.  $N_2$  and  $O_2$  are nonpolar since both ends of the molecules are equivalent. A polyatomic molecule may be nonpolar even if it contains polar bonds because, in such cases, the polar bonds are counteracting each other.  $CO_2$  and  $CH_4$  are nonpolar because of this geometric (symmetrical arrangement) effect.

Ball-and-stick models will be used to represent the shapes of molecules in this activity. Several molecular models will be built. The molecular formulas, the Lewis-dot structures, sketches of the molecules, the names of the molecular shapes, the approximate bond angles, and the polarities will be recorded in a data table.

### **Purpose**

To predict shapes, bond angles, and polarities of some molecules and to build models of these molecules confirming the predictions.

### **Safety**

There are no unusual hazards in this activity.

### **Procedure**

1. Construct a data table having eight columns with headings as follows: molecular formula, Lewis-dot structure, number of bond pairs, number of lone pairs, molecule sketch, molecular shape, bond angle, and polarity. Use the page's long axis for the column labels. Record data for each of the assigned molecules in the data table as the procedure is followed.
2. Write the molecular formula, and draw the Lewis-dot structure for each of the following molecules:  $CH_4$ ,  $H_3O^+$ ,  $N_2$ ,  $C_2H_2$ ,  $CH_2Cl_2$ , HF,  $Cl_2$ ,  $SO_2$ ,  $CH_4O$ ,  $NH_3$ ,  $C_2H_4$ ,  $SO_4^{2-}$ ,  $H_2$ ,  $H_2O_2$ ,  $CH_2O$ ,  $CO_2$ .

The formula should be in the first column and the Lewis-dot structure in the second column.

3. Using ball-and-stick models, build a model for each of the assigned molecules after completing Step 2 above. After completing each model, take it to your teacher to be checked. Draw a sketch of each model as soon as it is checked; then complete the remaining five entries in the data table.
4. After completing your table, your teacher will give you formulas for two unfamiliar molecules. Predict the shape, bond angle, and polarity after recording the formula and the Lewis-dot structure. Take your data table to your teacher to be initialed.
5. After your teacher has initialed your predictions, build the models to confirm them.
6. Return the model sets as your teacher directs.

### **Data Analysis**

1. Did your prediction of the geometry of the unknowns prove valid? Why or why not?
2. Did your prediction of the polarity of the unknowns prove valid? Why or why not?

### Implications and Applications

1.  $\text{CO}_2$  is nonpolar, but  $\text{SO}_2$  is polar. Explain.
2. Describe the electronic similarities between  $\text{NH}_3$  and  $\text{H}_3\text{O}^+$ . These species are called isoelectronic. Why?
3. Using your data table try to write some rules of thumb that would allow predictions of molecular geometry. These rules of thumb are generalizations and should include the total number of electron pairs, the number of bonding pairs, and the number of lone pairs on the central atom. Develop a table having columns containing number of electron pairs, number of bond pairs, number of lone pairs, molecular shape, and an example. The table should summarize the rules of thumb.
4. Develop some rules of thumb to help with determining molecular polarity. These rules should be in terms of the shape of the molecule and the kinds of atoms bonded to the central atom (all alike or some different, *etc.*).
5. Relate the Lewis-dot structure to the geometry of molecules.

#### Reference

*Doing Chemistry*. (1988). Washington, DC: American Chemical Society.



**LABORATORY**  
**ACTIVITY:**  
**TEACHER**  
**NOTES**

**Activity 1: Building Molecular Models**

**Major Chemical Concept**

This activity should provide the student with additional practice in drawing Lewis-dot structures, predicting molecular shapes from these drawings using the VSEPR model, and then constructing models of these molecules using appropriate modeling materials (*e.g.*, ball-and-stick kits, or Styrofoam® spheres of various sizes and colors. Gum drops and tooth picks may be used if other materials are not available.)

**Level**

This activity may be used for students at all ability levels. With basic students use only simple molecules such as  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ , *etc.* The general student should be able to use more complex molecules at least through the tetrahedral case such as  $\text{CH}_4$ , including polyatomic ions like  $\text{SO}_4^{2-}$ , and some simple two-center molecules such as  $\text{C}_2\text{H}_2$  and  $\text{H}_2\text{O}_2$ . For the honor students all cases may be treated.

**Expected Student Background**

Students should be familiar with writing Lewis-dot structures and applying the octet rule. They should recognize simple geometric shapes such as the triangle, tetrahedron, trigonal pyramid (square, trigonal bipyramid, square-based pyramid, octahedron, *etc.*, if more complex molecules and ions are included). Finally, it is assumed that—at minimum—covalent bonding (including polar bonding) has been taught.

**Time**

Teacher preparation time is very short—about 5-10 min to set out the molecular model kits. Students should be able to finish the activity in 40-50 min. It should only require 5-10 min to complete the unknowns.

**Safety**

Read the *Safety Considerations* in the *Student Version*. There are no unusual hazards in this activity. Remind students not to throw, roll, or otherwise damage the models, and to follow routine laboratory precautions.

**Materials** (For 24 students working in pairs)

If ball-and-stick models are used, one set per student pair is required. If Styrofoam® spheres are used, it is recommended that the denser type of spheres be used since they last longer.

- 96 Styrofoam® spheres, 3-in
- 180 Styrofoam® spheres, 2-in
- 240 Pipe cleaner sections about 1-in long (or toothpicks)
- 12 Drawing compasses
- 12 Metric/English scale rulers

**Advance Preparation**

If ball-and-stick models will be used, you should make all of the models in the activity to see what is involved for the student. It is also valuable to have a reference set available for students. It would be helpful to have solid models (made of poster board, old manila folders or construction paper) of the common geometric shapes ascribed to molecules.

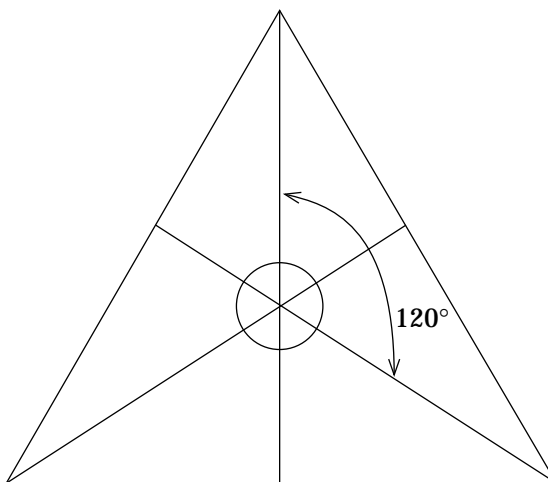
Make a list of “unknown” molecules to assign to students after they have completed the assigned list. The unknowns should consist of molecules similar to those used for the experimental procedure. For example, instead of  $\text{H}_2\text{O}$ ,  $\text{OF}_2$  could be used as an unknown. Make models of the unknowns to check for “impossible” ones. The unknowns should be easily predicted and constructed, particularly for the general and basic students.

Although ball-and-stick models are ideal for this activity, it is possible to have students build models from expanded polystyrene spheres. It is more difficult and time consuming, but not impossible. The following is a suggested procedure for this purpose.

Show students how to mark-off a sphere for the tetrahedral shape. If *Doing Chemistry* is available, use a video sequence from the videodisc B17391 to show how this may be done. The following description provides the needed steps.

Plane geometry allows one to calculate that the distance between any two tetrahedral points on the surface of a sphere is given by  $0.82 D$ , where  $D$  is the sphere's diameter. Mark any single point on the sphere. Set a compass to  $0.82 D$  for the diameter of the Styrofoam® sphere. The compass must be tight and able to hold the  $0.82 D$  distance. Place the compass point at the marked point and draw a circle on the sphere having  $0.82 D$  diameter. Mark a second point on the previously drawn circle, place the compass point there, and with the same compass setting mark two additional points on the circle. This gives four points on the sphere. Hold the sphere so that a point is at the top. Insert a toothpick vertically into the point. Then add toothpicks at the remaining three points in the same fashion. The bonds (toothpicks) should all be at the tetrahedral angle from each other.

Triangular planar templates made from cardboard should be provided. Draw an equilateral triangle large enough so that the size spheres used fit comfortably in the center. Draw a perpendicular line to each side of the triangle from the opposite vertices. The three lines should mark the center of the triangle. Using a compass set to the diameter of the sphere, place its point at the center of the triangle, draw a circle and cut it out. The spheres should now fit into the hole with the lines from the vertexes showing where toothpick bonds are to be placed (see Figure 1).



**Figure 1. Template for trigonal planar model.**

Students may use these templates to help them construct models from Styrofoam® spheres with correct angular relationships.

### Pre-Laboratory Discussion

Prior to having students build models, assign the task of completing Lewis-dot structures as homework the night before the laboratory. Briefly review drawing these structures. The Pauling-Giddings method (see *Chemical Bonding* module) is a quick and convenient way of determining how many bonds are on the central atom. The Lewis-dot structure is then easily drawn.



Demonstrate the method of making a tetrahedral template. Also show how the triangular templates are used.

If students are to use ball-and-stick models, demonstrate the correct manner of putting them together. In particular, point out that the sticks should not be jammed into the balls so tightly that removal is difficult. Show that for two center molecules, longer sticks should be used for C—C bonds and shorter ones for other bonds. Also show how springs are used to represent multiple bonds. Point out that springs are useful models for bonds since they stretch and bend as do chemical bonds. However, double and triple bonds restrict rotation between two adjacent bonded atoms. (A short piece of rubber tubing is helpful in removing jammed pegs when disassembling.)

Help students organize a data table. A simple format is shown here. Remember that there will be as many rows as there are molecules and ions plus an additional one for each unknown.

### Shapes of Covalent Molecules

Molecular formula	Lewis-dot formula	# Bond pairs	# Lone pairs	Ball/Stick model	Shape	Bond angle	Molecular polarity
CH <sub>4</sub>							
CH <sub>2</sub> Cl <sub>2</sub>							

The choice of which molecules and ions to have students model is critical. The ones given in the procedure section are suitable for general students. Some molecules may be too complex for basic students, and honor students probably need more challenge than that provided by this set. To provide more options, two additional listings are given. The first does not include molecules or ions having trigonal bipyramidal or octahedral central atoms. The second includes molecules and ions that do have trigonal bipyramidal and octahedral centers. If ordinary ball-and-stick models or Styrofoam® models are used, the models students can build will be restricted. Some ball-and-stick sets do have trigonal bipyramidal and octahedral centers. The choice of molecules and ions will depend upon what modeling material is available.

