**Che201**

# Molecular Geometry Based on the VSEPR Model

**Objectives:** Provide hands-on and visual interaction with three-dimensional shapes of molecules.

Use Lewis structures and the valence-shell-electron-pair repulsion (VSEPR) model to create and predict shapes of molecules.

Study the five most common VSEPR families of the general type $AB_x$ and the thirteen classes of the $AB_xE_y$ geometric arrangements.

Correlate shapes to the number of electron domains (bonding and non-bonding), and to the orbital hybridization of the central atom.

Predict the polarity of the geometric arrangements thus created.

**Prior Reading** Section 9.1-9.4 in Chemistry, 3rd Edition by Julia Burdge

**Introduction** In 1957, British Chemists Gillespie and Nyholm revived and extended the theory now known as the *valence-shell-electron-pair repulsion (VSPER) theory.* This qualitative theory extends the idea of Lewis structures with a few simple rules to allow the prediction of the shapes of molecules and ions. The basis of this theory is that electron pairs in the valence shell of an atom repel one another and therefore will arrange themselves to be as far apart as possible in order to minimize the repulsive interactions between them. Electron pairs can be referred to as electron domains and can be bonding (a single, double or triple bond) or nonbonding (lone pairs). The magnitude of the repulsion is greatest between nonbonding domains and decreases as follows:

Lone pair-lone pair (E-E) > lone pair-bonding pair (E-B) > bonding pair-bonding pair (B-B)

This experiment uses balloons to represent electron domains. At first, small balloons of equal size represent B atoms connected (or bonded) to a fixed central point representing the central atom A in the $AB_x$ family. Connecting 2, 3, 4, 5, or 6 of these small and equal balloons to a central point in various orientations will generate the 5 optimal geometries or shapes that allow the balloons to be as far apart as possible. The optimal shapes adopted by these bonding domains should be linear for 2 connected small balloons ($AB_2$), trigonal planar for 3 small balloons connected to a central point ($AB_3$), tetrahedral for 4 small balloons connected to a central point ($AB_4$), trigonal bipyramidal for 5 small balloons connected to a central point ($AB_5$), and octahedral for 6 small balloons connected to a central point ($AB_6$). The bond angles in these shapes are the bond angles associated with the respective geometric shapes ($180^o$ for the linear shape, $120^o$ for the trigonal planar shape etc). The equal size of each balloon and the symmetry of each ideal shape, predicts that each molecule represented by these geometries of all-bonding domains should be nonpolar.

Next, large and equal balloons represent E lone pairs of electrons on the fixed central point representing the central atom A in the $AB_xE_y$ class of molecules. Replacing one or more of the small balloons (bonding domains) with large balloons (representing lone electron pairs or nonbonding domains exhibiting greater repulsion and thus requiring more room) allows the balloons to adopt various spatial arrangements. The arrangements affording the most room for the balloons represent the shapes most energetically favored by these classes of compounds. The additional room required by the larger balloons mimics the increased repulsion and succeeds in minimizing angles between the small balloons (the bonded atoms in the molecule). Where the introduction of large balloons results in unsymmetrical arrangements, a polar molecule can be predicted.

## Procedure

### Part A

Select 6 balloons, each a different color, and inflate them to the size of a small cantaloupe. All 6 balloons should be the same size. Number each balloon 1-6. Mark the top of each balloon with a small dot. Create the shapes instructed below and evaluate them to answer the questions corresponding to each shape/section on the data sheet. Devise the best way to measure the dot to dot distances using a string and a meter stick and the best way to measure angles using a protractor. Decide the preferred shape based on the largest dot to dot distances and largest angles between balloon stems.

A1 Tie balloons #1 & 2 together and hold them so the distance from the dot of one balloon to the dot of the other balloon is greatest.

A2 Add a balloon #3, connecting all three tied ends together in the center. Position and reposition the three balloons, taking measurements from the dot of one balloon to the dot of another. Stop when you have created a shape the produces the greatest dot to dot distance.

A3 Add balloon #4, connecting all four tied ends together in the center. Place the balloons flat on the lab bench and hold them in place while measuring dot to dot distances of each balloon to its two nearest neighbors.

A4  Hold the four balloons in the air and allow them to point to the four corners of a tetrahedron.  Measure the dot to dot distance of each balloon to its nearest neighbor.

A5  Add balloon #5, connecting all five tied ends together in the center. Force four of the balloon to lie flat on the bench, with the fifth balloon sticking on top of them.  Find the greatest and the smallest dot to dot distances between adjacent balloons and record them.

