Name _____**Chem 162, Section**: _____**Group Number:** _____

ALE 12. Valence Shell Electron Pair Repulsion Theory (VSEPR)

(Reference: Section 10.2 - *Silberberg 5th edition*)

Why are molecules shaped the way they are?

The Model: Regions of Electron Density and AX_n Systems

After we've drawn a valid Lewis structure (or developed a set of resonance structures) for a compound, we can predict the molecular geometry (*i.e.* 3-D shape and bond angles). We start off by classifying each central atom (*i.e.*, one bound to two or more atoms) by the number of regions of electron density around it. A region of electron density is either a bond (of any bond order) or a lone pair of nonbonding electrons. Each bond (whether it be a single bond or a triple bond, or anything in between) and each lone pair counts as one "region of electron density".

All regions of electron density around a central atom repel each other. In order to minimize the repulsions, the regions of electron density arrange themselves around the atom so that they are as far away from each other as possible (while still belonging to the central atom).

If ***n*** is the number of regions of electron density ("**X**") around the central atom ("**A**"), then we classify it as "$\mathbf{AX}_{\boldsymbol{n}}$". By classifying each central atom as AX_n, we can predict the measurement of an angle X—A—X (*i.e.*, an angle between two regions of electron density with A at the vertex). The five commonly-encountered AE_n systems are: **AX_2, AX_3, AX_4, AX_5, and AX_6**.

Let's start off by looking at the first one, AX_2. To minimize the repulsions between neighboring regions of electron density around A, they get as far away from each other as possible. This has the effect of maximizing the measurement of the X—A—X angle. The maximum possible angle is 180°, so a central atom with two regions of electron density will be at the vertex of a 180° bond angle. If that atom determines the geometry of the molecule, it is called a linear molecule.

Key Questions

1a. In the gas phase, aluminum chloride is molecular. Aluminum is an example of an element that very often forms stable compounds that have Lewis structures that violate the Octet Rule. What is the preferred number of bonds of an atom in the Boron family? _____ in the Fluorine family?_____ Draw the Lewis structure of $AlCl_3$:

b. Classify the central atom in $AlCl_3$ as an AX_n system and predict what the measure of the Cl—Al—Cl bond angle is.

c. The molecular geometry of $AlCl_3$ is called "trigonal planar". Explain why.

2a. The molecular compound $SnCl_2$ has also been observed in the gas phase. Draw the Lewis structure of $SnCl_2$. (Like Al in $AlCl_3$, the Sn in $SnCl_2$ does not have an octet of valence electrons.)

b. Fact: The Cl—Sn—Cl bond angle in $SnCl_2$ has been determined to be 98.2°.
Which of the following does this fact suggest about the relative repulsions between lone pairs and bonding pairs? (Circle the correct answer.)

i. The repulsion between a lone pair and a bonding pair is greater than the repulsion between two bonding pairs.

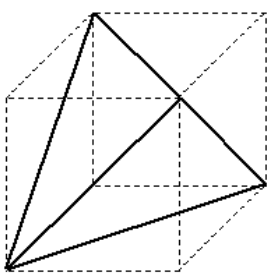
ii. The repulsion between a lone pair and a bonding pair is about the same as the repulsion between two bonding pairs.

iii. The repulsion between a lone pair and a bonding pair is less than the repulsion between two bonding pairs.

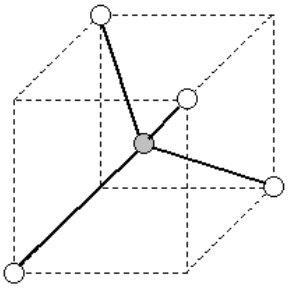
c. The name of the geometry of electron density around the Sn is called "***trigonal planar***". But the molecular geometry of $SnCl_2$ is called "angular" (or "bent" by other people). Why would the name of the molecular geometry (*i.e.*, geometry of "atomic connectivity") be different from the name of the geometry of electron density around a central atom?

The Model: Species with Tetrahedral Electron Densities

A ***tetrahedron*** is a four-sided polyhedron in which the faces are equilateral triangles. Starting with a cube, one can envision a tetrahedron as sitting in the cube such that the edges of the tetrahedron are coincident with the face diagonals of the cube (as shown below on the left).



an outlined tetrahedron



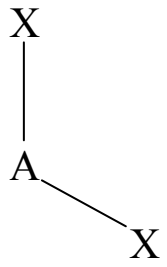
a tetrahedral structure

When there are four regions of charge around a central atom, the geometry of electron density around the atom is called ***tetrahedral***. The central atom A may be thought of as being in the center of a cube while the four regions of electron density are directed to different corners of the cube (as shown in the above figure on the right). The ideal X—A—X angle has a measurement of ***~109.5°***.

Key Questions

3. Use molecular models to build ***tetrahedral*** and ***square planar*** AX_4 models. Convince yourself and your teammates that a tetrahedral arrangement of electron density around a central atom has less repulsions than a square planar arrangement. Convince me in writing.

4. A ***tetrahedral*** arrangement of electron density is three dimensional. However, when we represent a tetrahedral structure on paper, it becomes 2-D. So that a reader will still "see" the 3-D nature of the tetrahedral structure, we use "bold wedges" (▬◀) to represent something coming toward us (*i.e.*, out of the plane of the paper) and "dashed wedges" (▮▮▮▮▮▮) to represent something going away from us (*i.e.*, into the plane of the paper). Any three points define a plane, so the central A and two of the regions of electron density (X's) are understood to be in the plane of the paper if they are connected by thin solid lines (as is shown to the right). Complete the above figure so that it depicts a tetrahedral arrangement of electron density around a central atom, using bold and dashed wedges to give it a 3-D look.



