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.

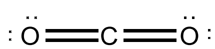
VSEPR (Valence Shell Electron Pair Repulsion) is a simple model that employs the concept that electrons, being negatively charged, are repulsive. Therefore, regions of electron densities will attempt to position themselves as far away from one another as possible. Regions of electron density are as follows:

- 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.

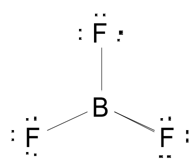
ANSWERS TO THE QUESTIONS

1. CO_2



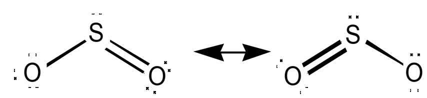
Molecular geometry: linear
Bond angle: 180
Hybridization: sp
Polarity: NP
IMF: LDF

2. BF_3



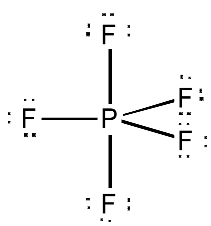
Molecular geometry: trigonal planar
Bond angle: 120
Hybridization: sp^2
Polarity: NP
IMF: LDF

3. SO_2



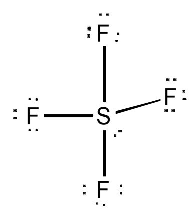
Molecular geometry: bent (2 resonance structures)
Bond angle: 118.7
Hybridization: sp^2
Polarity: P
IMF: LDF; dipole-dipole

4. PF_5



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

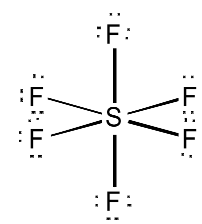
5. SF_4



Molecular geometry:
see-saw

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

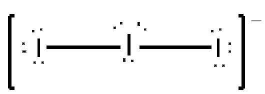
6. SF_6



Molecular geometry:
octahedral

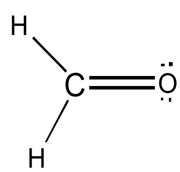
Bond angle: 90
Hybridization: sp^3d^2
Polarity: NP
IMF: LDF

7. I_3^-



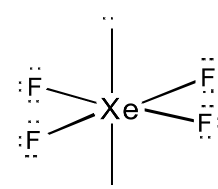
Molecular geometry:
linear
Bond angle: 180
Hybridization: sp^3d
Polarity: NP
IMF: NA

8. H_2CO



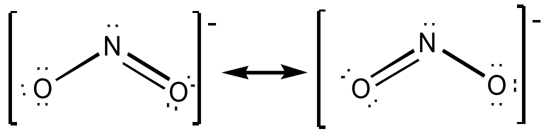
Molecular geometry:
trigonal planar
Bond angle: 114.9; 122.5
Hybridization: sp^2
Polarity: P
IMF: LDF, dipole-dipole

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____