N19 - VSEPR and the 3D Geometry of Molecules

Target:

I can identify the 3-dimensional shape of molecules.

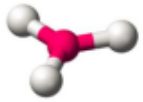
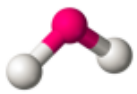
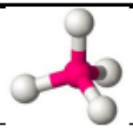
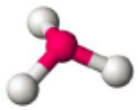
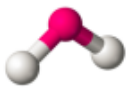
Link to YouTube Presentation: https://youtu.be/zvTSm6kT7C0

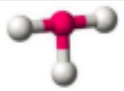
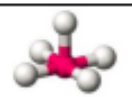
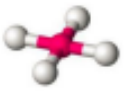
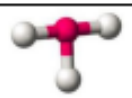
Make a big obvious note to yourself in your notebook...

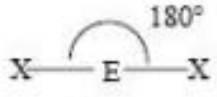
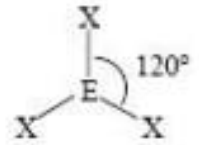
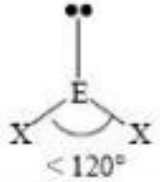
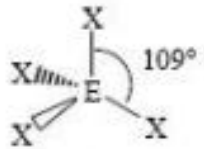
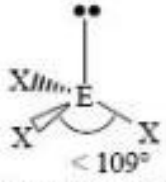
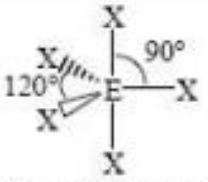
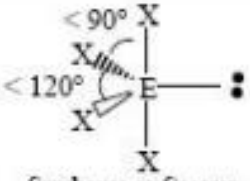
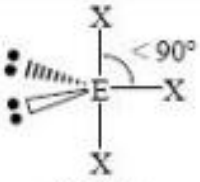
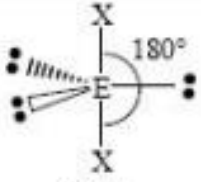
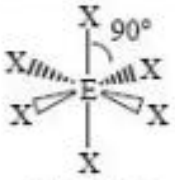
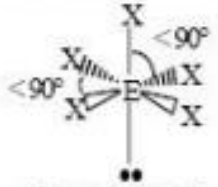
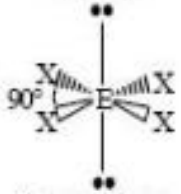
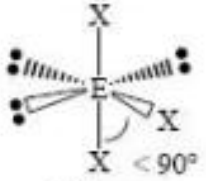
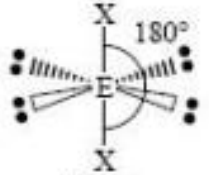
- **LOOK AT VSEPR CHART IN REFERENCE SHEET SECTION OF BINDER!!!!!**

VSEPR

Valence Shell Electron Pair Repulsion

Steric #	X	E	"generic" Looking at shape of everything attached	"specific" Only looking at shape of atoms		
Electron Pairs	**Bonded Pairs**	**Lone Pairs**	**Electron Geometry** (hybridization)	**Molecular Geometry** (AXE Formula)	**Bond Angles**	**3-D example**
2	1	1-3	Linear (sp)	Linear (AXE, AXE_2, AXE_3)	180	
	2	0		Linear (AX_2)		
3	3	0	Trigonal Planar (sp^2)	Trigonal Planar (AX_3)	120	
	2	1		Bent (AX_2E)	< 120	
4	4	0	Tetrahedral (sp^3)	Tetrahedral (AX_4)	109.5	
	3	1		Trigonal Pyramidal (AX_3E)	< 109.5	
	2	2		Bent (AX_2E_2)	<< 109.5	