A6  Hold the five balloons in the air and allow two of the balloons to be in the axial positions and the other three balloons to form a triangle in the equatorial plane between the two axial balloons.  Find the greatest and the smallest dot to dot distances between adjacent balloons and record them.

A7  Add balloon #6, connecting all six tied ends together in the center. Hold the balloons in the air and allow them to form different shapes while you note the dot to dot distances between adjacent balloons.  Next, allow two of the balloons to be in the axial positions and the other four balloons to form a square in the equatorial plane between the two axial balloons. Measure the dot to dot distance of each balloon to its nearest neighbor. Which shape produced the greatest dot to dot distance between adjacent balloons?

**Part B**

Select 3 new balloons, each a different color, and inflate them to the size of a basketball.  All 3 balloons should be the same size.  Letter each balloon A-C.  Mark the top of each balloon with a small dot.  Create the shapes instructed below and answer the questions corresponding to each shape/section on the data sheet.  Devise the best way to measure the dot to dot distances using a string and a meter stick and the best way to measure angles using a protractor.  Decide the preferred shape based on the largest dot to dot distances and largest angles between balloon stems.

B1  Replace balloon #6 with a larger balloon A in the preferred shape created in step A7.

B2  Remove balloons #5 and #4 and add a larger balloon B to the structure formed in step B1.  Hold the five balloons in the air and allow the two larger balloons A and B to be in the axial positions and the three smaller balloons #1-3 to form a triangle in the equatorial plane between the two axial balloons.

B3  Hold the five balloons in the air and allow the two larger balloons A and B to be in equatorial positions and the three smaller balloons to be two in axial positions and one in the remaining equatorial position.

B4  Hold the five balloons in the air and allow the two larger balloons A and B to be in an equatorial and an axial position and the tree smaller balloons to be two in equatorial and one in an axial position.

B5  Replace small balloon #3 with the third large balloon C in the shape created in step B4.  Hold the five balloons in the air and allow the two small balloons #1 and #2 to be in equatorial positions and the large balloons A and B in axial positions while large balloon C is in the third equatorial position.

B6  Hold the five balloons in the air and allow the two small balloons #1 and #2 to be in axial positions and the three large balloons A-C to be in equatorial positions.

B7  Hold the five balloons in the air and allow the two small balloons #1 and #2 to be one in an axial position and one in an equatorial position and two of the large balloons A and B to be in equatorial positions and the third C balloon to be in the remaining axial position.

**Pre-Laboratory Questions:** **Name________________**
**Date_________________**

1. What are the five basic common geometric arrangements or shapes of 2-6 total bonding domains and what are the bond angles associated with each shape?

| | Shape | Angle(s) |
|---|---|---|
| $AB_2$ | ________________ | ________________ |
| $AB_3$ | ________________ | ________________ |
| $AB_4$ | ________________ | ________________ |
| $AB_5$ | ________________ | ________________ |
| $AB_6$ | ________________ | ________________ |

2. The mathematical procedure for combining the wave functions is called *orbital hybridization*. What orbitals are combined in the case of carbon _____________ and what four equivalent hybrid orbitals are created this way? _____________ What is the name of the shape of these four equivalent hybrid orbitals?__________________

3. Draw the preferred Lewis structure (minimizing formal charges), predict the geometry or shape of the molecule or ion, and list the hybridized orbitals used by the central atom in the following molecules or ions.

$ClO_4^-$

$SF_4$

$BrF_5$

4. Why are larger balloons used to represent lone pairs of nonbonded electrons?

What does one or more lone pairs of electrons do to the bond angles in a molecule?

**Data and Results:** **Name___________________**
**Date____________________**

**Part A**

A1 The $AB_x$ class of this shape is ____, the B-A-B angle is ___and the shape is ___________

A2 The $AB_x$ class of this shape is ____, the B-A-B angle is ___and the shape is ____________

A3 The $AB_x$ class of this shape is ____, the B-A-B angle is ___and the shape is ____________
Dot to dot distance (cm) balloon 1 to its two neighbors _________, __________
Dot to dot distance (cm) balloon 2 to its two neighbors _________, __________
Dot to dot distance (cm) balloon 3 to its two neighbors _________, __________
Dot to dot distance (cm) balloon 4 to its two neighbors _________, __________

A4 The $AB_x$ class of this shape is ____, the B-A-B angle is ___ in this tetrahedral shape.
Dot to dot distance (cm) balloon 1 to its three neighbors ______, _____, ______
Dot to dot distance (cm) balloon 2 to its three neighbors ______, _____, ______
Dot to dot distance (cm) balloon 3 to its three neighbors ______, _____, ______
Dot to dot distance (cm) balloon 4 to its three neighbors ______, _____, ______

Which shape, that created in A3 or in A4, has the greater dot to dot distances and the greater B-A-B angle?_____________ (name the shape not the step).