#### Molecules and Ions for Kits *not* Having Trigonal Bipyramidal and Octahedral Centers

**Set A:** CH<sub>4</sub>, NH<sub>3</sub>, NO<sub>3</sub><sup>-</sup>, H<sub>2</sub>S, C<sub>2</sub>H<sub>2</sub>, CO<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub>, BCl<sub>3</sub>, C<sub>4</sub>H<sub>10</sub>

**Set B:** CHCl<sub>3</sub>, PCl<sub>3</sub>, NH<sub>4</sub><sup>+</sup>, O<sub>3</sub>, HCO<sub>3</sub><sup>-</sup>, N<sub>3</sub><sup>-</sup>, SF<sub>2</sub>, C<sub>2</sub>F<sub>4</sub>, C<sub>4</sub>H<sub>10</sub>, SO<sub>3</sub><sup>2-</sup>

**Set C:** CCl<sub>4</sub>, ClO<sub>3</sub><sup>-</sup>, H<sub>3</sub>O<sup>+</sup>, SO<sub>2</sub>, C<sub>2</sub>Cl<sub>4</sub>, SCN<sup>-</sup>, C<sub>3</sub>H<sub>6</sub>Cl<sub>2</sub>, Cl<sub>2</sub>O, BF<sub>3</sub>, CO<sub>3</sub><sup>2-</sup>

**Set D:** CH<sub>2</sub>Cl<sub>2</sub>, PH<sub>3</sub>, ClO<sub>4</sub><sup>-</sup>, HOCl, NH<sub>2</sub>OH, SiO<sub>2</sub>, C<sub>2</sub>Cl<sub>2</sub>F<sub>2</sub>, CH<sub>3</sub>OCH<sub>3</sub>, B<sub>2</sub>H<sub>4</sub>, SO<sub>3</sub>

These sets may also be used as sources of unknowns for the activity. Exercise judgment about which of these you assign to students, particularly some of the two- and three-center species. The idea for using unknowns is that the unknowns are within the ability of the student. Ions, other than simple ones, may prove difficult for the general student.

### Molecules and Ions for Kits Having Trigonal Bipyramidal and Octahedral Centers

**Set A:** CH<sub>4</sub>, B<sub>2</sub>H<sub>4</sub>, NCl<sub>3</sub>, H<sub>3</sub>O<sup>+</sup>, PCl<sub>5</sub>, CO<sub>3</sub><sup>2-</sup>, CS<sub>2</sub>, ICl<sub>4</sub><sup>-</sup>, H<sub>2</sub>S, C<sub>4</sub>H<sub>10</sub>

**Set B:** CHCl<sub>3</sub>, BF<sub>3</sub>, ClO<sub>3</sub><sup>-</sup>, NH<sub>4</sub><sup>+</sup>, I<sub>3</sub><sup>-</sup>, SO<sub>3</sub><sup>2-</sup>, C<sub>2</sub>H<sub>2</sub>, IF<sub>5</sub>, HOCl, C<sub>3</sub>H<sub>6</sub>Cl<sub>2</sub>

**Set C:** CCl<sub>4</sub>, CH<sub>2</sub>O, BrO<sub>3</sub><sup>-</sup>, PO<sub>4</sub><sup>3-</sup>, ClF<sub>3</sub>, NO<sub>3</sub><sup>-</sup>, SCN<sup>-</sup>, SF<sub>6</sub>, SO<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>F<sub>2</sub>

**Set D:** CH<sub>2</sub>Cl<sub>2</sub>, S<sub>2</sub>O<sub>3</sub><sup>2-</sup>, PH<sub>3</sub>, ClO<sub>4</sub><sup>-</sup>, ICl<sub>3</sub>, HCO<sub>3</sub><sup>-</sup>, SiO<sub>2</sub>, SiF<sub>6</sub><sup>2-</sup>, O<sub>3</sub>, C<sub>2</sub>H<sub>3</sub>Cl<sub>3</sub>

The sets having trigonal bipyramid and octahedral shaped species should prove more challenging and useful for honor students.

### Teacher-Student Interaction

Have students bring the models to you one at a time. Grade each one individually. If the first model is incorrect, give the student a second chance to complete the structure successfully. Mark students' data tables when they bring a correct model. It is highly desirable to have a complete model set available to show students the correct shapes. This immediate reinforcement should be helpful.

When students are completing their unknowns, circulate and give them hints. You may wish to use the unknowns to assess laboratory learning.

### Anticipated Student Results

The following sample data table shows anticipated student results.

Student answers to questions asked in the data analysis section will vary. It is anticipated that most students will be successful in completing the table, particularly after receiving help during the course of the activity. More difficulty will be encountered with predicting molecular polarity than the other parts of the procedure. Students should give some reason why the predictions were either valid or invalid.

### Answers to Implications and Applications

- CO<sub>2</sub> has only two regions of high electron density and both are due to two electron pairs (double bonds). Since there are only two electron pairs determining the geometry, they will lie on a line on opposite sides of the central carbon atom. The result is a symmetrical linear model that is nonpolar. In the case of SO<sub>2</sub>, there are three regions of high electron density; a single bond, a double bond, and a nonbonding pair of electrons. The three regions of electron density force a bent shape on the molecule since the nonbonding pair repels more strongly than do the bond pairs. The bent shape gives rise to a polar molecule.
- Electronically, NH<sub>3</sub> and H<sub>3</sub>O<sup>+</sup> are identical. In such cases structures are called **isoelectronic** meaning there are equal numbers of valence electrons in both.
- Possible Rules of Thumb for predicting molecular shapes: (*NOTE: You will probably need to help students devise rules of thumb.*) Determine the number of valence electron pairs, number of bond pairs, and number of nonbonding pairs (lone pairs) through Lewis-dot structures or the Pauling-Giddings Rule (see *Chemical Bonding* module). It is convenient to represent these cases with general formulas having *A* representing the central atom, *X* representing the attached atoms, and *E* representing lone pairs of electrons. (Students may not be able to develop these; you may have to provide this information.)

*Case 1.* Two electron pairs total with two bond pairs and no lone pairs predicts a linear structure. AX<sub>2</sub>



Molecular formula	Lewis-dot formula	# Bond pairs	# Lone pairs	Ball/Stick model	Shape	Bond angle	Molecular polarity
CH <sub>4</sub>	$\begin{array}{c} \text{H} \\   \\ \text{H} : \text{C} : \text{H} \\   \\ \text{H} \end{array}$	4	0	$\begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\text{H} \\   \\ \text{H} \end{array}$	Tetrahedral	109.5°	Nonpolar
CH <sub>2</sub> Cl <sub>2</sub>	$\begin{array}{c} \text{H} \\   \\ \text{H} : \text{C} : \text{Cl} \\   \\ \text{Cl} \end{array}$	4	0	$\begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\text{Cl} \\   \\ \text{Cl} \end{array}$	Tetrahedral	109.5°	Polar
CH <sub>4</sub> O	$\begin{array}{c} \text{H} \\   \\ \text{H} : \text{C} : \ddot{\text{O}} : \text{H} \\   \\ \text{H} \end{array}$	4(C) 2(O)	0(C) 2(O)	$\begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\ddot{\text{O}}-\text{H} \\   \\ \text{H} \end{array}$	Tetrahedral at C	109.5°	Polar
H <sub>2</sub> O	$\text{H} : \ddot{\text{O}} : \text{H}$	2	2	$\text{H}-\ddot{\text{O}}-\text{H}$	Bent	109.5°	Polar
H <sub>3</sub> O <sup>+</sup>	$\begin{array}{c} \text{H} : \ddot{\text{O}} : \text{H} \\   \\ \text{H} \end{array}$	2	2	$\begin{array}{c} \text{H} - \ddot{\text{O}} - \text{H} \\   \\ \text{H} \end{array}$	Pyramidal	109.5°	Polar
HF	$\text{H} : \ddot{\text{F}} :$	1	3	$\text{H} - \ddot{\text{F}}  $	Linear	180°	Polar
NH <sub>3</sub>	$\begin{array}{c} \text{H} : \ddot{\text{N}} : \text{H} \\   \\ \text{H} \end{array}$	3	1	$\begin{array}{c} \text{H} - \ddot{\text{N}} - \text{H} \\   \\ \text{H} \end{array}$	Pyramidal	109.5°	Polar
H <sub>2</sub> O <sub>2</sub>	$\text{H} : \ddot{\text{O}} : \ddot{\text{O}} : \text{H}$	2 Each	2 Each	$\text{H} - \ddot{\text{O}} - \ddot{\text{O}} - \text{H}$	Bent	109.5°	Polar
N <sub>2</sub>	$:\text{N} :: \text{N} :$	1 Each	1 Each	$ \text{N} \equiv \text{N} $	Linear	180°	Nonpolar
Cl <sub>2</sub>	$:\ddot{\text{Cl}} : \ddot{\text{Cl}} :$	1 Each	3 Each	$ \ddot{\text{Cl}} - \ddot{\text{Cl}} $	Linear	180°	Nonpolar
C <sub>2</sub> H <sub>4</sub>	$\begin{array}{c} \text{H} \quad \quad \text{H} \\ \diagdown \quad \diagup \\ \text{C} : \text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{H} \end{array}$	3 Each	0 Each	$\begin{array}{c} \text{H} \quad \quad \text{H} \\ \diagdown \quad \diagup \\ \text{C} = \text{C} \\ \diagup \quad \diagdown \\ \text{H} \quad \quad \text{H} \end{array}$	Planar	120°	Nonpolar
CH <sub>2</sub> O	$\begin{array}{c} \text{H} \\ \diagdown \\ \text{C} : \text{O} \\ \diagup \\ \text{H} \end{array}$	3 Each	0(C) 2(O)	$\begin{array}{c} \text{H} \\ \diagdown \\ \text{C} = \text{O} \\ \diagup \\ \text{H} \end{array}$	Planar	120°	Polar
C <sub>2</sub> H <sub>2</sub>	$\text{H} : \text{C} :: \text{C} : \text{H}$	2 Each	0 Each	$\text{H} - \text{C} \equiv \text{C} - \text{H}$	Linear	180°	Nonpolar
SO <sub>2</sub>	$\begin{array}{c} \quad \quad \ddot{\text{S}} \\ \diagdown \quad \diagup \\ \text{O} : \quad \text{O} \end{array}$	3(S)	1(S)	$\begin{array}{c} \quad \quad \ddot{\text{S}} \\ \diagdown \quad \diagup \\ \text{O} = \quad \text{O} \end{array}$	Bent	120°	Polar
CO <sub>2</sub>	$\ddot{\text{O}} :: \text{C} :: \text{O} \cdot$	2(C) 1(O) Each	0(C) 2(O) Each	$\ddot{\text{O}} = \text{C} = \ddot{\text{O}}$	Linear	180°	Nonpolar
SO <sub>4</sub> <sup>2-</sup>	$\begin{array}{c} \quad \quad \ddot{\text{O}} \\ \diagdown \quad \diagup \\ \ddot{\text{O}} : \text{S} : \ddot{\text{O}} \\ \diagup \quad \diagdown \\ \quad \quad \ddot{\text{O}} \end{array}$	4(S) 1(O) Each	0(S) 3(O) Each	$\begin{array}{c} \quad \quad \ddot{\text{O}} \\ \diagdown \quad \diagup \\ \ddot{\text{O}} - \text{S} - \ddot{\text{O}} \\ \diagup \quad \diagdown \\ \quad \quad \ddot{\text{O}} \end{array}$	Tetrahedral	109.5°	Nonpolar

- Case 2.* Three electron pairs total with three bond pairs and no lone pairs predicts a triangular planar (or trigonal planar) structure.  $AX_3$ .
- Case 3.* Three electron pairs total with two bond pairs and one lone pair predicts a bent (or angular) structure.  $AX_2E$ .
- Case 4.* Four electron pairs total with four bond pairs and no lone pairs predicts a tetrahedral structure.  $AX_4$ .
- Case 5.* Four electron pairs total with three bond pairs and one lone pair predicts a trigonal pyramidal structure.  $AX_3E$ .
- Case 6.* Four electron pairs total with two bond pairs and two lone pairs predicts a bent structure.  $AX_2E_2$ .
- Case 7.* Four electron pairs total with one bond pair and three lone pairs predicts a linear structure. (This is a trivial case since with only two atoms present, the resulting structure must be linear.)  $AXE_3$ .
4. Possible Rules of Thumb to predict molecular polarity. (*NOTE: You will probably need to help students develop these rules of thumb.*)
- Determine whether polar bonds are present by calculating the electronegativity difference between the two atoms. If no, then the molecule must be nonpolar. If yes, the molecule *may* be polar.
- Case 1.* Linear molecules with identical atoms attached to the central atom will always be nonpolar, *e.g.*,  $BeF_2$ .
- Case 2.* Triangular planar molecules with identical atoms attached to the central atom will always be nonpolar, *e.g.*,  $BCl_3$ .
- Case 3.* Bent molecules with two bond pairs and one lone pair will always be polar, *e.g.*,  $SnCl_2$ .
- Case 4.* Tetrahedral molecules with four bond pairs and with four identical atoms bonded to the central atom will be nonpolar, *e.g.*,  $CCl_4$ . If one, two, or three of the bonded atoms are different from the others, the molecule will be polar, *e.g.*,  $CHCl_3$ .
- Case 5.* Trigonal pyramidal molecules with three bond pairs and one lone pair will be polar, *e.g.*,  $NH_3$ .
- Case 6.* Bent molecules with two bond pairs and two lone pairs will be polar, *e.g.*,  $OF_2$ .
- Case 7.* Linear molecules with one bond pair and three lone pairs will be polar, *e.g.*,  $HCl$ .
5. The Lewis-dot structure provides the number of electron pairs surrounding the central atom making it possible to determine the number of bond pairs and lone pairs. This information is needed to predict the molecular structure.