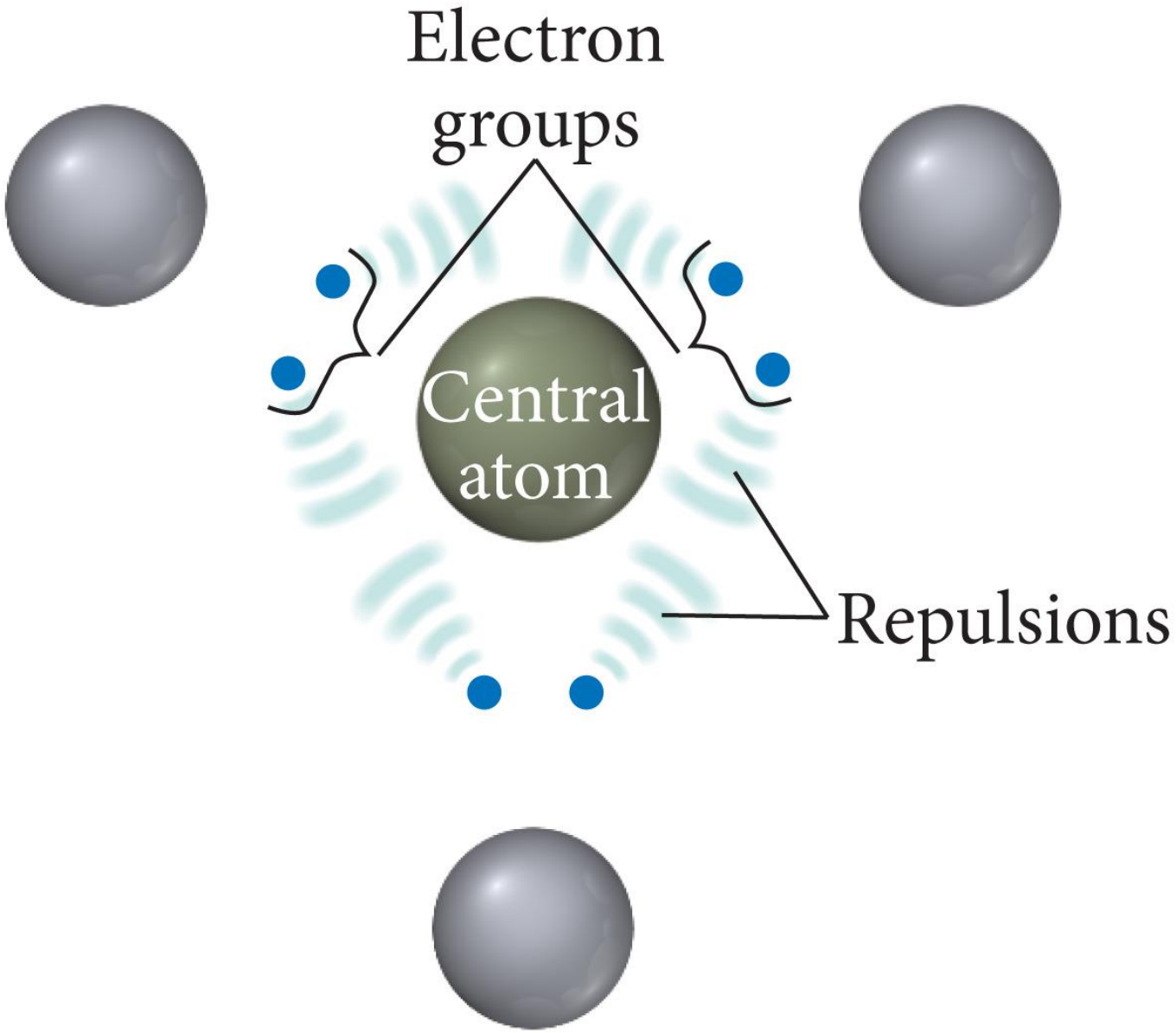
Steric #	X	E	"generic" Looking at shape of everything attached	"specific" Only looking at shape of atoms	*it is unclear if d orbitals hybridize – currently we think they do not.	
Electron Pairs	**Bonded Pairs**	**Lone Pairs**	**Electron Geometry** (hybridization)	**Molecular Geometry** (AXE Formula)	**Bond Angles**	**3-D example**
5	5	0	Trigonal Bipyramidal (sp^3d^*)	Trigonal Bipyramidal (AX_5)	90 Axial (above & below) 120 Equatorial (in plane)	
	4	1		Seesaw (AX_4E)	90 120 180	
	3	2		T-Shaped (AX_3E_2)	90 180	
	2	3		Linear (AX_2E_3)	180	
6	6	0	Octahedral (sp^3d^2*)	Octahedral (AX_6)	90	
	5	1		Square Pyramidal (AX_5E)	90 180	
	4	2		Square Planar (AX_4E_2)	90 180	
	3	3		T-Shaped (AX_3E_3)	90 180	
	2	4		Linear (AX_2E_4)	180	

VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 **Linear**				
3	 **Trigonal Planar**	 **Bent or Angular**			
4	 **Tetrahedral**	 **Trigonal Pyramid**	 **Bent or Angular**		
5	 **Trigonal Bipyramid**	 **Sawhorse or Seesaw**	 **T-shape**	 **Linear**	
6	 **Octahedral**	 **Square Pyramid**	 **Square Planar**	 **T-shape**	 **Linear**

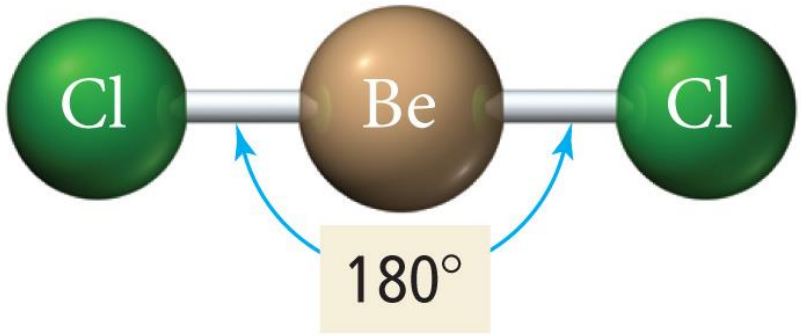
VSEPR Model

(Valence Shell Electron Pair Repulsion)

