Name _____ Date _____

Experiment 9, Structure of Molecules

Chemistry 201, Wright College, Department of Physical Science and Engineering

VSEPR Theory and Molecular Modeling with Ball-and-Stick Models

Many of the physical and chemical properties of molecules depend on the types of atoms in the molecule and the bonds that connect them. These properties are also affected by the way the atoms are arranged in space or the shape of a molecule. Therefore, the structural study of a chemical species (molecule, ion) is a very important field. Chemists can predict the shapes of many molecules from the chemical formula by drawing Lewis dot formulas and applying **Valence Shell Electron Pair Repulsion (VSEPR) theory**. VSEPR theory states that *electron pairs in a valence shell of an atom repel other electron pairs, and they minimize repulsion by making the angles between them as large as possible.*

In general, the electron geometry is based on the total number of electron pairs around the central atom. The molecular geometry is based on the balance of the bonding electron pairs and the lone pairs around the central atom. Generally, molecules are polar if the central atom has lone pairs of electrons (*except, linear molecular geometry of trigonal bipyramidal electron geometry and square planar molecular geometry of octahedral electron geometry).

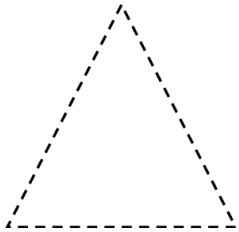
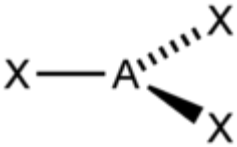
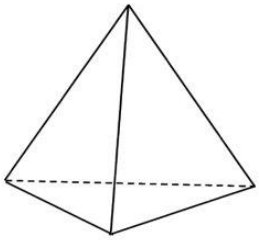
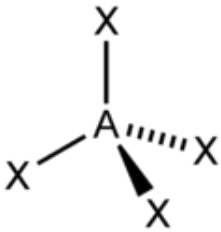
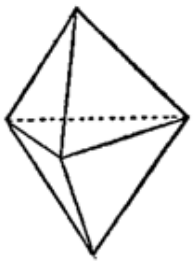
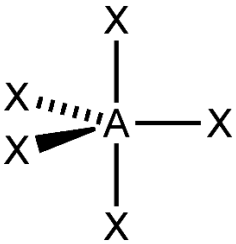
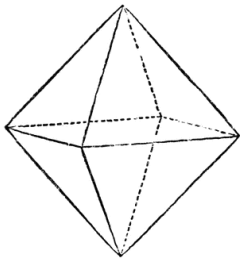
Summary of Molecular Structures and Polarity from the VSEPR Theory

Pairs of electrons around central atom	Electron Geometry	Bonding Pairs	Lone Pairs	Molecular Geometry	Example	Polarity
2	Linear	2	0	Linear	$BeCl_2$	No
3	Trigonal Planar	2	1	Bent	SO_2	Yes
		3	0	Trigonal planar	BCl	No
4	Tetrahedron	2	2	Bent	SCl_2	Yes
		3	1	Trigonal pyramidal	PCl_3	Yes
		4	0	Tetrahedron	CCl_4	No
5	Trigonal Bipyramid	2	3	Linear	$XeCl_2$	*No
		3	2	T-shape	ClF_3	Yes
		4	1	Seesaw	SCl_4	Yes
		5	0	Trigonal bipyramidal	PF_5	No
6	Octahedron	4	2	Square planar	XeF_4	*No
		5	1	Square pyramidal	BrF_5	Yes
		6	0	Octahedral	SeF_6	No

Molecular geometry of molecules and ions (based on electron geometry)

AX Type:	always linear	Examples: HCl, CO, OH^{1-}
AX_2 Type:	linear (linear) or bent (trigonal planar)	CO_2, H_2O, SO_2
AX_3 Type:	trigonal planar (trigonal planar) or trigonal pyramidal (tetrahedral)	SO_3, CO_3^{2-}, NH_3
AX_4 Type:	planar (octahedral), tetrahedral (tetrahedral), or seesaw (trigonal bipyramidal)	CH_4, XeF_4, SCl_4
AX_5 Type:	trigonal bipyramidal (trigonal bipyramidal) or square pyramidal (octahedral)	PCl_5, IF_5
AX_6 Type:	octahedral (octahedral)	SF_6