## Post-Laboratory Discussion

During the post-laboratory discussion, concentrate on helping students develop and apply the rules of thumb. These rules are not necessarily obvious, so have a “generic set” of molecular shapes available to use with the discussion. Model sets should also be available so students can construct the models and better follow development of the VSEPR concept. This exercise should serve well as a major teaching activity for the module.

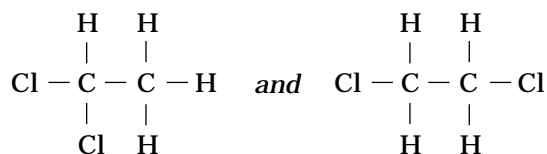
A generic set of molecular models may be constructed from 1- and 2-in polystyrene spheres, 1/8-in dowels, and some glue. These models prove helpful in demonstrating the shapes being considered.



One point that should be made in post-laboratory discussion is that the shapes shown by the models are idealized. Actual molecules deviate somewhat from the ideal shapes, particularly if there are different kinds of atoms bonded to the central atom (as in  $\text{CHCl}_3$ ). A distorted tetrahedron would be the result since the hydrogen atom is smaller than the chlorine atoms.

### Extensions

1. For some molecules with a given molecular structure it is possible to satisfy the octet rule with two, three, or more arrangements of the atoms. For example, it is possible to draw two different Lewis-dot structures for  $\text{C}_2\text{H}_4\text{Cl}_2$ .



In the first case both chlorine atoms are bonded to the same carbon atom, while in the latter case one chlorine atom is bonded to each carbon atom. Since there is free rotation about the  $\text{C}-\text{C}$  bond, the other three bonding positions on each  $\text{C}$  atom are equivalent. Such molecules with the same formula but different atomic arrangements are called isomers (see *Organic Chemistry* module). Find all the isomers of  $\text{C}_2\text{H}_2\text{Cl}_2$ . Draw the Lewis-dot structure, build the model, and describe the geometry and polarity of each isomer (three are possible). Note that the double bond between carbon atoms prevents free rotation, making the other bonding positions on the carbon atoms nonequivalent. These structural isomers are important in organic chemistry.

2. Stereoisomerism is another type of isomerism. Draw the Lewis-dot structures, build the models, and describe the geometry and polarity of each isomer of bromochlorofluoromethane,  $\text{CHBrClF}$ . If necessary, use a mirror with the first model you build to see how to build the second. Note that the difference is the same as the difference between your left hand and right hand; the structures are mirror images of each other. Stereoisomers displaying the phenomenon of “handedness” are important in organic and biochemistry.
3. It is possible for the same structure to have two or more different conformations. Different arrangements of atoms and groups in a molecule are possible as a consequence of rotation about single bonds. For example, cyclohexane,  $\text{C}_6\text{H}_{12}$ , exists in two conformations, the chair conformation and the boat conformation. Build a ball-and-stick model of cyclohexane (a ring compound) and try to form the two conformations. The difference is best seen when the models are viewed from the side (for honor students).

### Assessing Laboratory Learning

1. The unknown given to students is a good way to assess laboratory learning. Students who are successful have probably learned what was intended, provided that all unknowns are equally difficult. Assigning unknowns to be built from model kits can also be done after students have completed the activity as a form of “laboratory practical” test. Students should be required to draw the Lewis-dot structure, predict the shape and polarity, and then confirm the shape by building a model.
2. Students can be given several molecules or ions and asked to draw the Lewis-dot structures and to predict the shape and polarity as a paper and pencil test. In this type of assessment, both molecular and ionic species should be used.

CAUTION: Use appropriate safety guidelines in performing demonstrations.

## DEMONSTRATIONS

### Demonstration 1: Three-Dimensional Structure of Molecules

#### Purpose

To illustrate the three dimensional shape adopted by the electron pairs surrounding the central atom in a molecule or ion.

#### Materials

9 Balloons, 10-in

6 File cards, 3" x 5", used to identify bonded atoms and lone electron pairs

Double-sided transparent tape to attach file cards to balloons

#### Procedure

1. Instruct student volunteers to blow up the balloons to the same size. Tie the balloons together into sets as follows: one set of three tied together and three sets of two tied together.
2. Display the shape of one pair of balloons. Show that they are linear. Explain to students that this arrangement is analogous to a molecule such as  $\text{BeH}_2$ .
3. Display the three balloons tied together. Note that they form a planar triangle with bond angles of  $120^\circ$ . This arrangement represents a molecule such as  $\text{BCl}_3$ .
4. Take 2 two-balloon sets and push them together to form a square planar arrangement. Mention to the students that this is one possible way to represent a molecule like  $\text{CH}_4$ . Point out that the balloons are  $90^\circ$  apart. Then push or "pop" the one set against the other so that the balloons form a three-dimensional shape. Point out that this is a tetrahedral shape and that the electrons are farther apart than in the square planar arrangement.
5. Place a 3" x 5" card on one of the balloons in the tetrahedral arrangement to represent a nonbonding electron pair. Mention that the electron pair occupies the same space as a bond, perhaps even more. Note that the resulting pyramidal structure (pretending that the balloon with the card is not seen) represents a molecule like  $\text{NH}_3$  (three electron pair bonds, one unshared pair).
6. Place another 3" x 5" card on a second balloon to represent another nonbonding pair of electrons. Note the bent, planar shape as in  $\text{H}_2\text{O}$ , which has two bonded atoms and two unshared pairs (the balloons with the cards).
7. Display the tetrahedral arrangement once again with another card in place on a third balloon. Note that there is only one bonding site available, and that the resulting molecule is again linear. This is analogous to the bonding in  $\text{HF}$ .
8. Extend the demonstration by placing five balloons together (one set of two and the set of three). The balloon pair may be twisted around the center of the balloon trio. These five form a structure called trigonal bipyramidal, such as  $\text{PCl}_5$ .
9. Place six balloons together by twisting a balloon pair around the center of the balloon tetrahedron. An octahedral structure will form. Show the eight sides or faces that are the basis for the name. An example of an octahedral molecule is  $\text{SF}_6$ .



### Remarks

This demonstration may be used either for a pre-laboratory or post-laboratory discussion for *Activity 1*, or it may be used to introduce the VSEPR concept. Ten min of teacher preparation time is needed to try the demonstration prior to performing it for students. 20-30 min are needed to perform the demonstration.

There are no particular safety hazards involved with the demonstration. Have students inflate the balloons to get them involved. Instruct them to make the balloons nearly the same size.

It is helpful to have solids in the shape of a tetrahedron, a trigonal bipyramid, and an octahedron to show the origin of names given to molecular shapes while pointing out that the orientation of electron pairs determines the overall shape of the molecule. This fact is not always obvious to students. Otherwise, little discussion is needed other than to point out what each balloon set represents.

### Reference

(Based in part on: Demonstration B25 in *Doing chemistry*. (1988). Washington, DC: American Chemical Society.)

## Demonstration 2: Polar Molecules

### Purpose

This demonstration shows typical behaviors for a polar liquid (water) and a nonpolar liquid (hexane or kerosene).

### Safety

Hexane and kerosene are toxic by ingestion or absorption through the skin. Both are highly flammable and must not be used near open flames. Safety goggles must be worn.

### Materials

2 Burets, 50- or 100-mL and clamps; ringstand

2 Beakers, 400-mL or larger

Water, 100 mL

Hexane or other nonpolar liquid (*do not use toxic or carcinogenic liquids*), 100 mL

Hard rubber or glass rod (or use plastic pen and rub with paper toweling)

Cat fur or wool or silk (cat fur or wool with rubber rod or silk with glass rod)

### Procedure

Fill two burets with two liquids, water in one and a nonpolar liquid in the other. Have a rubber rod or glass rod and the material to rub it with nearby. Open the stopcock or adjust the clamp to obtain a thin, unbroken stream flowing into a beaker. Charge a rod by rubbing it with appropriate material. Bring the charged rod near the stream of liquid and have students state what is observed. If the stream is water, then the stream will be attracted to the rod and its path changed. Repeat with the other liquid.

(An alternate procedure is to use two paper cups, two bowls or beakers, and a balloon. Use water and kerosene for the liquids. First, use a small pin to put a small hole in the center of each paper cup's bottom. Then place one of the liquids in a cup and let it slowly stream into the bowl. Rub the balloon against a wool coat or sweater (or rub it against a person's hair), and then bring it close to the liquid stream. The bending of the water stream is quite obvious. Students seem to enjoy it more when it is done this way.)

*Remarks*

About 15 min are needed to get the materials together and try the demonstration. Only about 10-15 min are required to perform the demonstration.

The demonstration is probably best used in conjunction with the activity on molecular shapes. It could be used to pose a question that may be answered in terms of the polarity of molecules. In some respects it is counterintuitive since one does not ordinarily expect the result obtained.

There are variations to this demonstration. Its placement depends upon your preference and approach. It also fits well with a consideration of chemical bonding to illustrate polar molecules. It is included here to emphasize that molecular shape is important in determining molecular polarity.

Why is one stream attracted to the charged rod? (Bassam Z. Shakhashiri *Chemical Demonstrations: a Handbook for Teachers of Chemistry*, Volume 3. The University of Wisconsin Press, 1989, 329-332. I. D. Brindle and R. H. Tomlinson, *J. Chem. Educ.* 52:382 (1975).)

Polar molecules are themselves attracted to charges. Moreover, polar molecules support dissociation. Unless purified and stored with extreme care, polar liquids tend to form conducting solutions. The charged rod causes a net separation of charges in the bulk liquid. When droplets form at the end of the stream, they have a net charge and are attracted to the rod. (Friction of moving nonpolar liquids also causes charge separation; that is why gasoline tankers that move large amounts of liquid are grounded to receptacles as fuels are pumped. Failure to ground can lead to large static electric discharges and result in explosions.)