- **The structure around a given atom is determined (*mostly)* by minimizing electron pair repulsions.**
- **They try to maximize the distance between electrons**

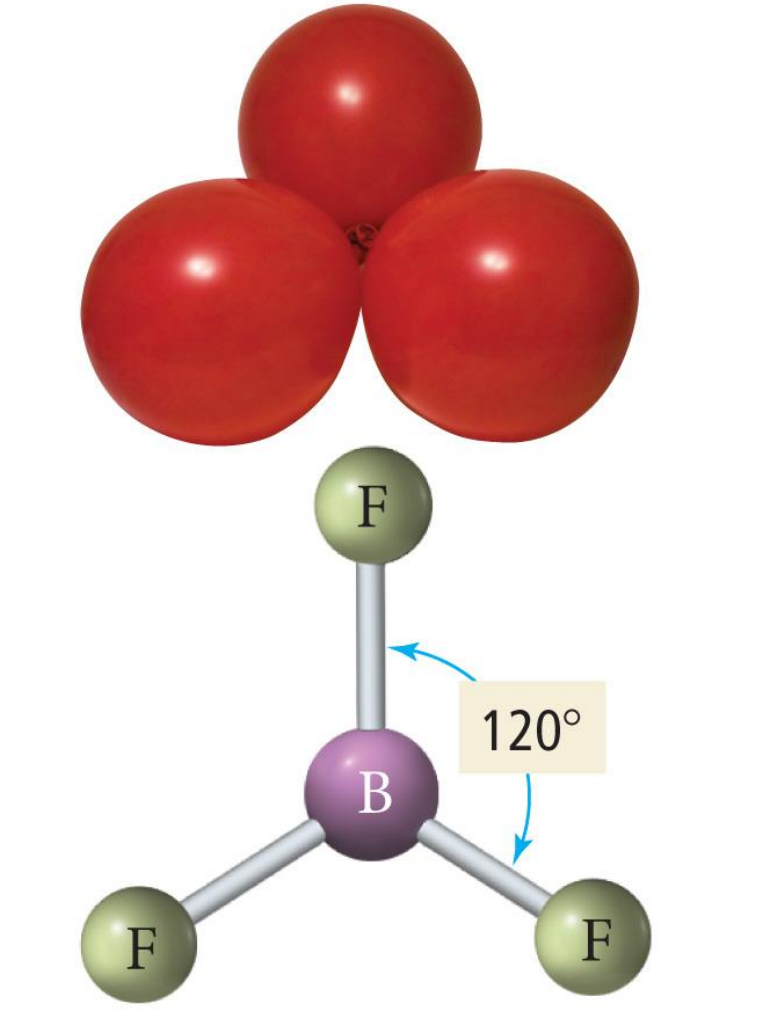

Electron groups
Central atom
Repulsions

Linear Geometry



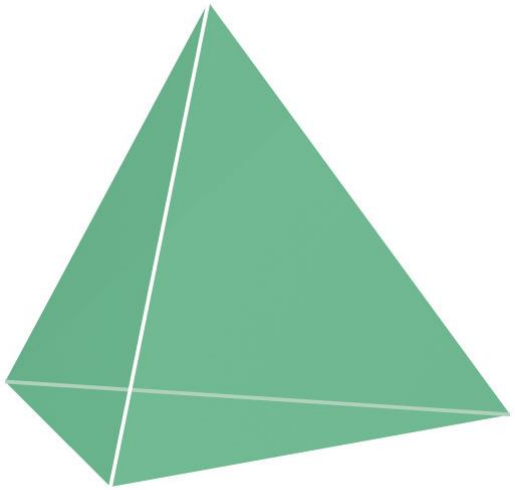
