Name____

Chemistry 117 Laboratory
University of Massachusetts Boston

MOLECULAR SHAPES

LEARNING GOALS

Almost everything that we do in Chemistry Lab this semester is going to involve measuring something. This first laboratory exercise has been designed around the following learning goals.

1. Practice the application of VESPR theory for predicting the 3-D shapes of molecules and complex ions.
2. Use a molecular model kit to help visualize the shapes predicted by VESPR theory.
3. Learn how electron pair repulsion from lone pairs impact bond angles.

INTRODUCTION

VESPR theory is used to predict the geometries around atoms in a molecule. The basic tenant of VESPR is that pairs of electrons around a central atom will spread out as far as possible to minimize repulsion.

Number of Electron Pairs	Domain Geometry	Bond angles
2	Linear	180 °
3	Trigonal Planar	120 °
4	Tetrahedral	109.5 °
5	Trigonal Bipyramidal	120 ° in plane 90 ° on axis
6	Octahedral	90 °

An electron pair around the central atom can be either a chemical bond (single, double or triple each count an electron pair) or a lone pair of electrons. The actual molecular geometry, or shape, about the central atom depends on how many of the electron pairs are bonds.

Table for Predicting Geometries around a Central Atom

# of Electron Pairs	Domain Geometry	# of bonds around the central atom	Shape	Examples
2	Linear	1 or 2	Linear	CO_2
3	Trigonal Planar	2	Bent	O_3
3	Trigonal Planar	3	Trigonal planar	SO_3
4	Tetrahedral	2	Bent	H_2O
4	Tetrahedral	3	Trigonal Pyramidal	NH_3
4	Tetrahedral	4	Tetrahedral	CHF_2Cl
5	Trigonal Bipyramidal	2	Linear	XeF_2
5	Trigonal Bipyramidal	3	T-shaped	ClF_3
5	Trigonal Bipyramidal	4	Seesaw	SF_4
5	Trigonal Bipyramidal	5	Trigonal Bipyramidal	PCl_5
6	Octahedral	4	Square Planar	XeF_4
6	Octahedral	5	Square Pyramid	ClF_5
6	Octahedral	6	Octahedral	SF_6

So the strategy is

1) Draw the Lewis dot structure
2) Count the total number of electron pairs around the central atom
3) Count the number of bonds around the central atom
4) Use the table above to predict the geometry around the central atom
5) Use the model kit to build a model of the molecule.

In this week's lab you will have the opportunity to visualize the geometric shapes defined by VSEPR theory. Throughout this exercise, the term “shape” refers to the molecule’s geometry (the geometrical arrangement of the atoms), which may be different from the idealized geometry of the electron domains (the domain geometry).

You should receive from your instructor a bag containing an assortment of parts from two types of molecular modeling kits. One of these is a “jack and straw” type kit; the other is a “ball and stick” molecular modeling kit typically used in organic chemistry courses. The straws and connectors represent bonds. The jacks and spheres represent atoms. Please verify that the bag includes at least the following:

6 straws
6 one-pronged jacks
1 each 2-, 3-, 4-, 5-, 6-pronged jacks
1 black, 1 brown, 4 white, and 3 red spheres
5 gray connectors

This bag must be returned with your worksheet.

IN THE LABORATORY

PART ONE

Place one-pronged jacks at one end of each straw to represent atoms.

1. A. Connect two straws to the 2-pronged connector. Obviously, the only way you can connect these is in a straight line. This geometry is similar to any linear triatomic molecule, such as gaseous $BeCl_2$ or CO_2. Draw the Lewis dot models for both molecules, and sketch a representation of their molecular shape.

B. Remove one straw from the previous model. You now have a model of a diatomic molecule, such as HCl, which is necessarily linear (two points define a straight line). Draw the Lewis structure of HCl, and sketch a representation of its shape.

2. **A** Connect three straws to a 3-pronged jack. They are in the same plane, a shape called trigonal planar. This geometry is similar to BF_3. Draw the Lewis dot structure, and sketch a representation of the molecular shape. Indicate the F-B-F angle on your molecular shape sketch.