*References*

Based in part on the demonstration "Bending a Stream of Water" in Summerlin, L., Borgford, C., and Ealy, J. (1987). *Chemical demonstrations: A sourcebook for teachers, Volume 2*. Washington, DC: American Chemical Society. CHEM STUDY film (video) on "Shapes and Polarities of Molecules" has a lengthy version of this demonstration (see *Media*).

Alternate procedure suggested by Doris Kolb.



### Demonstration 3: Demonstration Models

#### *Purpose*

To build a set of demonstration models that show the “ideal” geometry (shapes) for the molecular shapes taught using VSEPR theory.

#### *Materials*

15 Styrofoam® spheres, 76-mm diameter  
40 Styrofoam® spheres, 50-mm diameter  
8 Egg-shaped Styrofoam® figures, about 76- x 50- to 70-mm (lone pairs)  
9 Feet 3/16-in diameter Dowel stick  
Suitable glue for gluing Styrofoam® to wood  
Suitable device for measuring and marking angles on the 2” spheres  
Ice pick or carpenter’s awl or some other sharp-pointed tool  
Drawing compass and poster board  
Styroglue® (craft or hobby store)

#### *Procedure*

Use these models when introducing students to VSEPR theory. It shows students concrete examples of a rather abstract idea. Keep in mind that the shapes constructed are idealized. Begin with the simplest case,  $AX_3$ , and explain why that shape is assumed by the molecule in terms of minimizing electrostatic repulsion between the three regions of high electron density on the central atom. Continue in this fashion until all the molecular shapes that will be used by the class have been discussed. This may extend through the tetrahedral case, or may include all the cases, depending upon the ability of the class. Please note that the trigonal bipyramid is not intuitively the shape of choice for five electron pairs on the central atom; a square pyramidal arrangement with all angles equal to  $90^\circ$  seems more likely to students. A somewhat sophisticated geometric argument is required to illustrate that the trigonal bipyramidal shape minimizes repulsion between electron pairs.

#### *Remarks*

Building a set of models requires a substantial investment of time; therefore, the task must be started well in advance. However, once built, the models can be used again and again. An alternative is to purchase a demonstration-sized set of snap-together molecular models. Most major science suppliers have these available, but they are expensive.

Models are useful from the consideration of molecular geometry through the remainder of the course whenever models are needed.

1. To measure and mark angles on the Styrofoam® spheres, use the technique described in *Advance Preparation for Activity 1*. In addition to a triangular template to mark  $120^\circ$  angles, one to mark  $90^\circ$  angles is also needed. Both templates need a circular hole to fit the 76 mm spheres. The ice pick or carpenter’s awl are convenient to make holes for the dowel stick connectors.
2. Careful selection of glue is necessary since many modeling glues will dissolve polystyrene. Elmer’s™ glue works well if time is not important. Hobby shops and crafts shops will probably have an appropriate glue.

3. Egg-shaped Styrofoam® objects are available in hobby and crafts stores, particularly around Easter. These work well to represent nonbonding electron pairs.
4. Although it is not necessary, painting the spheres and egg shaped objects is a nice touch. Latex and acrylic based paints work well. Painting should be done prior to making the models.
5. Solicit volunteers from classes to help with the construction of models. This speeds up the process considerably. After school, during lunch or activity periods are convenient times to do this.
6. The only hazard in building the models is that some people are allergic to glues of one sort or another.

### Demonstration 4: Two-Dimensional Analogy of Molecular Geometry

#### *Purpose*

To demonstrate a magnetically driven, two-dimensional analogue of electron pair repulsion in molecules.

#### *Materials*

Package of stainless steel sewing needles, 4-5 cm long  
Strong permanent magnet or electromagnetic  
Pyrex™ or clear plastic cylinder, 15-20 cm diameter  
Bell wire (enough plastic coated copper wire to make 6-10 coils around a glass cylinder)  
6-V Dry cell battery or direct current power supply that can produce 6 V.  
Approximately 1 doz. Styrofoam® discs, 5/8-in diameter, cut from beverage cups or other sources (packing material pieces may be used).  
Wax

#### *Procedure*

Tell the class that they will be shown a two-dimensional analogy to molecular geometry. Then after connecting the direct current source to the wire coils, begin with one magnetized needle assembly in the water. It should stay near the center of the dish. Add additional needle assemblies, one at a time, and note the orientation about the first needle assembly. This behavior is analogous to that of atoms bonding with a central atom to produce a particular geometry.

#### *Remarks*

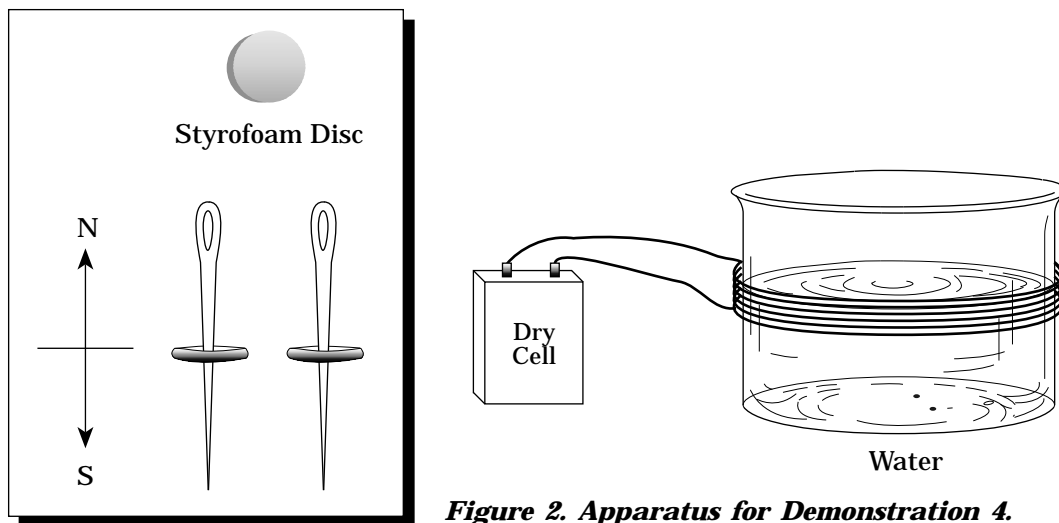
This demonstration makes more sense if it is presented *after* students' first introduction to VSEPR theory.

The demonstration may be performed in 15-20 min depending upon the points made to the class. Teacher preparation time is considerable. If materials are readily available, the preparation will take about one hour.

A clear Pyrex™ glass cylinder or clear plastic cylinder 15-20 cm in diameter works well for this demonstration. After waxing the inside of the dish above and below the wire turns, fill it with water to the middle of the wire coils. Magnetize about 12 needles with all points in the same direction on one pole of a strong magnet. Prepare each needle assembly by inserting the point of a needle through one of the Styrofoam® discs. Place one magnetized needle assembly in the water and attach the two ends of the wire to the current source. If the needle moves toward the outside of the dish, reverse the polarity of the



wire leads. The demonstration may be performed on an overhead projector by using a shallow dish (see Figure 2 for details of the setup).



**Figure 2. Apparatus for Demonstration 4.**

*Reference*

Based on a demonstration presented by A.C. Breyer at CHEM ED 77, Beaver College, Glenside, PA 19038.

**GROUP AND DISCUSSION ACTIVITIES**

**Key Questions**

1. **What are the basic assumptions of the Valence Shell Electron Pair Repulsion model of molecular structure?** *[Student answers will probably vary considerably. The answer given below is generally not published in introductory chemistry texts with the same amount of detail, and students' answers will probably give some vague idea about the first two of these. Typically, one high school chemistry textbook says that VSEPR theory states that because electron pairs repel, molecules adjust their shape so that the valence electron pairs are as far apart as possible. There are just four basic assumptions. One assumption is that all of the valence shell electron pairs of the central atom are about the same distance from the atom's nucleus. This is strictly exact for two, three, four, and six electron pairs that are bonding the central atom to a set of identical atoms or groups. The second is that electrons have the ability to rearrange themselves. The pairs arrange themselves so as to minimize repulsion. To do so they behave as if they are on the surface of a sphere behaving under an appropriate force law. This gives the most probable arrangement. The third assumption is that multiple bonds (double or triple covalent bonds) have about the same effect on molecular geometry as do single bonds. The final assumption is that nonbonding pairs occupy a larger volume of space than do bond pairs; hence they repel more strongly. Calculations based on electrostatic principles and the Pauli exclusion principle substantiate these assumptions.]*
2. **Based on VSEPR theory, what are the possible molecular shapes when representative elements form molecules?** *[See the Appendix for complete details in tabular form.]*

3. **Predict the molecular shapes of the following and predict whether each species is polar or nonpolar.** (a)  $\text{PH}_3$ , (b)  $\text{PH}_4^+$ , (c)  $\text{SO}_3^{2-}$ , (d)  $\text{BrO}_3^-$ , (e)  $\text{CaH}_2$ , (f)  $\text{H}_2\text{S}$ , (g)  $\text{PO}_4^{3-}$ , (h)  $\text{SiF}_4$ , (i)  $\text{SO}_3$ , (j)  $\text{ClO}_4^-$ , (k)  $\text{Cl}_2\text{O}$ , (l)  $\text{N}_2$ , (m)  $\text{CCl}_4$ , (n)  $\text{NCl}_3$ , (o)  $\text{HCN}$ , (p)  $\text{PCl}_5$ , (q)  $\text{SF}_6$ , (r)  $\text{Co}(\text{NH}_3)_6^{2+}$ . (HINT: First determine the number of bonds on the central atom.) [General students should be able to answer (a) through (o), and honor students should be able to answer all of them. (a) trigonal pyramidal; polar (b) tetrahedral; nonpolar (c) trigonal pyramidal; polar (d) trigonal pyramidal; polar (e) linear; nonpolar (f) angular (bent); polar (g) tetrahedral; nonpolar (h) tetrahedral; nonpolar (i) triangular planar; nonpolar (j) tetrahedral; nonpolar (k) bent (angular); polar (l) linear; nonpolar (m) tetrahedral; nonpolar (n) trigonal pyramidal; polar (o) linear; polar (p) trigonal bipyramidal; nonpolar (q) octahedral; nonpolar (r) octahedral; nonpolar.]
4. **Phosphorus forms  $\text{PCl}_3$  and  $\text{PCl}_5$ . Nitrogen forms  $\text{NCl}_3$  but not  $\text{NCl}_5$ . Explain why  $\text{NCl}_5$  does not exist.** [Due to the small atomic radii of Period 2 elements (see Periodicity module), the maximum coordination number (CN) of any element in Period 2 is four. Thus, it is not possible for  $\text{NCl}_5$  to exist. Furthermore, nitrogen does not have any low-lying d orbitals available to form the required bonds. Phosphorus can utilize the 3d orbitals in forming the extra bonds.]
5. **Explain what is meant by a polar molecule.** [A polar molecule is one in which there is an asymmetric distribution of charge. Due to both differences in electronegativity between the atoms forming bonds and the shape of the species, electron density is not evenly distributed, resulting in apparent separation of charge.]
6. **Must a polar molecule contain a polar bond? Explain.** [Yes. Otherwise, there will be no permanent separation of charge.]
7. **The bond angles in  $\text{NH}_3$ ,  $\text{H}_2\text{O}$ , and  $\text{CH}_4$  are  $107^\circ$ ,  $104.5^\circ$ , and  $109.5^\circ$ , respectively. How can these values be justified if the central atom in each has four electron pairs in its valence structure?** [ $\text{CH}_4$  has four bond pairs and no lone pairs,  $\text{H}_2\text{O}$  has two bond pairs and two lone pairs,  $\text{NH}_3$  has three bond pairs and one lone pair. Lone pairs exert a greater repulsion than do bond pairs. As the number of lone pairs increases, the bond angle of the bond pairs decreases.]
8. **Challenge question: predict the shapes and polarities of the following molecules and/or ions.** (a)  $\text{BeH}_2$ , (b)  $\text{BCl}_3$ , (c)  $\text{SiH}_4$ , (d)  $\text{Sb}(\text{OH})_6^-$ , (e)  $\text{CO}_3^{2-}$ , (f)  $\text{Al}(\text{H}_2\text{O})_6^{3+}$ , (g)  $\text{SbCl}_5$ , (h)  $\text{TeCl}_4$ , (i)  $\text{BrF}_3$ , (j)  $\text{BrF}_5$ , (k)  $\text{NO}_2^-$ , (l)  $\text{N}_2\text{O}$ . [(a) linear; nonpolar, (b) triangular planar; nonpolar, (c) tetrahedral; nonpolar, (d) octahedral; nonpolar, (e) triangular planar; nonpolar, (f) octahedral; nonpolar, (g) trigonal bipyramidal; nonpolar, (h) distorted tetrahedron (seesaw); polar, (i) T-shaped; polar, (j) square pyramidal; polar, (k) bent; polar, (l) linear; polar.]

