# Molecular Geometry
## Investigating Molecular Shapes with VSEPR using J-Mol software

### OBJECTIVE
Students will explore Lewis structures of selected substances and then represent the structures on paper after building models using molecular model kits. The molecular geometry of the molecule, hybridization, the polarity and the IMF's will be determined for each of the substances.

### LEVEL
Chemistry

### NATIONAL STANDARDS
UCP.2, UCP.5, B.2

### CONNECTIONS TO AP
AP Chemistry:

I. Structure of Matter B. Chemical Bonding 2. Molecular models a. Lewis structures b. Valence bond; hybridization of orbitals, resonance, sigma and pi bonds c. VSEPR

### TIME FRAME
45 minutes

### MATERIALS
(For a class of 28 working in pairs)

14 model sets

14 Computers with internet access

### TEACHER NOTES
Each student pair will need a model kit containing 4, 5, and 6 holed central atoms.. If you are using model kits it is a good idea to explain the relationship between the number of holes on the central atom and the sites of electron density in a Lewis structure. Constructing double bonds should also be discussed.

This lesson is designed to follow an introduction to Lewis structures for covalent compounds. Students should also have been introduced to the concept of hybridization. During a pre-lab discussion you should demonstrate the Lewis structures and corresponding geometries for several of the example compounds in the reference table on the student pages.

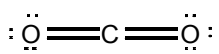
VSEPR (Valence Shell Electron Pair Repulsion) is a simple model that employs the concept that electrons, being negatively charged, are repulsive. Therefore, regions of electron densities will attempt to position themselves as far away from one another as possible. Regions of electron density are as follows:

- Single bond
- Double bond
- Triple bond
- Lone pair

These regions get increasingly more repulsive moving down the list. You will find a table of basic VSEPR molecular geometries, along with examples of molecular species that exhibit that molecular geometry, on the student instruction page. Note that lone pairs are more repulsive than any of the bonds. This is because they are only influenced by one nucleus rather than two nuclei. For this reason, lone pairs take up more space and will cause the other bond angles to be smaller. In general, each lone pair will collapse the bond angle by approximately $2^o$ per lone pair.

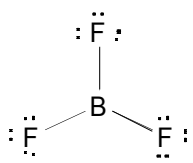
## ANSWERS TO THE QUESTIONS

1. $CO_2$



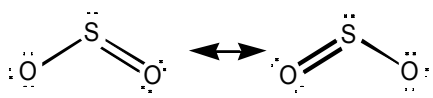
Molecular geometry: linear
Bond angle: 180
Hybridization: sp
Polarity: NP
IMF: LDF

2. $BF_3$



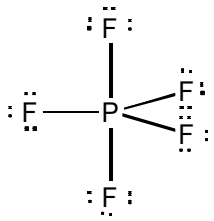
Molecular geometry: trigonal planar
Bond angle: 120
Hybridization: $sp^2$
Polarity: NP
IMF: LDF

3. $SO_2$



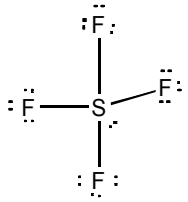
Molecular geometry: bent (2 resonance structures)
Bond angle: 118.7
Hybridization: $sp^2$
Polarity: P
IMF: LDF; dipole-dipole

4. $PF_5$



Molecular geometry: trigonal bipyramid
Bond angle: 90, 120
Hybridization: $sp^3d$
Polarity: NP
IMF: LDF

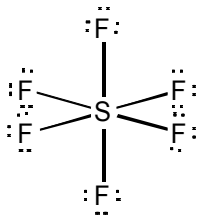
5. $SF_4$



Molecular geometry: see-saw

Bond angle: 87.4
Hybridization: $sp^3d$
Polarity: P
IMF: LDF, dipole-dipole

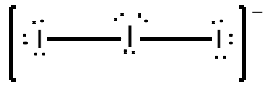
6. $SF_6$



Molecular geometry: octahedral

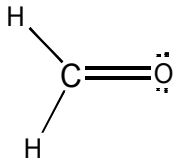
Bond angle: 90
Hybridization: $sp^3d^2$
Polarity: NP
IMF: LDF

7. $I_3^-$



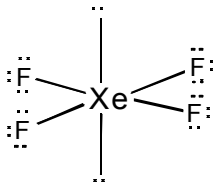
Molecular geometry: linear
Bond angle: 180
Hybridization: $sp^3d$
Polarity: NP
IMF: NA