B. Remove one of the straws from the previous model. The remaining two straws define a "bent" or "angular" molecule similar to SO_2. Draw the Lewis dot structure(s), and sketch the molecular shape. Indicate the approximate O-S-O bond angle in SO_2 on your molecular shape sketch. Is it the same, smaller, or greater than the F-B-F angle in BF_3? Explain.

3. A. Now connect four straws to a 4-pronged jack. You should see the shape of a tetrahedron. This is the geometry of CH_4. The H-C-H angle in CH_4 is the perfect tetrahedral angle, 109.5^o. Draw the Lewis dot structure of CH_4, and sketch the three-dimensional molecular shape.

B. Remove one of the straws from the previous model. The remaining shape is a trigonal pyramid. This shape is the shape of an NH_3 molecule. Draw the Lewis dot structure, and sketch the three-dimensional molecular shape. Is the H-N-H angle in NH_3 the same, smaller, or greater than the H-C-H angle in CH_4? Explain.

C. Remove another straw from the previous model. You should have two straws defining a "bent" or "angular" geometry. This geometry is similar to that of H_2O. Draw the Lewis dot structure, and sketch the molecular shape. Compare and contrast the H-O-H angle in H_2O with the H-C-H angle in CH_4, the H-N-H angle in NH_3, and the O-S-O angle in SO_2 (see 2B, above). Explain the differences.

4. A. Now connect five straws to a five-pronged jack. The resulting shape is a trigonal bipyramid (sometimes abbreviated *tbp*), composed of three equatorial positions in a trigonal plane with two axial positions perpendicular to this plane on both sides. In most *tbp* molecules, the two axial bonds have one length and the three equatorial bonds have a different length (most often shorter). This is the shape of PCl_5. Draw the Lewis dot structure, and sketch the three-dimensional molecular shape. Indicate the equatorial and axial positions on your sketch.

B. In molecular shapes based on five electron domains about a central atom (*tbp* domain geometry), any lone pairs preferentially occupy equatorial positions. Remove one equatorial straw from the previous model. The remaining shape is called an irregular tetrahedron or "seesaw." This is the geometry of SF_4. Draw the Lewis dot structure, and sketch the three-dimensional molecular shape. There are two different F-S-F bond angles in SF_4. Indicate the two angles on your molecular shape sketch, and indicate whether they are the same, smaller, or greater than the comparable angles in a perfect trigonal bipyramid. Explain. Do you expect all the S-F bonds in SF_4 to have the same length? Explain.

C. Remove another equatorial straw. This leaves the two axial straws and one equatorial straw. We call this geometry, for obvious reasons, "T-shaped." ClF_3 adopts this geometry. Draw the Lewis dot structure, and sketch a representation of the molecular shape. Is the F-Cl-F angle the same, smaller, or greater than 90^o? Explain. Do you expect all three Cl-F bond lengths to be the same? Explain.

D. Remove the last equatorial straw. You should now be left with a linear geometry with the straws in a straight line. This is the same geometry as XeF_2. Draw the Lewis dot structure, and sketch a representation of their molecular shape. Do the lone pairs around Xe cause any deviations from linear geometry? Explain why or why not.

5. A. Assemble six straws around a 6-pronged jack. This shape is called octahedral. Each straw makes a 90^o angle with four other straws and a 180^o angle with the straw opposite it. Note that all six positions in the octahedron are geometrically equivalent, unlike the positions in the *tbp* geometry we have just seen. SF_6 is an example of a molecule that has this geometry. Draw the Lewis dot structure, and sketch the three-dimensional molecular shape.

B. Remove one of the straws. It doesn't matter which one, because all six are geometrically equivalent. The shape that is left is called a square pyramid. BrF_5 adopts this geometry. Draw the Lewis dot structure, and sketch the three-dimensional molecular shape. Do you expect the F-Br-F angles in BrF_5 to be the same, smaller, or greater than 90^o? Explain.

