WS 7: The VSEPR Model: Part 2: Molecular Geometries: Where do the lone pairs go?

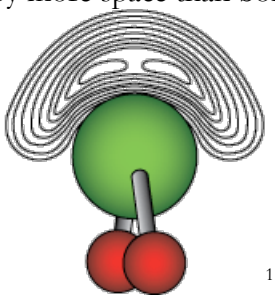
We see that the Electron Domain Geometries don't give information about the placement of the lone pairs around the central atom. In this handout, we will practice drawing VSEPR molecules with the lone pairs, connecting Electron Domain Geometries with Molecular Geometries.

- Molecular geometries are based on the VSEPR or Electron Domain Geometries.
- While the Electron Domain Geometries show all the bonding regions, nonbonding pairs are not part of the description of the molecular geometry.

SUMMARY:

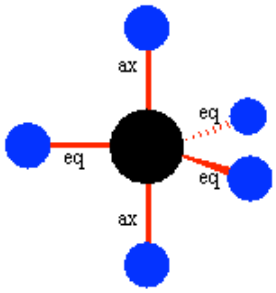
- Draw the lewis structure of the molecule or ion
- Count the number of electron domains around the central atom, remembering that each lone pair, each single bond, each double bond, and each triple bond count as one reagion of electron density or 1 domain. (a triple bond is one domain, not three!)
- Arrange the domains around the central atom to minimize 90° lone-pair lone-pair repulsions.
    - Lone-pairs occupy more space than bonding regions.

This map is a little closer to the the true electron density of the two lone pairs of the oxygen in water.



[1]

    - Lone pairs lead to distortion in the molecular geometry.
- The arrangement of the bonding regions determines the molecular geometry
- The 90° lone-pair issue becomes important when central atoms violate the octet rule.
    - Trigonal bipyramidal-Lone pairs must go equatorial
    - Octahedral: lone pairs must go axial



[2]

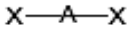
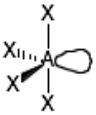
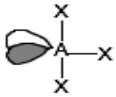
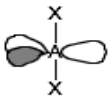
[1] http://xaktly.com/Images/Chemistry/VSEPR/Water_VSEPRImage02.png

[2] http://www.angelo.edu/faculty/kboudrea/general/shapes/shape5_equatorial.gif

Part 1: Electron Domains and Molecular Geometries

Placement of the lone pairs:

Table 1:Formulas, Electron Pair Geometry, and Molecular Geometry

		No. of regions					
Formula	Example	Lone	Bonding	Total	Shape	RED	Molecular geometry
AX_2	$BeCl_2$	0	2	2		Linear	Linear
AX_3	BF_3	0	3	3		Trigonal planar	Trigonal planar
AX_2E	$SnCl_2$	1	2	3			Bent
AX_4	CF_4	0	4	4		Tetrahedral	Tetrahedral
AX_3E	NF_3	1	3	4		Tetrahedral	Trigonal pyramidal
AX_2E_2	OF_2	2	2	4		Tetrahedral	Bent
AX_5	PCl_5	0	5	5		Trigonal bipyramidal	Trigonal bipyramid
AX_4E	SF_4	1	4	5		Trigonal bipyramidal	Irregular tetrahedron, distorted tetrahedron, seesaw
AX_3E_2	ClF_4	2	3	5		Trigonal bipyramidal	T-shaped
AX_2E_3	XeF_2	3	2	5		Trigonal bipyramid	Linear

Formula	Example	No. of regions: Lone	Bonding	Total	Shape	RED	Molecular geometry
AX_6	SF_6	0	6	6		Octahedral	Octahedral
AX_5E	BrF_5	1	5	6		Octahedral	Square pyramid
AX_4E_2	XeF_4	2	4	6		Octahedral	Square planar

Part 2: Drawing Molecules

molecualr fomula → Lewis Structure → Electron Domain Group → VSEPR → 3-D drawing

For the next section of the text, you need to be able to draw three-dimensional models of molecules. Fortunately, there are basic rule that you can follow to help you in this process.

Rules:

- Look at your Lewis structure. The central molecule is the starting point for drawing 3–D representations.
- You have three fundamental positions on the molecule that you need to draw: in the plane, out of the plane away from you, and out of the plane towards you.
- For regions of electron density in the plane of the paper, draw a line
- For regions of electron density out of the plane of the paper away from you, draw a dotted line.
- Put lone pairs in a lobe shaped orbital. These are easiest to draw in the plane of the paper.
- For regions of electron density out of the plane and toward you, draw a dark wedge or slanted triangle.

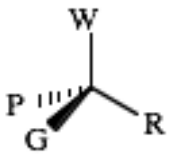


Figure 1: Reference model

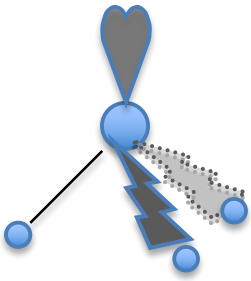
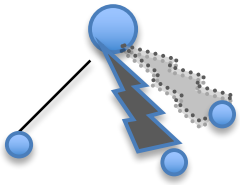
1. Practice drawing the shapes of molecules listed in the table below. Show lone pairs in orbitals. Use the drawings in your book and table 1 to help you. There might be more then one shape for some of the families

Table 2:Practice drawing Molecular Geometries

:Shape name of electron domains	Molecular geometries
Linear Hint: these shapes are in your book	Example 
Trigonal planar (and related shapes)	
Tetrahedral (and related shapes)	
Trigonal bipyramidal (and related shapes)	
Octahedral and related shapes.	

- Working with the information for drawing **Lewis structures**, and the information about molecular and electron geometries, draw the electron domain and the molecular geometry for each structure.
- Remember, the electron geometry of a molecule shows lone pairs and bonding pairs, the molecular geometry does not show lone pairs about the central atom.
- Molecules that exhibit three-dimensionality shape must be represented with wedge and dot drawings. Please give reasonable drawings. If the molecule has resonance, draw only one of the resonance structures. If you need more room, use the back of the page. Please keep your work organized and the molecules in order. **(My picture looks funny because I don't have a molecular drawing program. I think you get the general idea. Use your drawing skills and draw the best you can. Lone pairs are in teardrop shapes, not hearts)**

Table 3:Practicing Drawing Electronic and Molecular Geometries of Specific Molecules

NH_3		NO_3^{1-}	
Electron Geometry	Molecular Geometry	Electron Geometry	Molecular Geometry
			
ICl_2^{1-}		ICl_4^{+}	
Electron Geometry	Molecular Geometry	Electron Geometry	Molecular Geometry

CO_2		CH_4	
Electron Geometry	Molecular Geometry	Electron Geometry	Molecular Geometry
BF_3		PCl_5	
Electron Geometry	Molecular Geometry	Electron Geometry	Molecular Geometry
SF_6		XeF_4	
Electron Geometry	Molecular Geometry	Electron Geometry	Molecular Geometry