### Counterintuitive Examples and Discrepant Events

1. Distribution of four electron pairs about a central atom leads to two possible structures, the square plane and the tetrahedron. Since the square planar structure is two-dimensional and easy to visualize, students often think that this structure is optimal for minimal repulsion. They must see models in order to understand that the tetrahedral angle exceeds  $90^\circ$ .



2. Predicting the geometry of five electron pairs is counterintuitive. Experiment shows that five electron pairs lead to a trigonal bipyramidal structure. Such a structure has two different angles; the trend in equivalent angles is broken. Analysis shows that for regular, isogonal polyhedra, only the tetrahedron, the octahedron, the icosahedron, the cube, and the dodecahedron are possible. The trigonal bipyramid is not. It is impossible to distribute five equivalent vertices into a convex polyhedron with five equivalent angles between its center and its vertices. The nonequivalent positions for coordination number = 5 lead to another counterintuitive example. All lone pairs are found in the equatorial positions ( $120^\circ$  separation) rather than the axial positions ( $180^\circ$  separation; see *Appendix*).
3. A third counterintuitive example is the fact that distribution of six electron pairs around a central atom can lead to a square planar molecular shape. A good example is  $\text{XeF}_4$  (see *Appendix*).

## Analogies and Metaphors

### What's in a name?

1. The word "polar" is associated with ice caps, bears and regions of the earth. Few people, except chemists, think in terms of polar molecules.
2. What if polar molecules did not exist? How would our lives be affected if water were not a polar molecule? Consider the hydrogen compounds of some Period 2 elements:  $\text{BH}_3$ ,  $\text{CH}_4$ ,  $\text{NH}_3$ ,  $\text{OH}_2$  and  $\text{FH}$ . Of these five compounds,  $\text{OH}_2$  is the only liquid at room temperature.  $\text{OH}_2$  also has the highest boiling point, highest heat capacity and the lowest density in the solid state. All of these unusual properties are due to the polar nature of  $\text{OH}_2$ ; if  $\text{OH}_2$  behaved like its periodic analogs, carried to its ultimate conclusion, life as we know it would not exist [see Speakman, J. C. (1966). *Molecules*].

## Pictures in the Mind

1. Molecular models are visual aids commonly used by chemistry teachers. To provide students with a hands-on activity that enhances their visualization of the three-dimensional arrangement of bond angles in common molecules, the following activity is recommended.

To illustrate the spatial distribution of electron pairs achieving maximum spatial separation, use a piece of Play-Doh™ or modeling clay and four toothpicks per student. After materials have been distributed, instruct students to place two toothpicks in the Play-Doh™ so that they are separated as far apart as possible. The students will quickly realize that toothpicks placed at a  $180^\circ$  angle produce this result. Have them repeat with three and then four toothpicks. It is *not* recommended that this activity be extended to the trigonal bipyramidal structure since it is a counterintuitive arrangement (see *Counterintuitive Examples* and *Discrepant Events*). The activity might work with six toothpicks to produce an octahedral arrangement. (This idea was suggested by K. Elsen, Mount Mary College, Milwaukee, WI.)

2. Constructing models of polyhedra constitutes an excellent group activity or homework exercise. Templates can be reproduced and assembled with minimal materials: Old manila folders, scissors, glue, and transparent tape. The activities that follow work well if done as part of the pre-laboratory exercise.

**Tetrahedron** Using a drawing compass, draw a circle with a 10-cm radius close to the edge of an 8 1/2 x 11" piece of heavy paper. Maintaining the same radius, place the compass point at Point A (Figure 3), and draw an arc that intersects the circle at Point B. Place the compass point on Point B and repeat to intersect the circle at Point C; repeat the procedure for Point D. Connect Points A, B, C and D with the center of the circle (E) as shown in Figure 4a. Then extend the lines A-B and D-C as shown in Figure 4b, and add tabs for gluing.

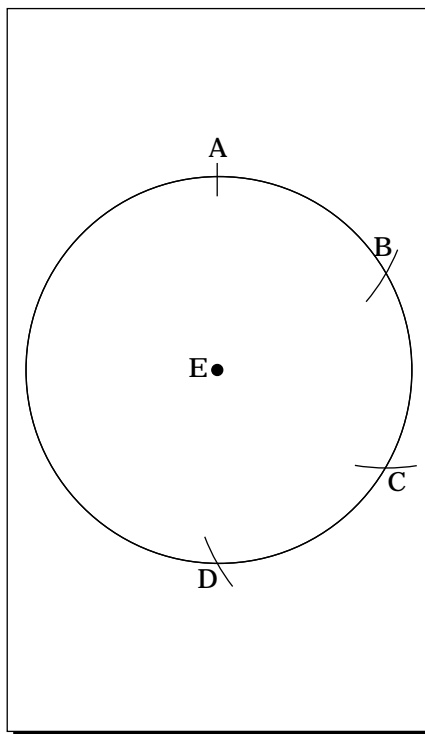


Figure 3. Arcing a circle.

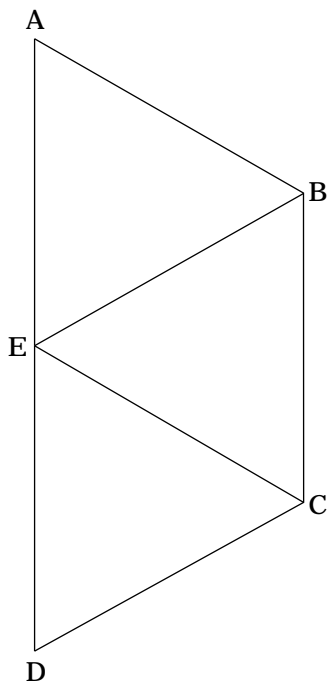


Figure 4a. Connecting points with center of circle.

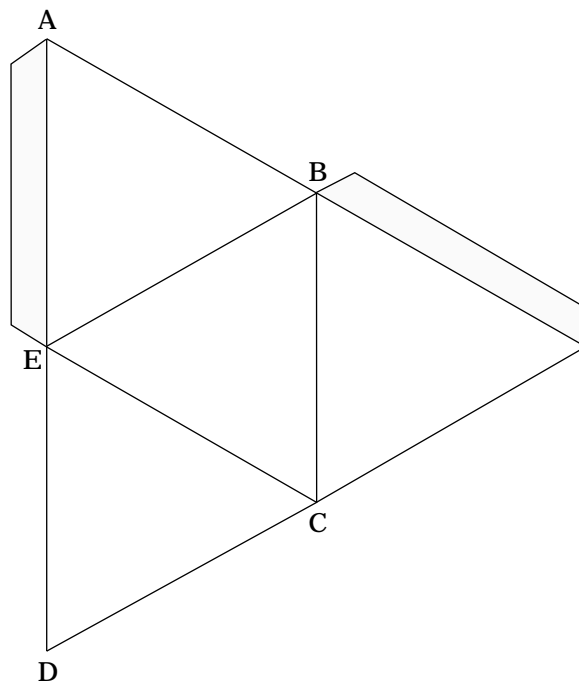
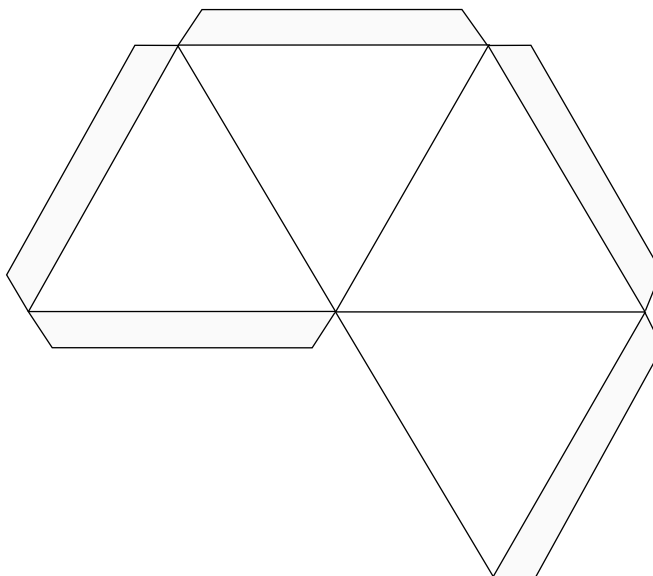


Figure 4b. Adding tabs.



**Octahedron** To form an octahedron, reproduce the template provided in the *Appendix* and assemble it. Alternatively, use the same method as for the tetrahedron, but lay off *four* radii around the circle. Connect the radii as shown in Figure 5.

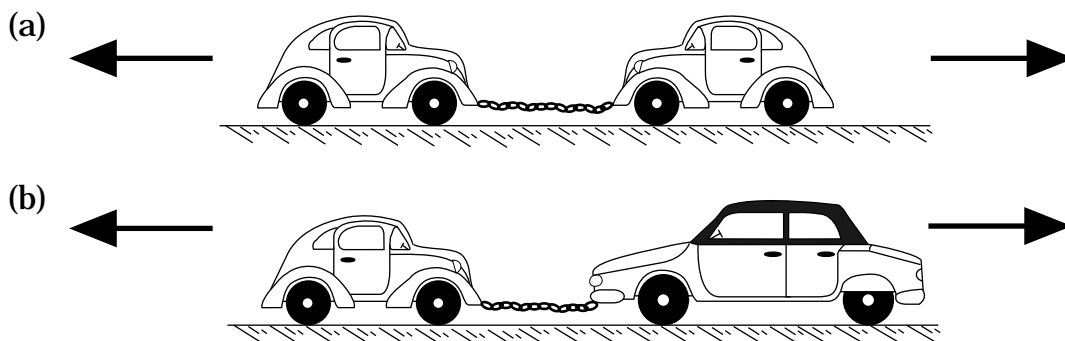


**Figure 5. Connecting radii.**

Make a second half like the first half. After being certain that the tabs are folded flat, glue the two halves together, putting the two square based pyramids base to base.