8. $H_2CO$



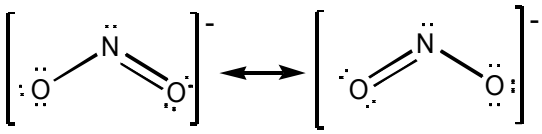
Molecular geometry: trigonal planar
Bond angle: 114.9; 122.5
Hybridization: $sp^2$
Polarity: P
IMF: LDF, dipole-dipole

9. $XeF_4$



Molecular geometry: square planar
Bond angle: 90
Hybridization: $sp^3d^2$
Polarity: NP
IMF: LDF

10. $NO_2^-$



Molecular geometry: bent
(2 resonance structures)
Bond angle: 116.4
Hybridization: $sp^2$
Polarity: P
IMF: NA

# Molecular Geometry
## Investigating Molecular Shapes with VSEPR using J-Mol software

The shape of a molecule will dictate many physical and chemical properties of a substance. In biological systems many reactions are controlled by how substrate and enzyme molecules fit together. Physical properties of substances, such as solubility and boiling point are also influenced by molecular geometry.

### PURPOSE
Students will explore Lewis structures of selected substances and then represent the structures on paper after building models using molecular model kits. The molecular geometry of the molecule, hybridization, the polarity and the IMF's will be determined for each of the substances.

### MATERIALS
14 model sets

14 Computers with internet access

### PROCEDURE
1. All of the substances on your student answer page are covalent molecules or polyatomic ions.

2. Draw Lewis dot structures in the space provided on your student answer page. Use the VSEPR theory to predict the molecular geometry of each molecule or ion listed on your student answer page.

3. Use the model kits provided to build each chemical species.

4. Use the J-Mol software to find the species and compare your model to the computer model.

5. Follow the instructions to find the bond angle for the central atom. Write this number in the space provided.

6. Write the hybridization of the orbitals in the space provided for each substance.

7. Use the software to find the molecular dipole. If there is a dipole, the molecule is polar. If there is no dipole, the molecule is nonpolar. Write this answer in the space provided. Draw an arrow on all polar substances showing the net pull on the central atom.

8. Predict the type(s) of intermolecular forces that might be found in a pure sample of each of the substances. Write your answer in the space provided.

Name _____

Period _____

# Molecular Geometry
## Investigating Molecular Shapes with VSEPR

VSEPR (Valence Shell Electron Pair Repulsion) is a simple model that employs the concept that electrons, being negatively charged, are repulsive. Therefore, regions of electron densities will attempt to position themselves as far away from one another as possible. Regions of electron density are as follows:

- Single bond
- Double bond
- Triple bond
- Lone pair

These regions get increasingly more repulsive moving down the list. The following table is provided as a reference for basic VSEPR molecular geometries. In the table that follows, M represents the central atom, X represents the terminal or surrounding atoms and E represents lone pairs of electrons.

| Regions of Electron Density | Representative Formula | Example | Molecular Geometry | Hybridization |
|---|---|---|---|---|
| 2 | $MX_2$ | $CO_2$ | Linear (180°) | sp |
| 3 | $MX_3$ | $BF_3$ | Trigonal planar (120°) | $sp^2$ |
| 3 | $MX_2E$ | $SO_2$ | Bent (118°) | $sp^2$ |
| 4 | $MX_4$ | $CH_4$ | Tetrahedral (109.5°) | $sp^3$ |
| 4 | $MX_3E$ | $NH_3$ | Trigonal pyramidal (107°) | $sp^3$ |
| 4 | $MX_2E_2$ | $H_2O$ | Bent (105°) | $sp^3$ |
| 5 | $MX_5$ | $PF_5$ | Trigonal bipyramidal | $sp^3d$ |
| 5 | $MX_4E$ | $SF_4$ | See Saw | $sp^3d$ |
| 5 | $MX_3E_2$ | $ICl_3$ | T-shaped | $sp^3d$ |
| 5 | $MX_2E_3$ | $I_3^-$ | Linear | $sp^3d$ |
| 6 | $MX_6$ | $SCl_6$ | Octahedral | $sp^3d^2$ |
| 6 | $MX_5E$ | $XeF_5^+$ | Square pyramidal | $sp^3d^2$ |
| 6 | $MX_4E_2$ | $ICl_4^-$ | Square planar | $sp^3d^2$ |

## QUESTIONS

**1. $CO_2$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**2. $BF_3$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**3. $SO_2$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**4. $PF_5$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**5. $SF_4$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**6. $SF_6$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**7. $I_3^-$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____NA_

**8. $H_2CO$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**9. $XeF_4$**

Molecular geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF _____

**10. $NO_2^-$**

Molecular
geometry _____

Bond angle _____

Hybridization _____

Polarity _____

IMF ____NA____