CHE 2060: Principles of Organic Chem

> VSEPR & molecular geometry

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2. Intro to organic structure & bonding, II

Valence shell electron pair repulsion (VSEPR) and molecular geometry

This material is adapted from Flowers et al, 'Chemistry', OpenStax, 2018

Please note that Wikipedia has an excellent VSEPR page with clear models and explanations of each molecular and electron pair geometry: https://en.wikipedia.org/wiki/VSEPR_theory

What is VSEPR?

Valence shell electron pair repulsion (VSEPR), allows for *some prediction* of molecular structure and geometry from the bonding patterns of the molecule's central atom.
- VSEPR is **not** a perfect predictor!

VSEPR uses the **electrostatic repulsion** of the pairs of electrons that make up both covalent bonds and lone pairs to assume that those pairs will repel one another, seek to **maximize the inter-pair distance** between one another and thus determine the **molecule's shape or geometry**.

VSPER starts with Lewis dot structures and then counts:
1. The **number of atoms** bonded to the central atom; and
2. The **number of lone electron pairs** on the central atom.
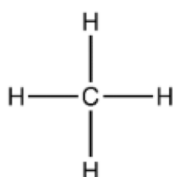
VSEPR charts (1)

Number of regions	Two regions of high electron density (bonds and/or unshared pairs)	Three regions of high electron density (bonds and/or unshared pairs)	Four regions of high electron density (bonds and/or unshared pairs)	Five regions of high electron density (bonds and/or unshared pairs)	Six regions of high electron density (bonds and/or unshared pairs)
Spatial arrangement	180° **sp**	120° **sp^2**	109.5° **sp^3**	90° 120° **sp^{3}d**	90° 90° **sp^{3}d^2**
Line-dash-wedge notation	H—Be—H	H–B(–H)(–H)	H–C(–H)(–H)(–H)	F–P with F, F, F, F	S with F, F, F, F, F, F
Electron pair geometry	Linear; 180° angle	Trigonal planar; all angles 120°	Tetrahedral; all angles 109.5°	Trigonal bipyramidal; angles of 90° or 120° An attached atom may be equatorial (in the plane of the triangle) or axial (above or below the plane of the triangle).	Octahedral; all angles 90° or 180°

VSEPR charts (2)

atoms bonded to the central atom

	Number of electron pairs	Electron pair geometries: 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
sp	2	180° X—A—X Linear				
sp²	3	120° Trigonal planar	<120° Bent or angular			
sp³	4	109° Tetrahedral	X<109° Trigonal pyramid	<<109° Bent or angular		
sp³d	5	120° 90° Trigonal bipyramid	<120° <90° Sawhorse or seesaw	<90° T-shape	180° Linear	
sp³d²	6	90° Octahedral	<90° Square pyramid	90° Square planar	X<90° T-shape	180° Linear

VSEPR charts (3)

# lone e- pr	# atoms bonded	e- pair geometry		Molecular geometry	Bond Angle (°)
0	2	linear **sp**		linear	180
0	3	trigonal planar	**sp²**	trigonal planar	120
1	2	trigonal planar		bent	< 120
0	4	tetrahedral		tetrahedral	109.5
1	3	tetrahedral	**sp³**	trigonal pyramidal	< 109.5
2	2	tetrahedral		bent	<109.5
0	5	trigonal bipyramidal		trigonal bipyramidal	90, 120, 180
1	4	trigonal bipyramidal	**sp³d**	seesaw	90, 120, 180
2	3	trigonal bipyramidal		T-shaped	90, 180
3	2	trigonal bipyramidal		linear	180
0	6	octahedral		octahedral	90, 180
1	5	octahedral	**sp³d²**	square pyramidal	90, 180
2	4	octahedral		square planar	90, 180

http://intro.chem.okstate.edu

Here's a simple example

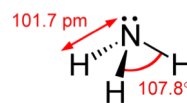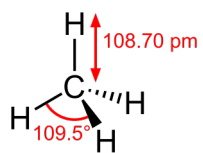Let's look at the gas beryllium fluoride, BeF2.
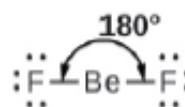
Electron pair vs molecular geometry?

Let's compare methane (CH4) and ammonia NH3.
- Begin with their Lewis structures.
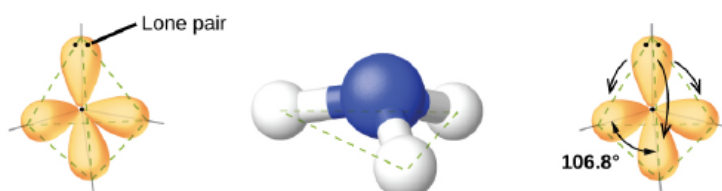
Lone pairs distort geometry

Notice that methane has perfect tetrahedral angles of 109.5°.
* But the inter-hydrogen angles of ammonia are closer, 107.8°.

Why?
The lone pair is more electronegative– more repulsive - than the covalent bonds and pushes the bonds further away and closing the angles to less than 109.5°.

Strength of repulsion:
lone pair – lone pair > lone pair – bond pair > bond pair - bond pair

## Lone pairs occupy equatorial positions

The **geometrical location of lone pairs** isn't random, but is determined by their greater repulsive power.
* Lone pairs **occupy more space** than bonded atoms.
* **Equatorial** positions offer more space than axial positions.

Notice that lone pairs always occupy equatorial positions here in trigonal bipyramidal geometries.
* The number of lone pairs changes the apparent – or **molecular geometries** – of molecules even when the central atoms has a constant orbital hybridization.
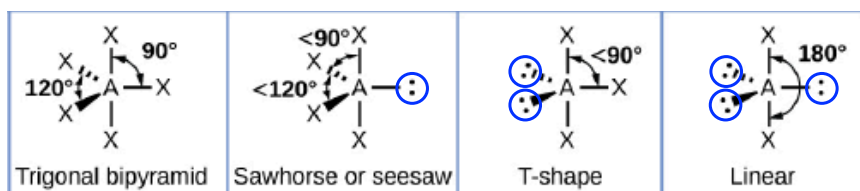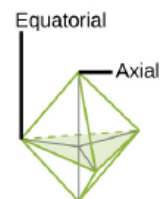
Try this:

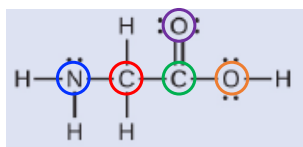Use VSEPR to predict: 1) electron pair geometry; and 2) molecular geometry of
- CO_2
- BCl_3

VSEPR exercises:

For each non-H atom of the amino acid glycine, use VSEPR to predict:
(1) orbital hybridization;
(2) electron pair geometry; and
(3) molecular geometry

VSEPR exercises:

Use VSEPR to predict: (1) electron pair geometry; & (2) molecular geometry of
- CO_3^{-2} ion
- NH_4^{+1} ion
- PF_5
- H_2O
- H_3O^{+1} ion
- SF_4
- XeF_2
- XeF_4

Can you?

(1) Explain what VSEPR stands for?

(2) Explain why the concept of repulsion can determine molecular shape?

(3) Explain the steps required to use VSEPR to determine orbital hybridization, electron pair geometry and molecular geometry?

(4) Apply VSEPR to predict orbital hybridization, electron pair and molecular geometry?

(5) Describe why lone pairs have more 'repulsive power' than covalent bonding pairs of electrons?

(6) Explain why the number of lone pairs can change molecular geometry?