(a) Linear geometry

Trigonal Planar Geometry

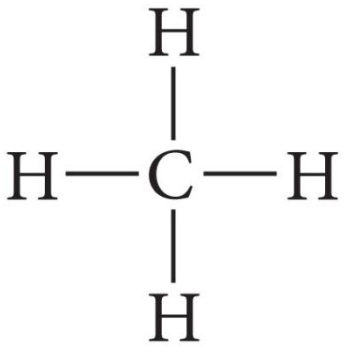


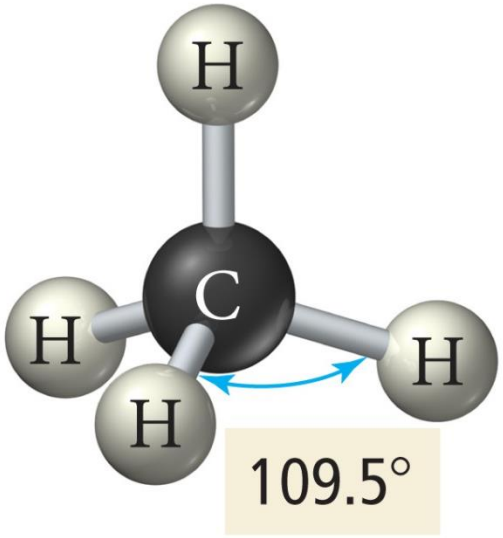
(b) Trigonal planar geometry

Tetrahedral Geometry



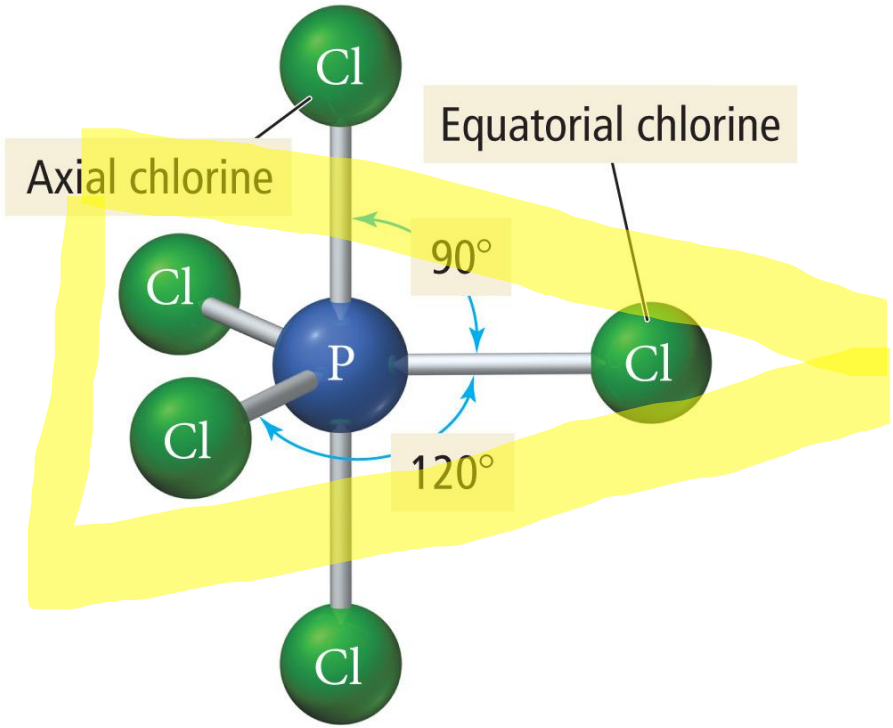
Tetrahedron

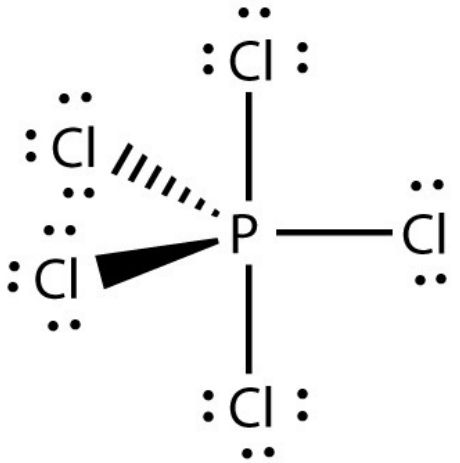




Tetrahedral geometry