C. Remove the straw opposite the one you removed in the previous model. This should leave four straws in the same plane as the central jack. This shape, called square planar, is the geometry that describes a XeF_4 molecule. Draw the Lewis dot structure, and sketch the three-dimensional molecular shape. Do you expect the F-Xe-F angles in XeF_4 to be the same, smaller, or greater than 90^o? Explain.

PART TWO

In this section we will be using the organic chemistry modeling kit. The following exercise represents the oxidation of methane. Some of these ideas will be familiar from your current chemistry experience; some may be covered more fully later.

1. Using the gray connectors ("single bonds"), connect four white spheres ("hydrogen") to the black sphere ("carbon"). This model represents methane, CH_4. This is odorless "natural gas" and has been produced predominantly on Earth as a byproduct in the digestion of plant life. Ironically, much of the value attributed to methane and other hydrocarbons compounds is in their usefulness once they react with oxygen in one way or another, a process called oxidation. The hydrocarbons, however, began as highly oxidized molecules. Over time they have been digested or experienced such extreme pressures that they have lost their original oxygen composition. Because of this, and because we are depleting our hydrocarbon reserves, there is a huge incentive to use plant sources directly for our hydrocarbon needs. Next time you hear about renewable or bio-feedstocks, see if you can tie it into what you do here today.

2. Remove a hydrogen from the end of its connector and replace it with a red sphere ("oxygen"). Now connect the hydrogen to the oxygen using another connector. This model represents methanol, CH_3OH. Methanol is commonly referred to as wood alcohol. Unlike ethanol ("drinking alcohol," C_2H_5OH), methanol is highly toxic. Draw the Lewis structure for methanol. Estimate the size in degrees of the H-C-H and C-O-H angles in the actual molecule. Note that neither of these is 90^o!

3. Locate the five-holed brown sphere, which can be used to represent a central carbon atom with *sp*^{2} hybridization. Using the gray connectors ("single bonds"), connect two white spheres ("hydrogen") to two of the three holes that make a trigonal planar arrangement with each other. Attach another gray connector to the third hole, and attach a red sphere ("oxygen"). In this case, the connector to the oxygen atom represents a double bond. This model represents CH_2O, formaldehyde. If you have ever had a dissection laboratory, you may be familiar with aqueous solutions of formaldehyde as a preservative for animal tissue. Methanol is converted to formaldehyde by the liver. This is one reason why ingesting "wood alcohol" is highly toxic! Draw the Lewis structure of formaldehyde. Estimate the size in degrees of the H-C-O angle in the actual molecule. Note that this angle is neither 90^o nor 109.5^o!

4. Remove one of the hydrogen atoms and its connector from the previous model, and reattach it to the oxygen atom. Then, add another oxygen atom with a connector to the position where you removed the hydrogen. You have now made a model of HCO_2H, formic acid. Non-stinging ant species produce this organic acid in their abdomens and inject it into their victims after first biting, generally as a defense mechanism. Some birds put ants in their feathers because the ants squirt formic acid, which gets rid of parasites. Draw the Lewis structure for formic acid. On your Lewis model, indicate the approximate sizes in degrees of the following angles in the actual molecule: H-C-O, O-C-O, C-O-H. Do you expect both C-O bond lengths to be the same? Explain.

5. Remove the remaining hydrogen atom from the previous model, and reattach it to the oxygen atom that does not already have a hydrogen atom. In its place, attach an oxygen atom with a connector. You have now made a model of H_2CO_3, carbonic acid. This molecule is a minor component in an aqueous solution of carbon dioxide, familiar as carbonated water or "club soda." The major components in carbonated water are dissolved $CO_2(aq)$ and $H_2O(l)$. That "psst" sound you hear when you open a soda bottle is the sound of $CO_2(g)$ being released. Draw the Lewis structure of carbonic acid, H_2CO_3. Are all three C-O bonds the same length? If not, indicate which C-O bond is longer or shorter than the other two.

When you are finished, place all the kit's pieces in the zipper bag and return it with your worksheet!

Turn in your data sheet (pg 3-12) before you leave lab. There is no additional component to this report. That is correct. You get a free 30 points.

See you in CHEM 118!!!