**Trigonal Bipyramid** To form a trigonal bipyramidal structure, glue two tetrahedra base to base.

3. Polar covalent bonding in a linear molecule. Which of these sketches can be compared to a polar covalent bond?



**Figure 6. Polarity analogy.**

**TIPS FOR THE TEACHER** **Language of Chemistry**

The following is a minimal glossary of terms for molecular geometry:

**bond pair** bonding electron pair on the central atom (frequently referred to as X in generic formulas).

**coordination number** number of neighboring groups in contact with a central atom.

**electronic geometry** arrangement of bonding and nonbonding electron pairs around a central atom.

**lone pair** nonbonding electron pair on the central atom (frequently represented as E in generic formulas).

**molecular geometry** shape of a molecule resulting from covalent bonding of ligands around a central atom. Molecular geometry is not synonymous with electronic geometry (see *Common Misconceptions* for a detailed discussion).

**polygon** plane form made up of a number of straight sides.

**polyhedron** solid formed by a number of polygonal faces.

**polytope** general term for a solid figure like a polyhedron.

**stereochemistry** study of the geometric arrangement of atoms or groups of atoms around the central atom(s) in a molecule or polyatomic ion.

**steric number** number of bond pairs and lone pairs of electrons surrounding the central atom in a molecule.

## Pattern Recognition

Refer to *Answers to Implications and Applications for Activity 1* for some fairly simple rules of thumb (ROTs) to help students predict both molecular geometry and molecular polarity.

## Common Student Misconceptions

**“The number of electron pairs surrounding a central atom is equivalent to the molecular geometry of the resultant molecule.”**

The word geometry has *two* different meanings when applied to molecules.

- Electronic geometry and molecular geometry have different meanings!
- Molecular geometry and shape of a molecule are the same thing.

The central organizing principle that is responsible for molecular geometry is the *number of valence pairs of electrons* that surround a central atom. That number determines the *electronic* geometry. The valence electrons distribute around a central atom in order to minimize mutual repulsion. Location of these electron pairs results in spontaneous placement at the vertices of two-dimensional polygons (*e.g.*, triangle or square) and three-dimensional polyhedra (*e.g.*, tetrahedron and octahedron).

It is first necessary to assess the number of bonds present around a central atom. The “demand/supply rule” provides a rapid answer (see *Chemical Bonding* module). A linkage is a connection between two atoms. A linkage may be a single, double, or a triple bond. When the number of linkages equals the number of valence electron pairs around the central atom, the situation is simple (an example is  $\text{CH}_4$ ). The number of linkages plus the number of lone pairs is called the steric number of the central atom. The steric number always determines the electronic geometry. If the steric number is the *same* as the number of linkages, then the molecular and electronic geometries are the same. If the number of linkages is less than the steric number, it is the steric number that determines the shape of the molecule. Some examples are the following.  $\text{CH}_4$  has four linkages (C—H connections) and a steric number of four,



so the central C atom is at the center of a tetrahedron, four H atoms are the vertices, and both the electronic and the molecular geometry are tetrahedral.  $\text{H}_2\text{O}$  has two linkages (H—O connections) and two lone pairs, so the steric number is four, the *electronic geometry* is tetrahedral, and the *molecular geometry* is called bent. The steric number is also four in  $\text{NH}_3$  so the central N atom is also at the center of a tetrahedron. The electronic geometry is tetrahedral; the molecular geometry is trigonal pyramidal (the three linkages define a triangular plane below (or above) the central N atom).  $\text{SO}_2$  has two linkages (two S—O connections, one is a single bond, one is double bond), and one lone pair, so the steric number is three. In this case the S atom is at the center of a triangle, the two O atoms are at two of the vertices and the lone pair is at the position of the third vertex. The electronic geometry is triangular, but the molecular geometry (shape) is angular, or bent.

### Problem Solving

*HOT TIP: Use the “ultrafast method” to determine the electronic geometry (without taking the time to determine the Lewis structure first)!*

Although this method is *based on* our knowledge of Lewis structures it is a quick trick to find electronic geometry and then molecular geometry. The advantage of the method is that you do not have to determine the Lewis structure first, saving considerable time. The method is very easy to apply to molecules containing a single central representative element (the Li, Be, B, C, N, O, F, and Ne families; H and He normally are not “central atoms”). It is best for beginners to restrict their practice to these families of molecules. They are, by far, the most common. There are only three “rules.”

1. First, count the number of valence electrons for the *central atom* of the family. If the central atom is C, count “4.”
2. Next, look at the atoms that are bonded to the central atom, and count the following for each of these: H, F, Cl, Br, I—1; O, S—0. (It is rare that atoms bonded to a central atom are not in this list.)
3. Add the number of electrons for the central atom and for *each* of the bonded atoms, add or subtract the charge on the species if it is not a neutral molecule, then divide the total number of electrons by two to obtain the number of repelling pairs of electrons. Remember, two pairs gives linear electronic geometry, three pairs are triangular, four pairs are tetrahedral, five pairs are triangular bipyramidal, six pairs are octahedral.

Examples:

1. **Water,  $\text{H}_2\text{O}$**

O is the central atom, so count 6 electrons and count 1 for each H atom, giving

$$\frac{[6 + 2(1)]}{2} = 4 \text{ pairs—the tetrahedral geometry.}$$

O is at the center of the tetrahedron, and the two H atoms are at two of the four vertices. The other two vertices are occupied by lone pairs. The electronic geometry is tetrahedral; the molecular geometry is bent

2. **Sulfate ion,  $\text{SO}_4^{2-}$**

S is the central atom, count 6 for it, 4 O atoms are bonded to it, count 0 for

each of these, and the ion has a charge of 2-, so

$$\frac{[6 + 4(0) + 2]}{2} = 4 \text{ pairs}$$

Thus, the ion is tetrahedral (four pairs) with the S atom at the center, and four O atoms at the vertices.

### 3. Xenon tetrafluoride, XeF<sub>4</sub>

Xe is the central atom, count 8 for it, each of the four bonded fluorines counts 1 each, so

$$\frac{[8 + 4(1)]}{2} = 6 \text{ pairs.}$$

The electronic geometry is octahedral 6 pairs. The four F atoms are at the vertices of a square, so the molecular geometry is square planar.

As early as 1852, E. Frankland proposed the idea of valence. A. Kekulé, in 1858, and A. W. H. Kolbe, in 1859, extended this concept by proposing the quadrivalency of the carbon atom; Kekulé then suggested that carbon atoms could bond to one another in indefinite numbers to form a chain. A. S. Couper, in the same year, introduced the concept of a valence bond and drew the first structural formulas.

A. M. Butlerov, in 1861, introduced the term chemical structure and stressed the importance of writing a single formula for a compound showing how the atoms were linked together in one of its molecules.

The tetrahedral structure of the carbon atom was independently recognized two months apart in 1874 by J. H. van't Hoff and J. A. Le Bel. A. Werner worked on deducing the stereochemistry of complex compounds from 1893 to 1905. In 1916, G. N. Lewis introduced his theory of valence, which was followed by a period of development leading to the quantum mechanical valence bond and molecular orbital theories. Linus Pauling is frequently called the father of modern structural chemistry. During the time period 1930-1933, he published seven papers applying quantum mechanics to chemical bonding that elucidated the nature of the chemical bond. Pauling received the 1954 Nobel Prize in chemistry for this work.

In 1962, Neil Bartlett synthesized a xenon compound, the first recorded instance of the preparation of a noble gas compound. The study of noble gas compounds has contributed greatly to our understanding of chemical bonding and molecular structure.

Dorothy Crowfoot Hodgkin spent most of her career teaching and doing research using X-ray crystallographic analysis. This method led to the structure determination of a number of complex molecules from natural sources including penicillin, vitamin B<sub>12</sub>, and insulin. Hodgkin was awarded the 1964 Nobel Prize in chemistry for this work.

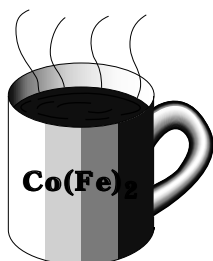
W. N. Lipscomb, Jr. during the period of time, 1952-1976, did pioneering research on the structure of the boron hydrides that led to a better understanding of molecular structure and chemical bonding. For this work, he received the Nobel Prize in 1976.

Isabella L. Karle developed an analytical technique to use with X-ray diffraction that has made important contributions in the field of X-ray crystallography. This work enabled her husband, Jerome Karle, to gain acceptance for his work on key mathematical techniques through which X-ray crystallography can be used directly to determine the three-dimensional structure of natural substances.

## HISTORY: ON THE HUMAN SIDE



## HUMOR: ON THE FUN SIDE



1. Ball-and-stick models are frequently referred to as “chemical tinker toys.”
2. When using Styrofoam® spheres for models, welcome students to the “ball room.”
3. A cup of coffee is the model for  $\text{Co(Fe)}_2$ .

### 4. Word Search (see *Appendix* for master copy)

P P A O V Y Z V Y R I A P E N O L  
M O L E C U L A R G E O M E T R Y  
O X L D J R Y A F C T N J F P Y S  
V N J Y T Z I T P T V L Q U Q H C  
J I J F G P W V M Z A M H I V C V  
R Y L O K O E Y M P L V J Q O U Z  
I P B I I L N O R D E H Y L O P G  
A T E X R Y J J E R N F E D J Q R  
P T G S Y T L J A C C N J G S M C  
D F D X V O C B K V E T X V F Q E  
N R W K G P U A P T Z V O Z C E S  
O C J S T E R I C N U M B E R D W  
B S T E R E O C H E M I S T R Y R

Words about the concepts in this module can be obtained from the clues given. Find these words in the block of letters:

1. Bonding electron group contributing to entry 8 (two words).
2. Nonbonding contributor to entry 8 (two words).
3. Shape of a molecule (two words).
4. Plane form made up of a number of straight sides.
5. Solid formed by a number of polygonal faces.
6. General term for a solid figure like a polyhedron.
7. Geometric arrangement of atoms or groups around the central atom in a molecule.
8. Number of bond pairs and lone pairs of electrons surrounding the central atom in a molecule (two words).
9. Combining ability of an atom based upon the number of electrons in its outer shell.
10. Acronym for theory to describe the forces resulting in the geometry of a molecular species.

Answers: 1. BOND PAIR 2. LONE PAIR 3. MOLECULAR GEOMETRY  
4. POLYGON 5. POLYHEDRON 6. POLYTOPE 7. STEREOCHEMISTRY  
8. STERIC NUMBER 9. VALENCE 10. VSEPR

5. See cartoons at end of module.

**MEDIA**

Many computer programs that use graphics to show molecular structure are available. Prices vary, and programs can be found for almost any microcomputer.