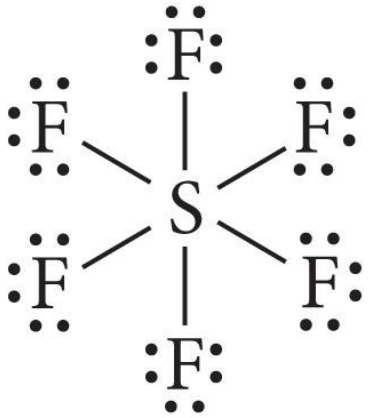
Trigonal Bipyramidal

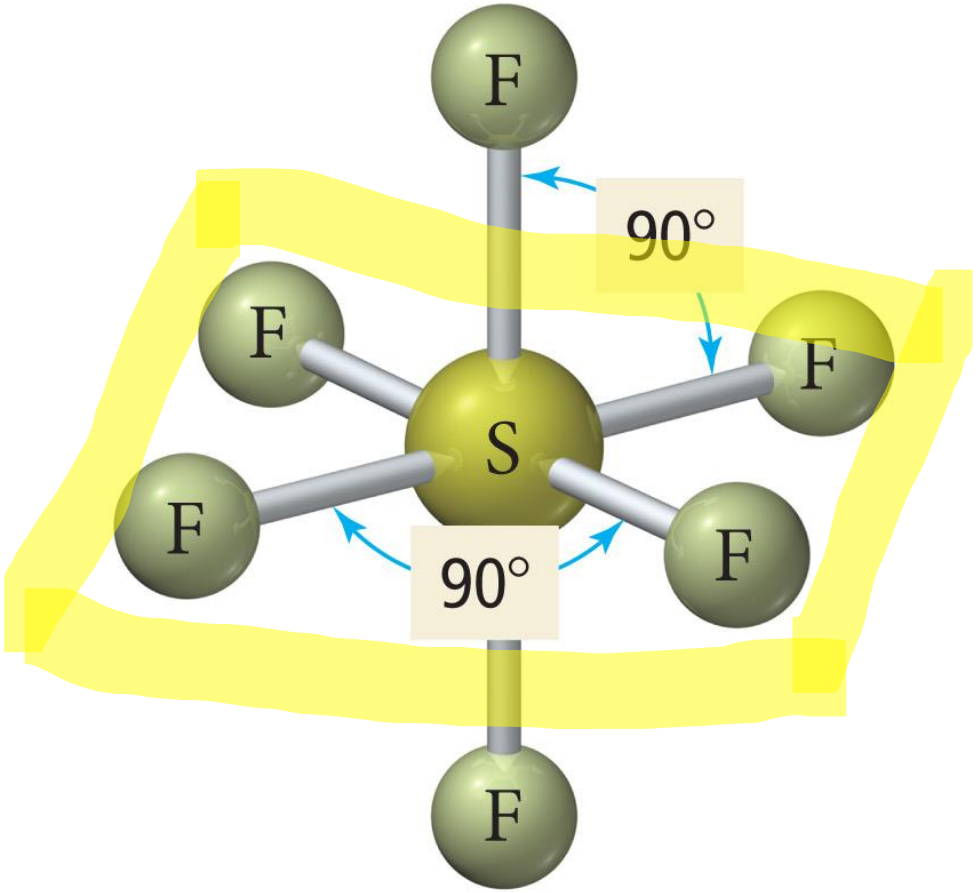




Trigonal bipyramidal geometry

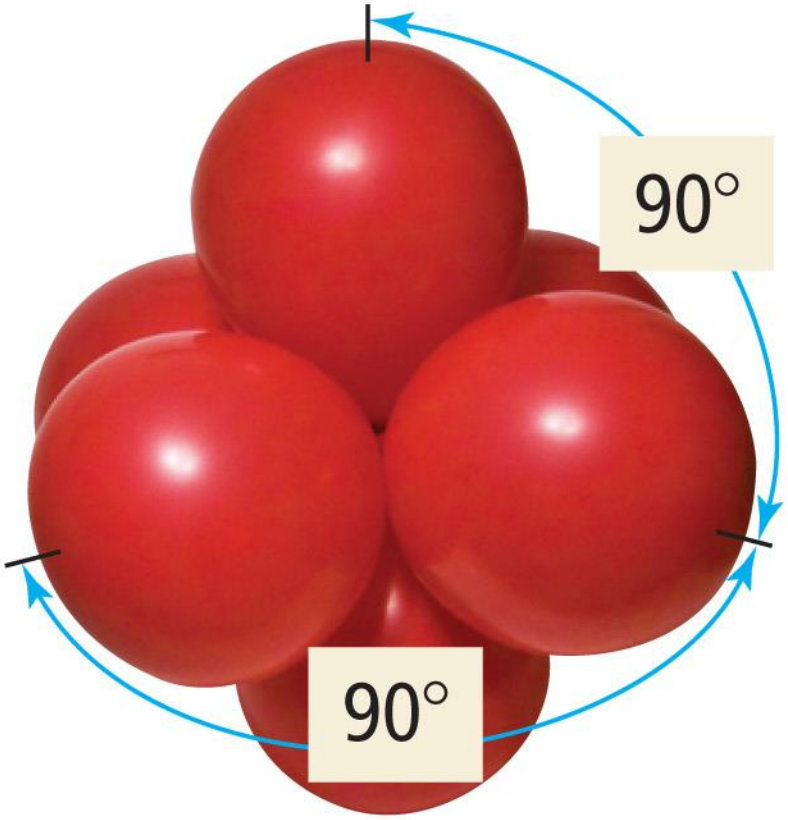
Octahedral Geometry

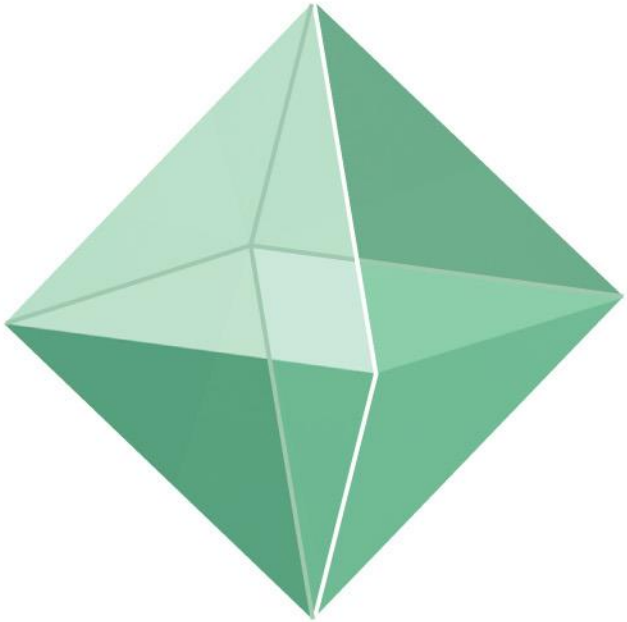




Octahedral geometry

Octahedral Geometry





Octahedral geometry

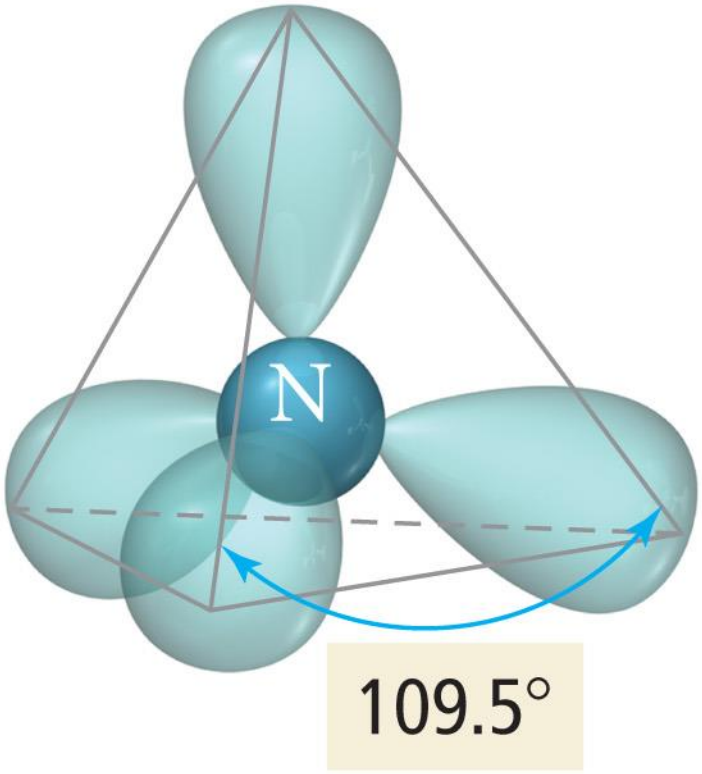
