**Name \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Period \_\_\_\_\_ Date \_\_\_\_\_\_\_\_\_\_**

**Determining Shapes of Molecules and Polarity**

**Background Information:**

The most common chemical bond between two atoms is a covalent bond and occurs in molecules and polyatomic ions. The covalent bond consists of at least one pair of electrons shared between two atoms. In addition to the shared electrons in the bonds, the atoms in molecules have unshared electrons. The negative charge of the electrons causes them to repel each other so that electron pairs, whether shared or unshared, are as far apart as possible. This is the premise of the VSEPR Theory. VESPR Theory states that bonding and non-bonding electron pairs in a molecule will adopt a geometry or shape in which the distance between the electron pairs is maximized from one another in order to minimize the repulsions. (Xie, 2005)

By writing a Lewis electron structure for a molecule, the number of shared electron pairs (bonds) and unshared electron pairs around a central atom can be counted. Once the number of shared and unshared electron pairs around a central atom is known, the shape of the molecule can be determined. If there are more unshared electron pairs and bonds around the central atom the angle between bonding atoms is less, and if there are fewer unshared electron pairs and bonds around the central atom, the angle between bonding atoms is greater. As these angles vary, the molecular shape will vary. See Table 1. This is shown by examining diagrams of CO2 and CH4. Carbon dioxide has 2 bonds and no unshared pairs on the central ‘C’ atom and the angle between the bonding oxygen atoms is 180˚ which results in a linear shape. Methane (CH4) has 4 bonds and no unshared pairs on the central atom and the angle between the bonding hydrogen atoms is 109˚ which results in a tetrahedral shape.

|  |  |
| --- | --- |
| CO2 | CH4 |
| http://chemlabs.uoregon.edu/GeneralResources/models/grf/CO2.gif | http://chemlabs.uoregon.edu/GeneralResources/models/grf/CH4.gif |

Molecules composed of covalently bonded atoms are described as polar or nonpolar depending on their shape and the distribution of electrons. For a molecule to be polar, it must have an **uneven** distribution of electrons which makes one end of the molecule more negative and one end more positive. Nonpolar molecules have a perfectly symmetrical or **even** electron distribution which causes both sides of the molecule to be electrically balanced. If there are more unshared electron pairs on one side of a molecule than the other, the molecule is polar. And, if there are more electronegative atoms on one side of the molecule than the other, the molecule is polar.

In this experiment, you will write Lewis Electron Dot Structures to determine the number of shared and unshared electron pairs around a central atom and build models of some simple molecules. Based on the model of the molecule, the shape and the polarity can be determined.

Xie, L. (2005, April 4). *Vsepr theory*. Retrieved from <http://www.uwosh.edu/faculty_staff/xie/tutorial/vsepr.htm>

**Pre-Lab Questions**:

1. Identify the following compounds as covalent or ionic and draw Lewis Electron Structures.
2. CaBr2 b. BaS
3. CF4 d. SeO3
4. Examine your Lewis Structures for CF4 and SeO3. Which of these molecules would have the greater bond angle? Explain why.

3. Go to the phet website and choose “Chemistry”, “Molecule Shapes” tab “Model”. Make models for CF4 and SeO3. Check the boxes for ‘show bond angles’, ‘show lone pairs’, and ‘molecular geometry’. Verify or revise your answer above regarding the bond angles.

**Table 1: Shapes of Molecules; Number of Bonds and Unshared E- Pairs on Central Atom**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Bonds on Central Atom** | **Unshared E- Pairs on Central Atom** | **Shape** | **Ideal Bond Angle (example bond angle)** | **Example** | **Image** |
| 2 | 0 | linear | 180° | [CO2](http://en.wikipedia.org/wiki/Carbon_dioxide) | [Linear-3D-balls.png](http://en.wikipedia.org/wiki/File:Linear-3D-balls.png) |
| 3 | 0 | trigonal planar | 120° | CH2O | [Trigonal-3D-balls.png](http://en.wikipedia.org/wiki/File:Trigonal-3D-balls.png) |
| 2 | 1 | bent | 120° (119°) | SO2 | [Bent-3D-balls.png](http://en.wikipedia.org/wiki/File:Bent-3D-balls.png) |
| 4 | 0 | tetrahedral | 109.5° | CH4 | [AX4E0-3D-balls.png](http://en.wikipedia.org/wiki/File:AX4E0-3D-balls.png) |
| 3 | 1 | pyramid | 109.5° (107.5°) | NH3 | [NH3 One Carbon Three Hydrogen](http://newenergyandfuel.com/wp-content/uploads/2008/09/nh3.png) |
| 2 | 2 | bent | 109.5° (104.5°) | H2O | [Bent-3D-balls.png](http://en.wikipedia.org/wiki/File:Bent-3D-balls.png) |
| 1 | 1, 2, 3 | linear | No angle | O2 | Structure |

**Materials:** Ball and stick model kit

**Procedure:**

1. Make a data table that includes: Molecular Formula, Lewis Structure (make this column big), Sketch of Ball and Stick Model, Shape of Molecule, Molecular Polarity
2. Include the following molecules: H2, HBr, NCl3, H2S, CH2Br2, HOCl, SeO2,

N2, SO3, SiH4, OF2, H2CO, PH3, CH3Cl, HCN, CS2, CH3SH, NO2+, CO3-2, C2H3F

1. With your partner, build models of basic molecules using the provided kit.
2. Sketch the models into your data table, and determine the shape and the molecular polarity.
3. Use the black ball(s) (4 holes) for your central atom(s) and multi colored balls for bonding atoms.
4. Use short sticks for single bonds and long sticks for double or triple bonds.
5. To check the shape, use Phet simulation from CU or <http://www.chemeddl.org/>.

For Phet, go to: http://phet.colorado.edu/en/simulation/molecule-shapes

Click on “Play with Sims”. Select “chemistry”. Select “Molecule Shapes”. Click on “Run Now”. Choose the “Model” Tab. Now, build your molecule and compare shapes. You a can also use “Build a Molecule” and the “Larger Molecule” tab.

**Analysis Questions:**

1. Describe the difference between bonding or shared electrons and unshared (nonbonding) electrons.
2. How many shared electron pairs and unshared electron pairs are on the central atom, P, in PH3? What shape is the result of this combination of shared and unshared electron pairs?
3. Determine the shapes of SO3 and SO3-2. Explain why the shapes are different.

Hint: Draw Lewis Structures first.

1. Which molecule has a greater bond angle: CS2 or SO2? Explain why referring to diagrams.
2. Identify the side of the molecule that is more negative and the side that is more positive in each of the following molecules: CO HF HCN Hint: Consider electronegativity

Explain each answer.

1. Explain why CF4 is nonpolar and CHF3 is polar.
2. Explain why CS2 is nonpolar and SO2 polar.