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Molecule Shapes Simulation

Go to our class web site and tap on the Digital Content tab. Then scroll down to the end of Unit 3 for the simulation. In this simulation, you'll be exploring the shapes of various molecules and what happens to the shape when more 'stuff' is added to a molecule.

Part 1: Electron Domains

1. Explore the *Model* screen of the simulation. As you explore, answer the following questions:
   A. How does adding an **atom** affect the position of existing atoms or lone pairs?

   B. How does adding a **lone pair** affect the position of existing atoms and lone 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?

5. Can you force the atoms into new configurations by pushing atoms around? What does this suggest about the configuration of atoms in real molecules?

6. What is the difference between *Electron Geometry* and *Molecule Geometry*?

7. In one or two grammatically correct sentences, write a definition for the term *Molecule Geometry*.

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Part 2: Drawing Molecules to Show 3-Dimensionality (Model 2)

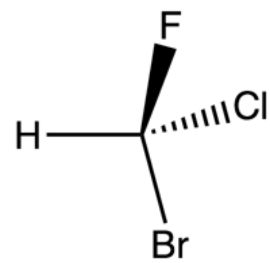
Line, Wedge and Dash Drawings

Line: In the plane of the paper:

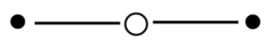
Wedge: Coming forward, in front of the plane of the paper: 

Dash: 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 _____



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		Linear	180°
3	○		
4	○		
5	○		
6	○		

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3. In the *Model* screen, build a molecule with 5 atoms attached to the central atom. Look at the molecule geometry and electron geometry. **Predict** what will happen to the molecule geometry as you replace atoms with lone pairs.

Your Prediction:

4. In the following table draw the **molecule geometry**. As a group, make a **prediction for each first**, and then compare you answers with the simulation.

Number of Domains Around Central Atom	1 Lone Pair	2 Lone Pairs	3 Lone Pairs	4 Lone Pairs
3				
4				
5				
6				

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Part 3: Comparing Model vs. Real Molecules

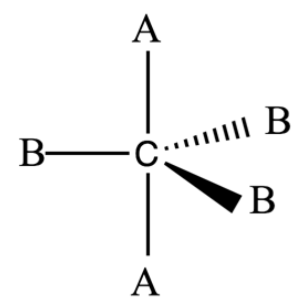
1. Explore the *Real Molecules* screen.
   C. List the molecules that show a **difference in bond angle** between 'Real' and 'Model'. Note: differences in bond angle may be small.

Molecule	Number of Lone Pair Domains

   D. What do all of the molecules in the table have in common?

   E. What trend do you observe that distinguishes lone pairs from bonding pairs?

2. Use the simulation to build a system with 5 domains. This is called a trigonal bipyramidal structure. The two different sites in a trigonal bipyramid are labeled as A and B in the drawing to the right.
   F. Each A tom is adjacent to 3 B atoms. What is the A-C-B bond angle?



   G. Each B atom is adjacent to 2 A atoms and 2 B atoms. What is the B-C-B bond angle?

   H. In a system with 4 atoms and 1 lone pair, predict whether the lone pair will be in a B site or an A site. Explain.

   I. Examine the molecule SF_4 in the Real Molecules screen to check your prediction from question C. Which interactions are more important in determining where the lone pair will go?