Octahedron

The Effect of Lone Pairs

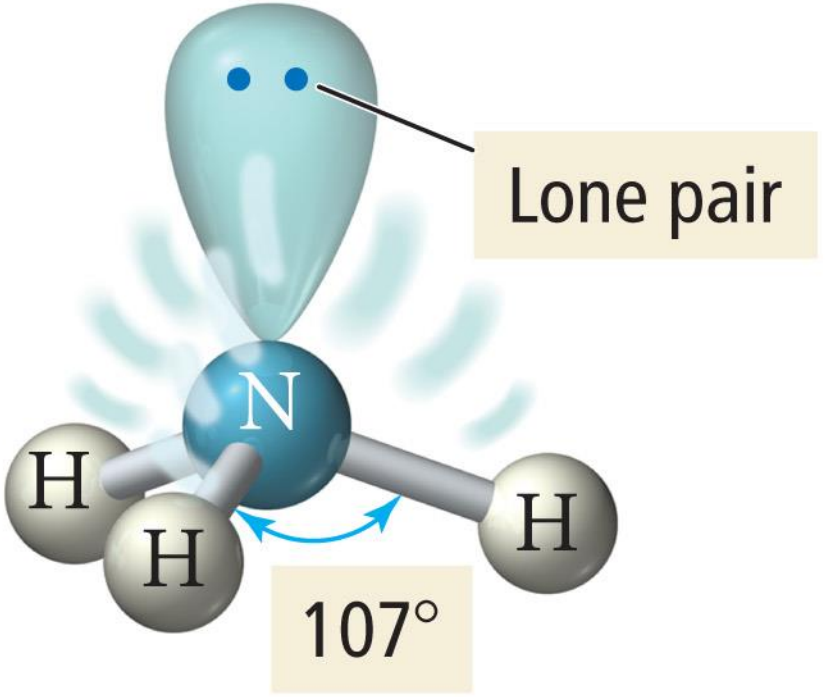
- Lone pair = “occupy more space”
- This affects the bond angles, making the bonding pair angles smaller than expected.
- Pushes the atoms out of the way
- Relative sizes of repulsive force interactions is as follows:

Lowest: **Bonding Pair – Bonding Pair**
Medium: **Lone Pair – Bonding Pair**
Highest: **Lone Pair – Lone Pair**

Bond Angle Distortion from Lone Pairs

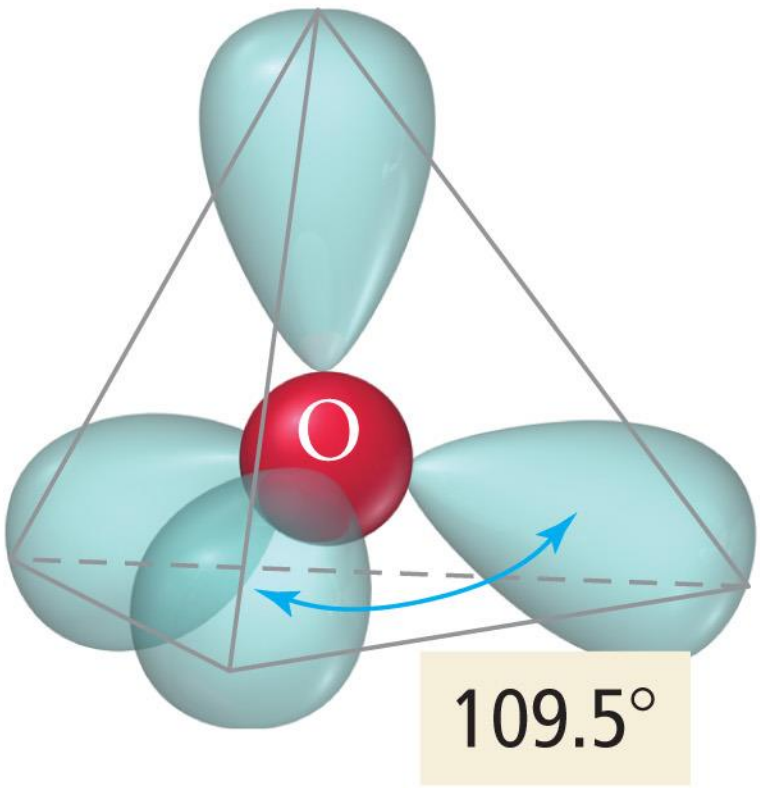


Ideal tetrahedral geometry

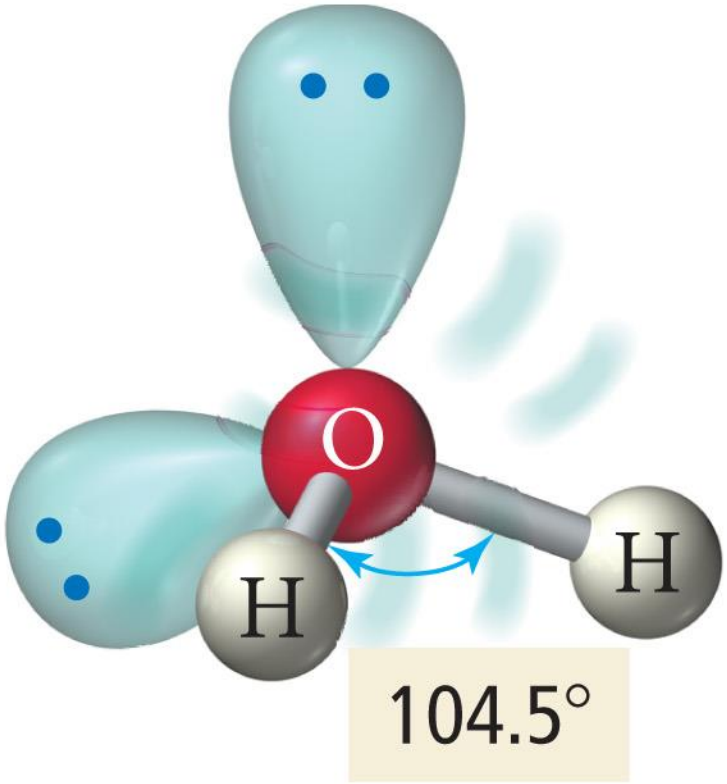


Actual molecular geometry

Bond Angle Distortion from Lone Pairs



Ideal tetrahedral geometry



Actual molecular geometry

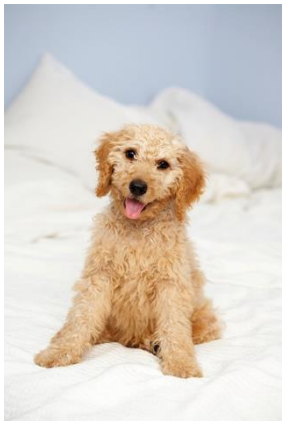
Hybridization - The Blending of Orbitals