Electron Arrangements with Minimum Repulsion

# Areas of e^- Density	Electron Geometry	Arrangement	
2	Linear		
3	Trigonal Planar		
4	Tetrahedral		
5	Trigonal Bipyramidal		
6	Octahedral		

Determination of hybridization and bond angles:

# of electron sets	Electron Geometry	Hybridization	Bond angle
2	Linear	sp	180°
3	Trigonal Planar	sp^2	120°
4	Tetrahedron	sp^3	109.5°
5	Trigonal Bipyramid	sp^3d	90° and 120°
6	Octahedron	sp^3d^2	90°

PROCEDURE

The objective of this exercise is to predict the structure and simple properties of a molecule based on its Lewis electron dot formula and the Valence Shell Electron Pair Repulsion (VSEPR) theory.

For the given molecules, apply the following guidelines and label as shown for the CO_2 example.

1. Draw the Lewis electron dot formula:

a. Calculate the total number of valence electrons. If it's a cation, subtract electrons equal to the charge. If it's an anion, add electrons equal to the charge.

b. The least electronegative atom should be placed at the center of the molecule. The H atom is an exception, it must always be an outer atom. Use a pair (2) of electrons between the central atom and each outer atom. Subtract electrons from total.

c. Distribute remaining electrons around the outer atoms and obey the octet rule. The H atom is an exception, it can never have more than 2 (bonding) electrons. Subtract electrons from total.

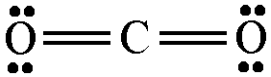
d. Distribute remaining electrons to the central atom. Subtract electrons from total.

e. Check: Does the central atom have at least 8 electrons? If yes, done. If no, move nonbonding electron pairs from the outer atoms in to form multiple bonds.

2. Count the total number of pairs of electrons (bonding and lone pairs) around the central atom and determine the electron geometry. From the electron geometry, determine the hybridization and the bond angles.

3. Identify the number of bonding pairs of electrons and the number of nonbonding pairs of electrons around the central atom. Determine the molecular geometry and polarity.
4. Select the ball in the model kit that represents the central atom. Add outer atoms to the bonding electron pairs in the central atom to have a particular 3-D structure (molecular geometry).

EXAMPLE: Carbon dioxide, CO_2

CO_2		Lewis Dot Structure	Molecular Geometry drawing
Total # of valence electrons	16		**O------C------O**
Central Atom	C		
# of pairs of electrons around the central atom	"2"		
Electron geometry	linear		
Bond angles	180°		
Hybridization	sp		
# of lone pairs on central atom	0		
# of bonding pairs on central atom	"2"		
Molecular geometry	linear		
Polar or nonpolar?	nonpolar		

Multiple bonds are counted as "1" pair of electrons. Therefore, CO_2 has "2" pairs of electrons around the C atom. Thus the electron geometry is linear.

For trigonal bipyramidal molecular geometry drawings, lone pairs should be in the equatorial positions.

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REPORT SHEET

Structure of Molecules

PBr_5		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

H_2O		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

XeF_4		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

SCl_6		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

SCl_4		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

PCl_3		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

SO_2		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

IF_5		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

CCl_4		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

BF_3		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

ClF_3		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

XeF_2		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

BeH_2		Complete Lewis Structure-show bonds and electron dots	Molecular Geometry drawing
Total # of valence electrons			
Central Atom			
# of pairs of electrons around the central atom			
Electron geometry			
Bond angles			
Hybridization			
# of lone pairs on central atom			
# of bonding pairs on central atom			
Molecular geometry			
Polar or nonpolar?			

1. Predict the H—O—H bond angle in H_3O^+. Draw a structure to illustrate.

2. Predict the F—Sn—F bond angle in SnF_6^{2-}. Draw a structure to illustrate.

3. Why is the H—O—H bond angle in a water molecule (H_2O) smaller than the H—C—H bond angle in methane (CH_4).

4. Draw the structure for $SCl_3F_2^+$. Place the F atoms in the axial positions and the Cl atoms in the equatorial positions. Label all bond angles.