A5 $AB_x$ class of this shape is ____, the B-A-B angle from an axial balloon to an equatorial balloon is ___and the B-A-B angle from an equatorial to an equatorial balloon is ____.
The shape is ____________
Greatest dot to dot distance (cm) is ____________between balloon #__ and balloon #__
Smallest dot to dot distance (cm) is ____________between balloon #__ and balloon #__

A6 $AB_x$ class of this shape is ____, the B-A-B angle from an axial balloon to an equatorial balloon is ___and the B-A-B angle from an equatorial to an equatorial balloon is _____.
The shape is ____________
Greatest dot to dot distance (cm) is ____________between balloon #__ and balloon #__
Smallest dot to dot distance (cm) is ____________between balloon #__ and balloon #__

Is the "smallest dot to dot distance" bigger in the shape created in step A5 or in step A6?
_____________ (name the shape not the step).

A7 The $AB_x$ class of the shape producing the greatest dot to dot distance (cm) is ____, the B-A-B angle is ___and the shape is ____________

**Part B**

B1 The $AB_xE_y$ class of this shape is _____, the domain shape (formed by ALL the balloons) is ___________ while the molecular shape (formed by only the smaller balloons) is ____________.

B2 The $AB_xE_y$ class of this shape is _____, the domain shape (formed by ALL the balloons) is ___________ while the molecular shape (formed by only the smaller balloons) is ____________.

B3 The $AB_xE_y$ class of this shape is _____, the domain shape (formed by ALL the balloons) is ___________ while the molecular shape (formed by only the smaller balloons) is ____________.

B4 The $AB_xE_y$ class of this shape is _____, the domain shape (formed by ALL the balloons) is ___________ while the molecular shape (formed by only the smaller balloons) is ____________.

Which molecular shape, that created in B2, B3 or B4, has the largest angle between large & small balloons thus giving them the most room and minimizing their repulsive interactions? ____________________ (name the shape not the step).

B5 The $AB_xE_y$ class of this shape is _____, the domain shape (formed by ALL the balloons) is ___________ while the molecular shape (formed by only the smaller balloons) is ____________.

B6 The $AB_xE_y$ class of this shape is _____, the domain shape (formed by ALL the balloons) is ___________ while the molecular shape (formed by only the smaller balloons) is ____________.

B7 The $AB_xE_y$ class of this shape is _____, the domain shape (formed by ALL the balloons) is ___________ while the molecular shape (formed by only the smaller balloons) is ____________.

Which molecular shape, that created in B5, B6 or B7, has the largest angle between large balloons thus giving them the most room and minimizing their repulsive interactions? ____________________ (name the shape not the step).

**Post-laboratory Questions:** Name___________________
Date____________________

1. Draw a possible Lewis structure for a $IF_7$ molecule. List two possible names for this shape ______________________ or _________________________.
What hybridized orbitals are used by the central iodine atom in this molecule?__________

2. Complete the following table. Some are done for you.

| Molecule | Total Domains | Bonding Domains | Nonbonding Domains | Hybrid Orbitals | Orbital Diagram of Hybridized Orbitals | VSEPR Class | Shape | Polar? Y/N |
|---|---|---|---|---|---|---|---|---|
| $BeCl_2$ | 2 | 2 | 0 | sp | ↑ ↑ | $AB_2$ | linear | N |
| $BF_3$ | | | | | | | | |
| $SnCl_2$ | | | | | ↑↓ ↑↑ | | | |
| $CH_4$ | | | | | | | | |
| $NH_3$ | | | | | | | | |
| $H_2O$ | | | | | | | | |
| $PCl_5$ | | | | | | | | |
| $SF_4$ | | | | | ↑↓ ↑↑↑ ↑ | $AB_4E$ | | |
| $BrF_3$ | | | | | | | | |
| $XeF_2$ | | | | | | | | |
| $SF_6$ | | | | | | | | |
| $IF_5$ | | | | $sp^3d^2$ | | | | |
| $XeF_4$ | | 4 | 2 | | ↑↓ ↑↓ ↑ ↑ ↑↑ | | sq planar | |