1. Software published by *JCE: Software*, a publication of the *Journal of Chemical Education*, Department of Chemistry, University of Wisconsin-Madison, 1101 University Avenue, Madison, WI 53706-1396: (608) 262-5153 (voice) or (608) 262-0381 (FAX).
  - a. *Bravais*, by Philip Pavlik. Vol. III B, No. 1, for IBM PS/2 PC-compatible computers.
  - b. *Alkane Isomers*, by Richard R. Hiatt. Vol. VI V, No. 1, for IBM PS/2 PC-compatible computers.
  - c. *MolVib: Visualizing Molecular Vibrations*, by Daniel Huber. Vol. III C, No. 1, for the Apple Macintosh.
  - d. *Proton NMR Spectrum Simulator*, by Kersey Black. Vol. II C, No. 1, for the Apple Macintosh.
  - e. *Evolution of Bonding Theory*, by David Whisnant. Vol. II A, No. 1, for the Apple II computer.
  - f. *Crystal Lattice*, by David Trapp. Vol. IV A, No. 1, for the Apple IIGS computer.
2. Software published by Falcon Software, Box 200, Wentworth, NH 03282; (603) 764-5788.
  - a. *Lewis Structures and Molecular Geometry*, by Jeffrey R. Buell, Andrew F. Montana and Patrick A. Wegner. For the Apple Macintosh. \$95 for individual copies.
  - b. *Molecular Editor*, by Allan Smith. For the Apple Macintosh. \$50 for individual copies.
  - c. *Valence Shell Electron Pair Repulsion Theory*, by Michael P. Doherty. For IBM computers. \$50 for individual copies.
  - d. *SpectraBook* for Windows and *SpectraDeck* for Macintosh – An Annotated Collection of IR, NMR, CMR and Mass Spectra, by Paul F. Schatz. \$95 for individual copies.
  - e. *The Schatz Index* for Macintosh, by Paul F. Schatz. The IR and NMR spectra, physical information, references, synonyms and safety data for 400 organic compounds. \$200 for individual copies.
  - f. IR and NMR Simulators of Macintosh and MS-DOS. These simulators are low-cost and easy to use; they are no-maintenance simulations of the real instruments. Data sets for 300 compounds are available separately. \$95 for individual copies of NMR simulator, \$75 for individual copies of IR simulator, \$200 for IR data set, \$250 for NMR data set.
3. Software published by Project SERAPHIM, Department of Chemistry, University of Wisconsin-Madison, 1101 University Avenue, Madison, WI 53706-1396: (608) 263-2837 (voice) or (608) 262-0381 (FAX).
  - a. For the Apple II computer running on ProDOS: AR 303.
  - b. For the Apple II computer: AP 301, AP 310, AP 704, AP 705, AP 706.
  - c. For IBM PCs and PC-compatibles: PC 2801, PC 2802, PC 2803, PC 3501.



4. Videodiscs published by *JCE: Software*, a publication of the *Journal of Chemical Education*, Department of Chemistry, University of Wisconsin-Madison, 1101 University Avenue, Madison, WI 53706-1396: (608) 262-5153 (voice) or (608) 262-0381 (FAX).

“Carbon and Its Bonds,” “Chiral Molecules and Polarized Light,” “From an Amino Acid to a Peptide Chain,” “The Alpha Helix,” “Hair and Silk,” “The Boat and Dock Model, and “DNA Structure, Synthesis of Messenger RNA, Protein Synthesis,” seven chapters on *The World of Chemistry: Selected Demonstrations and Animations: Disc II* (double sided, 60 min.), Special Issue 4.
5. *MacMolecule*, V. 1.7, by Eugene Meyers, Carlos Blanco, Richard B. Hallick and Jerome Jahnke, Department of Computer Science, University of Arizona, Tucson, AZ 85721. Interactive 3D molecular modeling curriculum development shareware program featuring a video animation generation program and a molecular image database. For Apple Macintosh computer with math coprocessor.
6. Materials and devices from ICE—Institute for Chemical Education, Department of Chemistry, University of Wisconsin-Madison, 1101 University Avenue. Madison, WI 53706-1396: (608) 262-3033 (voice) or (608) 262-0381 (FAX).
  - a. The Solid State Model Kit.
  - b. The Optical Transform Kit.
7. CHEM Study films/videos available from Ward’s Natural Science Establishment, Inc., 5100 West Henrietta Road, P.O. Box 92912, Rochester, NY 14692-9012; (800) 2660.
  - a. *Shapes and Polarities of Molecules*. This video develops the relationship between polarity and structure from an experimental point of view. The molecular dipole model is extended to explain differences in solubility, conductivity and chemical reactivity.
  - b. *Molecular Spectroscopy*. Laboratory experiments, molecular models and animation show the infrared light absorption process and its relation to molecular properties. The video stresses the concept of natural molecular vibrational frequencies and includes the method of using infrared spectroscopy to identify molecules and determine their structure.
8. *Ball and Stick* for the Macintosh computer is available on some bulletin boards and from Educorp Computer Services, 7434 Trade Street, San Diego, CA 92121-2410; (800) 843-9497; (619) 359-2502.
9. *VSEPR* (for the Macintosh; requires HyperCard) is available from John Gelder, Department of Chemistry, Oklahoma State University, Stillwater, OK 74078; (800) 633-1176.
10. *Molecular Editor*, for the Macintosh is available from Jan Biros, Microcomputing Department, Drexel University, Philadelphia, PA 19104. This is a software-based molecular model kit.

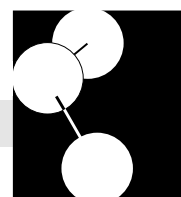
11. *Modeler: Molecular Design Editor* and *Molecular Animator* are two programs available from Sargent Welch, P.O. Box 1026, Skokie, IL 60076-1026; (800) 677-0624. Written for both Apple II and IBM-PC computers, they allow viewing ball-and-stick molecular models from different angles by rotation. Each program is approx. \$100.

Ball-and-stick models and Styrofoam® spheres of various sizes are available from most major scientific supply houses. For example, Sargent-Welch, Cenco, Science Kit, Ward's, Flinn Scientific and Fisher Scientific all have a variety of kits available at reasonable prices. Flinn Scientific has an inexpensive Styrofoam® sphere kit with a tetrahedral template included. Another source is your local hobby shop.

There are several molecular model kits that are relatively inexpensive and designed for use by large student groups. For example, one kit contains twelve packets that allows students to construct models with linear to tetrahedral centers. Most inexpensive kits are variants of ball-and-stick models. Orbit® and Minit® model systems are also available either in individual student kits or class kits that may be made up into individual packets using zip-closure plastic bags. Supplier: Aldrich Chemical Company, Inc., 1001 West Street Paul Avenue, Milwaukee, WI 53233, 1-800-558-9160.

## EQUIPMENT

# Links/Connections



## WITHIN CHEMISTRY

Molecular geometry can be linked to physical properties and chemical properties of substances. Pertinent modules are *Chemical Bonding*, *Organic Chemistry*, *Chemistry in Medicine*, *Polymers*, and *Enzymes*.

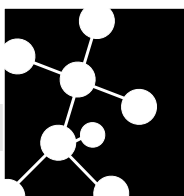
1. When retinal, a compound located in the retina of the eye, absorbs photons of visible light, its molecules change from the *cis* form to the *trans* form. This change in molecular geometry causes a signal to be transmitted from the retina along the optic nerve to the brain.
2. In diamonds, silicates, and carborundum (SiC), the atoms are arrayed in tetrahedral geometry, whereas in graphite, the carbon atoms have a trigonal planar arrangement.
3. In organic chemistry, sulfur tetrafluoride (SF<sub>4</sub>) and xenon oxytetrafluoride (XeOF<sub>4</sub>) are used as fluorinating agents. SF<sub>4</sub> has a see-saw (irregular tetrahedral) shape, whereas the xenon compound has a square pyramidal shape. What might you expect the geometry of SOF<sub>4</sub> to be? (*Trigonal bipyramid*)
4. To determine the molecular geometry of a molecule, one must ascertain the location of the constituent atoms. Diffraction methods involve the formation of diffraction-interference patterns that result from the scattering of X-rays (X-ray diffraction), electrons (electron diffraction), or neutrons (neutron diffraction). Spectroscopic methods that include microwave, Raman, and infrared spectroscopy rely upon energy transfer interactions between electromagnetic radiation and matter.

## BETWEEN CHEMISTRY AND OTHER DISCIPLINES

Shapes of many molecules have been directly linked to their function in biological systems. Molecular geometry concepts and techniques are highly applicable in molecular biology, pharmacology, genetic engineering, medicine, *etc.*

## TO THE CONTEMPORARY WORLD

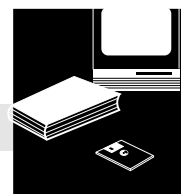
1. **Drugs.** The physiological activity of many prescription and OTC drugs is due to the shape of specific functional groups in the molecule (see *Chemistry in Medicine* module).
2. **Crystal Structure.** The shape of an individual molecule dictates the crystal structure of its aggregates.
3. **Biochemistry** Enzymes owe their activity to active sites that interact with substrates with the correct geometry. Since enzymes are crucial to the functioning of all living things, there is a direct, personal link between molecular geometry and life. Furthermore, the conformations of proteins, nucleic acids, and other substances making up the human body determine its macroscopic structure.
4. **Societal** Synthetic polymers are extremely important substances to a highly developed technological society. The desirable properties of polymers depend on molecular conformation, but because of these same properties, polymers are also disposal problems and environmental pollutants.



# Extensions

1. Research methods to measure the polarity of some covalent molecules.
2. What contributions did Jacobus van't Hoff make to understanding three-dimensional structures of molecules?
3. Make models of a family of compounds such as  $\text{H}_2\text{O}$ ,  $\text{H}_2\text{S}$ ,  $\text{H}_2\text{Se}$ , and  $\text{H}_2\text{Te}$  and relate bond angles to the predictions of VSEPR theory.
4. How did Linus Pauling use quantum mechanical theory to describe chemical bonds?
5. There are some compounds in which one atom has more electrons than the corresponding noble gas.  $\text{PCl}_5$ ,  $\text{SF}_6$ , and  $\text{IF}_7$  are examples. Write electron configurations for the central atoms in each one, and draw Lewis-dot structures for the compounds. Using the valence configuration of the central atoms, develop a VSEPR procedure to describe these molecules.
6. Using appropriate sized spheres and connectors, construct a model set including the following:  $\text{AX}$ ,  $\text{AX}_2$ ,  $\text{AX}_3$ ,  $\text{AX}_2\text{E}$ ,  $\text{AX}_4$ ,  $\text{AX}_3\text{E}$ ,  $\text{AX}_2\text{E}_2$ ,  $\text{AX}_5$ ,  $\text{AX}_4\text{E}$ ,  $\text{AX}_3\text{E}_2$ ,  $\text{AX}_2\text{E}_3$ ,  $\text{AX}_6$ ,  $\text{AX}_5\text{E}$ , and  $\text{AX}_4\text{E}_2$ .

# References



Module developed by Royace Aikin, Daniel Kallus, and Russell D. Larsen, the Texas team.

Brey, W. (1965). *Physical methods for determining molecular geometry*. New York, NY: Reinhold.

An excellent summary of the many instrumental methods used to determine molecular geometry.

Brooks, D. W. (Producer). (1989). *Doing chemistry*. [Videodiscs, computer program, and supporting materials]. Washington, DC: American Chemical Society.

This is an excellent teacher resource. It provides hard copy of all the experiments and demonstrations; it also provides a planning toolkit, all of the experiments and demonstrations on videodisc, a computer program to interface the videodiscs with a Macintosh computer, and other useful information on computer disc. It is quite interesting and informative to watch a chemical reaction such as a dust explosion one frame at a time, which is possible with this resource.