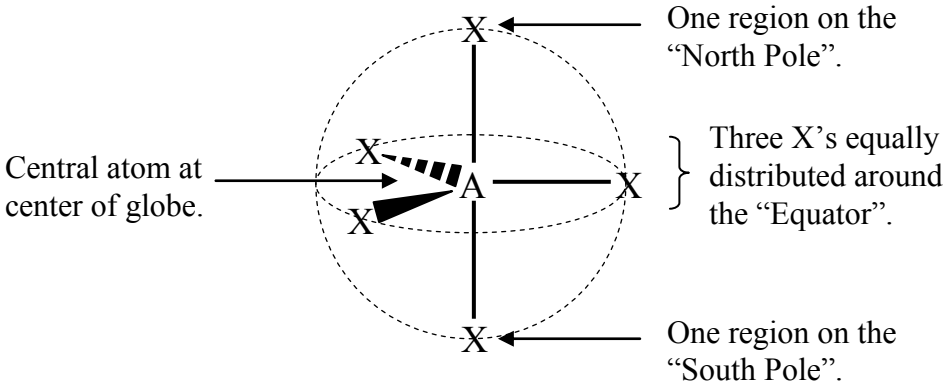
5. When a central atom has four regions of electron density around it but one or two of the regions are lone pairs, the molecular geometry is called "***trigonal pyramidal***" or "***bent***", respectively, instead of "tetrahedral".

a. Draw Lewis structures of H_2O and NH_3.

b. Redraw H_2O and NH_3, this time using bold and dashed wedges to represent bonds to the hydrogen atoms or lone pairs (whichever is appropriate) coming out and going into the plane of the paper. Briefly explain the reason why the molecular geometry of H_2O is called "bent" and why the molecular geometry of NH_3 is called "trigonal pyramidal".

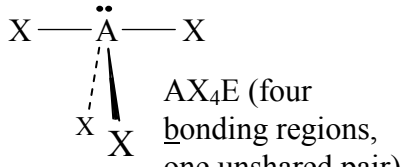
The Model: Species with Trigonal Bipyramidal Electron Densities

In an AX_5 system, the central atom is surrounded by five regions of electron density. In order to minimize repulsions, the electron density takes a ***trigonal bipyramidal*** shape, which may perhaps best be visualized superimposed on a "globe":



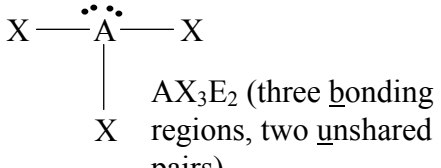
We learned before (Question 2b) that the repulsion between lone pairs and bonding pairs is greater than the repulsion between two bonding pairs. Even greater repulsions exist between two lone pairs. 120° interactions between two lone pairs are okay, but two lone pairs are NEVER observed in Nature to be 90° from each other.

When a compound has a central atom surrounded by five regions of charge, one or more of which is a lone pair, in order to minimize repulsive forces, the following molecular shapes are observed:



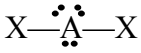
AX_4E (four bonding regions, one unshared pair)

"**See saw**"



AX_3E_2 (three bonding regions, two unshared pairs)

"**T-shaped**"



AX_2E_3 (two bonding regions, three unshared pairs)

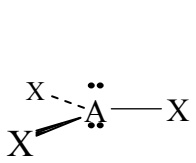
"**Linear**"

Key Questions

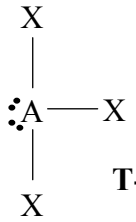
6. Now consider *all* of the possible ideal bond angles that are likely to be observed in a molecule in which the central atom has *five regions* of electron density around it—i.e. AX_5.
   a.) What is *the angle of* X—A—X for regions of electron density on the "Equator"?

   b.) What is *the angle of* X—A—X for one region of electron density on the "Equator" and another on a "pole"?

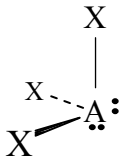
7. In an AX_3E_2 system (*i.e.*, one in which the central atom has three regions of bonding electron density and two lone pairs), the three possible molecular shapes are:



Trigonal planar



T-shaped



distorted trigonal pyramidal

a. Build each of these, one at a time, with molecular models. Use hydrogen (white) to represent the X and small gray connectors to represent lone pairs. In each, determine the number of 90° interactions between two lone pairs ("E-E") and lone pairs and bonding pairs ("E-X") and enter this information in the table below. Fill in the table on the Recorder's Report.

	Trigonal planar	**T-shaped**	**distorted trigonal pyramidal**
90° E-E			
90° E-X			

b. Briefly explain why <u>*only*</u> the T-shaped geometry exists and <u>*not*</u> the other two.

8a. Draw Lewis structures for $XeOF_4$ and XeF_4. (*Hint*: A noble gas has 8 valence electrons.)

b. Both $XeOF_4$ and XeF_4 are classified as $\mathbf{AX_6}$ systems and, therefore, possess octahedral electron density geometries. But the molecular geometry of $XeOF_4$ is called "square pyramidal" and the molecular geometry of XeF_4 is called "square planar". Explain why these molecules are given these names instead of "octahedral". [*Hint*: Redraw $XeOF_4$ (the four fluorine atoms are in the same plane) and XeF_4, this time using bold and dashed wedges to represent bonds to fluorine atoms coming out and going into the plane of the paper.]