Name\_\_\_\_\_ Date

## **ACTIVITY: Molecule Shapes Computer Simulation**

MODEL 1: (http://phet.colorado.edu/en/simulation/molecule-shapes)

## PART I: ELECTRON DOMAINS

1) Explore the *Model* screen of the simulation. As you explore, answer the following questions.

A) How does adding an atom ("bonding") affect the position of existing atoms or lone electron pairs?

B) How does adding a **lone pair (of electrons)** affect the position of existing atoms and lone electron pairs?

2) Is the effect of adding **bonded atoms** and **lone pairs** to the central atom similar? Explain why this could be the case.

We can think of a bond or a lone pair of electrons as a "domain" of electrons. **Single bonds, double bonds, and triple bonds each count as ONE domain.** 

3) How do the electrons in bonds (bonding domains) differ from lone pairs (non-bonding domains)?

4) What happens to the **bond angle** when you add or remove an electron domain? (HINT: under "Options" you can click on the box that says "Show Bond Angles")

5) What is the difference between *Electron Geometry* and *Molecule Geometry*? (HINT: under "Name" you can click on the boxes that say "Molecule Geometry" and "Electron Geometry")

6) In one or two sentences, write a clear definition / explanation for the term *Molecule Geometry*.

## PART 2: DRAWING MOLECULES TO SHOW 3-DIMENSIONALITY

MODEL 2: Line, Wedge and Dash Drawings	
Line: In the plane of the paper:	
Wedge: Coming forward, in front of the plane of the paper:	
<b>Dash</b> : Going backward, behind the plane of the paper:	_
1) Where is each of the 5 atoms in the molecule CHFClBr? In the plane of the paper: In front of the plane of the paper: Behind the plane of the paper:	H C

2) Using the *Model* screen, add bonding domains (●) to the central atom (○). Using lines, wedges and dashes from Model 2, draw each molecule's shape.

Bonding Domains Around Central Atom	Drawing of Shape	Electron Geometry	Bond Angles	
2	•-0-•	Linear	180º	
3	0			
4	ο			

3) In the following table, sketch and record the **molecular geometry** and make a sketch of the molecule **\*Possible molecule geometries are: Bent, linear, tetrahedral, trigonal planar & trigonal pyramid\*\*** 

Predict First, Then Compare with the Simulation						
Number of Domains Around Central Atom (Bonds and Lone Pairs)	0 Lone Pairs	1 Lone Pair	2 Lone Pairs	3 Lone Pairs		
2						
3						
4						

## EXERCISES:

\*Possible electron geometries are: \*Possible molecule geometries are: \*Possible bond angles are: Bent, linear, tetrahedral, trigonal planar & trigonal pyramid\*\* Bent, linear, tetrahedral, trigonal planar & trigonal pyramid\*\* 90°, 109.5°, 120°, 180°\*\*

1) A molecule has 2 double bonds on the central atom and no lone pairs. Predict the electron geometry. Predict the molecule geometry. What do you think the bond angles would be?

Electron geometry:\_\_\_\_\_

Molecule geometry:\_\_\_\_\_

Bond angles:

2) For each of the molecules below, determine the electron geometry, molecule geometry, and label the bond angles. Draw pictures to show your geometries.

A) CCl<sub>4</sub> (4 Cl atoms, no lone pairs on C)

B)  $PF_3$  (3 F atoms, 1 lone pair on P)

C) OF<sub>2</sub> (2 F atoms, 2 lone pairs on O)

D) H<sub>2</sub>O (Oxygen in center; 2 H atoms; 2 lone pairs on O)