Day, Jr., Clyde, M., and Selbin, J. (1962). *Theoretical inorganic chemistry*. New York, NY: Reinhold.

Although some of the material in this textbook is dated, it still is a valuable resource for chemical bonding and molecular structure.

McQuarrie, D. A., and Rock, P. A. (1984). *General chemistry*. New York, NY: W. H. Freeman and Company.

This book is an excellent general chemistry reference for the teacher. It contains extensive coverage of the same topics taught in a typical high school chemistry course, but in greater depth.

Parry, R. W., Bassow, H., and Merrill, P. (1987). *Chemistry: Experimental foundations*. Englewood Cliffs, NJ: Prentice-Hall, Inc.

The only CHEMS derived text currently published. Very good information, especially how to present chemistry from an experimental point of view. The companion teacher's guide is a must.

Ryschkewitsch, G. E. (1963). *Chemical bonding and the geometry of molecules*. New York, NY: Reinhold.

A plausible exposition of modern thoughts in structural chemistry.

Speakman, J. C. (1966). *Molecules*. New York, NY: McGraw-Hill.

Summerlin, L. R., Borgford, C. L., and Ealy, J. B. (1987). *Chemical demonstrations: A sourcebook for teachers, (2)*. Washington, DC: American Chemical Society.

Many of the demonstrations are highly useful in an introductory chemistry course. This should be a part of every chemistry teacher's library.

Toon, E. R., and Ellis, G. L. (1973). *Foundations of chemistry (2nd Ed.)*. New York, NY: Holt.

This high school chemistry textbook is loaded with valuable information about all aspects of general chemistry. It provides more historical data than most

current high school textbooks and has nice vignettes about outstanding scientists. Another useful feature is the inclusion of special sections, *e.g.*, chromatography.

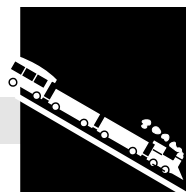
Wilbraham, A. C., Staley, D. D., Simpson, C. J., and Matta, M. S. (1987). *Addison-Wesley chemistry* (Teacher's Edition). Menlo Park, CA: Addison-Wesley.

A good, solid high school chemistry textbook that may be used by both novice and experienced teachers. Other equally good textbooks are available.

Zumdahl, S. S. (1986). *Chemistry*. Lexington, MA: Heath.

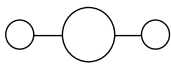
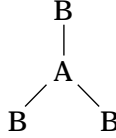
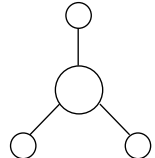
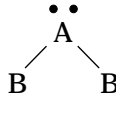
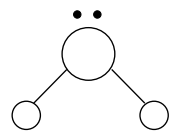
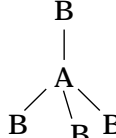
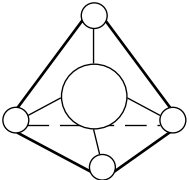
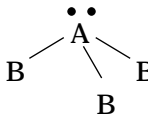
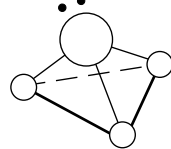
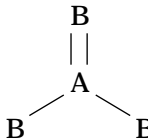
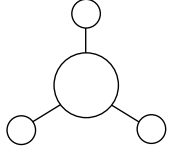
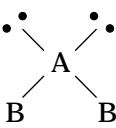
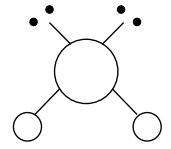
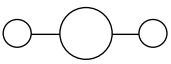
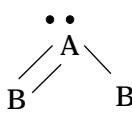
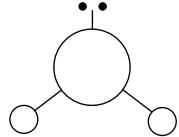
A well written and understandable freshman chemistry textbook. It can serve as an invaluable resource for the teacher.

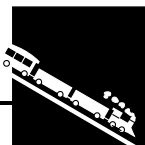
# Appendix



- **Transparency Masters**
  1. Molecular Shapes of Species Containing Representative Elements
  2. Molecular Shapes of Species Containing 5, 6, or 7 Electron Pairs
  3. Octahedron Template
  4. Word Search
- **Humor**

## Molecular Shapes of Species Containing Representative Elements

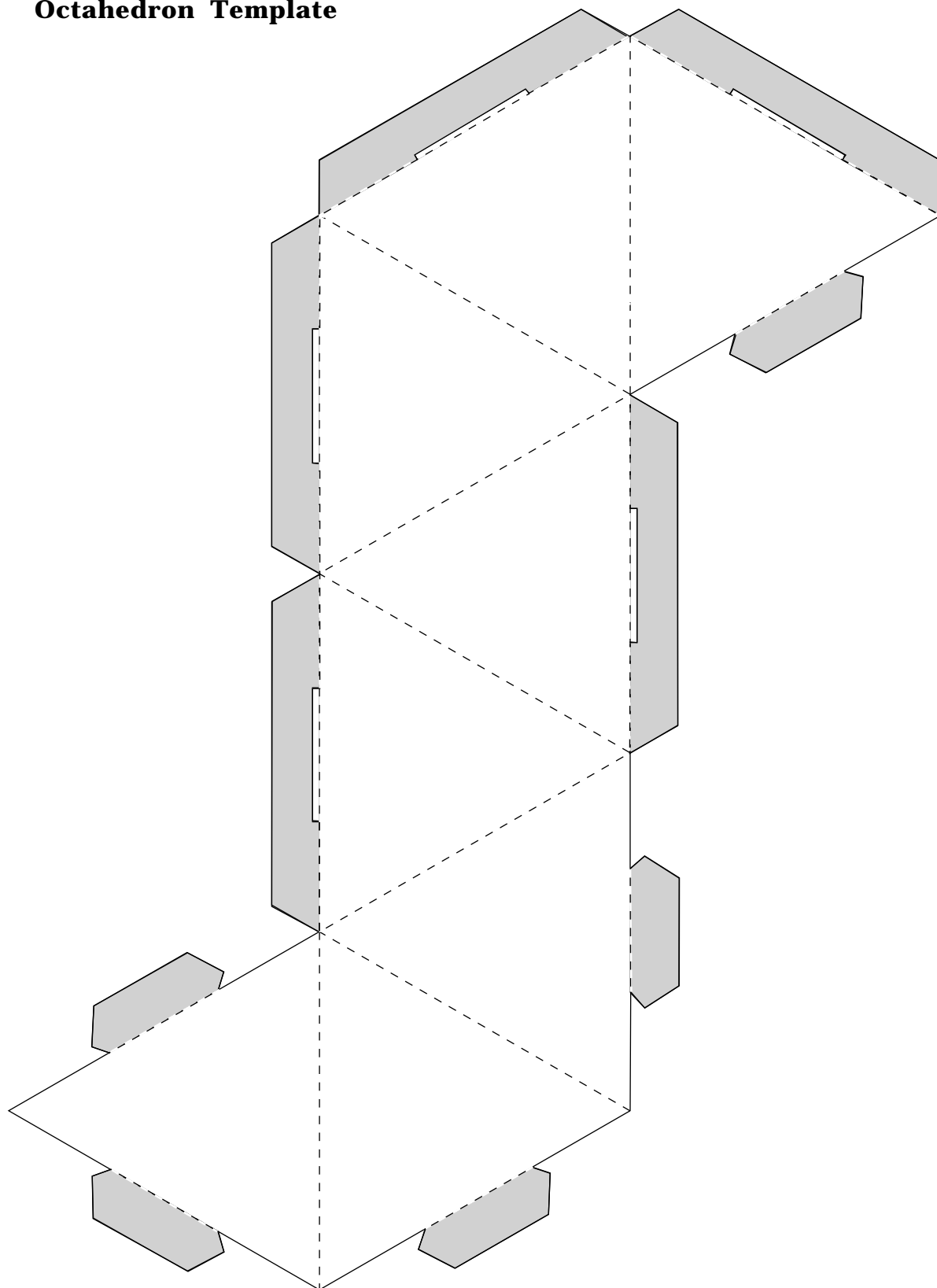
Name of shape	Formula	No. of unbonded electron pairs (lone pairs)	No. of electron pairs in valence level of central atom	Lewis structure	Representation of shape
Linear	AB <sub>2</sub>	Zero	2	B—A—B	BeF <sub>2</sub> 
Trigonal planar	AB <sub>3</sub>	Zero	3		BF <sub>3</sub> 
Angular	AB <sub>2</sub>	One	3		SnCl <sub>2</sub> 
Tetrahedral	AB <sub>4</sub>	Zero	4		CCl <sub>4</sub> 
Pyramidal	AB <sub>3</sub>	One	4		NH <sub>3</sub> 
Trigonal planar	AB <sub>3</sub>	Zero	4		SO <sub>3</sub> 
Angular	AB <sub>2</sub>	Two	4		H <sub>2</sub> O 
Linear	AB <sub>2</sub>	Zero	4	B=A=B	CO <sub>2</sub> 
Angular	AB <sub>2</sub>	One	4		SO <sub>2</sub> 

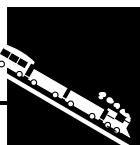


## Molecular Shapes of Species Containing 5, 6, or 7 Electron Pairs

Name of shape	Formula	No. of unbonded electron pairs (lone pairs)	No. of electron pairs in valence level of central atom	Lewis structure	Representation of shape
Trigonal bipyramidal	AB <sub>5</sub>	Zero	5		PCl <sub>5</sub>
Seesaw	AB <sub>4</sub>	One	5		SF <sub>4</sub>
T-shaped	AB <sub>3</sub>	Two	5		ClF <sub>3</sub>
Linear	AB <sub>2</sub>	Three	5		XeF <sub>2</sub>
Octahedral	AB <sub>6</sub>	Zero	6		SF <sub>6</sub>
Square-based pyramidal	AB <sub>5</sub>	One	6		IF <sub>5</sub>
Square planar	AB <sub>4</sub>	Two	6		XeF <sub>4</sub>
Pentagonal bipyramidal	AB <sub>7</sub>	Zero	7		IF <sub>7</sub>

**Octahedron Template**





## Word Search

P P A O V Y Z V Y R I A P E N O L  
M O L E C U L A R G E O M E T R Y  
O X L D J R Y A F C T N J F P Y S  
V N J Y T Z I T P T V L Q U Q H C  
J I J F G P W V M Z A M H I V C V  
R Y L O K O E Y M P L V J Q O U Z  
I P B I I L N O R D E H Y L O P G  
A T E X R Y J J E R N F E D J Q R  
P T G S Y T L J A C C N J G S M C  
D F D X V O C B K V E T X V F Q E  
N R W K G P U A P T Z V O Z C E S  
O C J S T E R I C N U M B E R D W  
B S T E R E O C H E M I S T R Y R

Words about the concepts in this module can be obtained from the clues given. Find these words in the block of letters:

1. Bonding electron group contributing to entry 8 (two words).
2. Nonbonding contributor to entry 8 (two words).
3. Shape of a molecule (two words).
4. Plane form made up of a number of straight sides.
5. Solid formed by a number of polygonal faces.
6. General term for a solid figure like a polyhedron.
7. Geometric arrangement of atoms or groups around the central atom in a molecule.
8. Number of bond pairs and lone pairs of electrons surrounding the central atom in a molecule (two words).
9. Combining ability of an atom based upon the number of electrons in its outer shell.
10. Acronym for theory to describe the forces resulting in the geometry of a molecular species.



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