Poodle

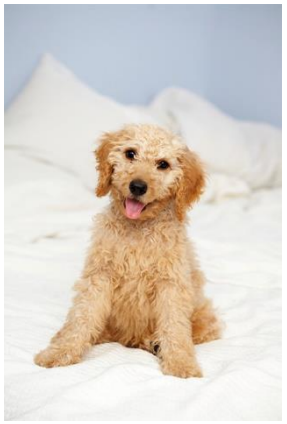
\+

Labrador

=



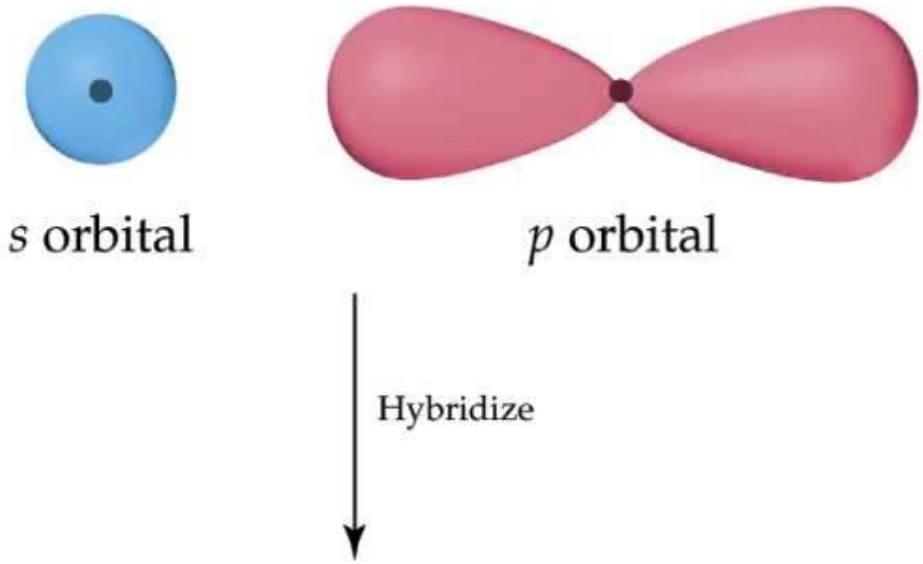
Labradoodle



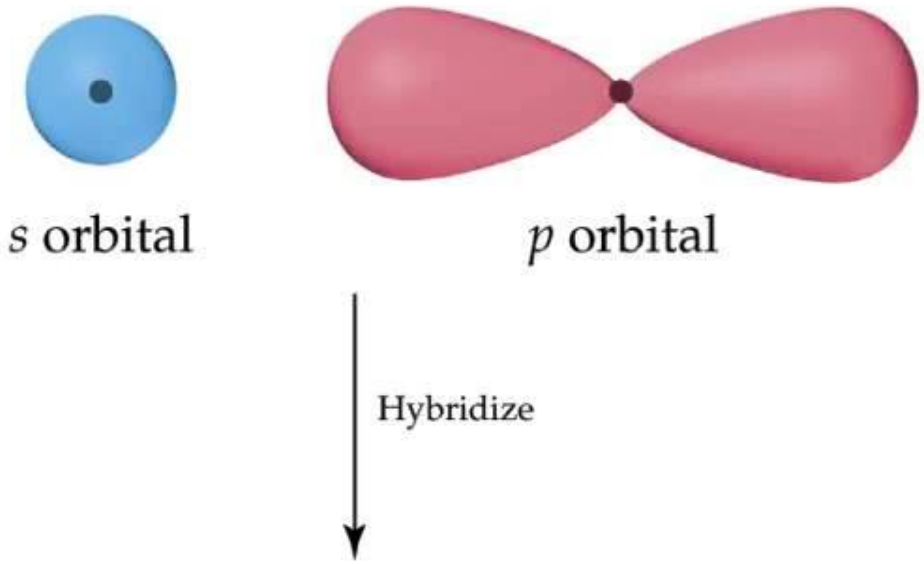
Labradoodle

Hybridization is the combining of two or more orbitals of nearly equal energy within the same atom into orbitals of equal energy.

sp Hybridization



sp Hybridization

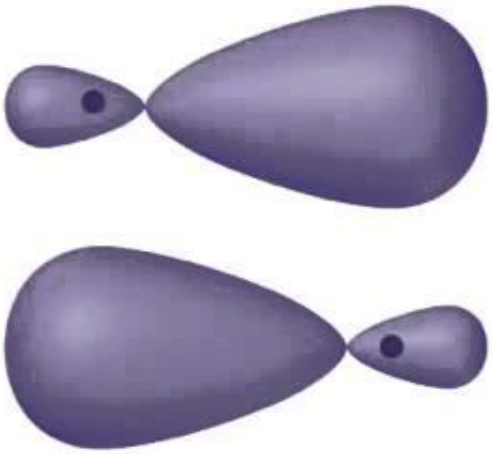


sp Hybridization

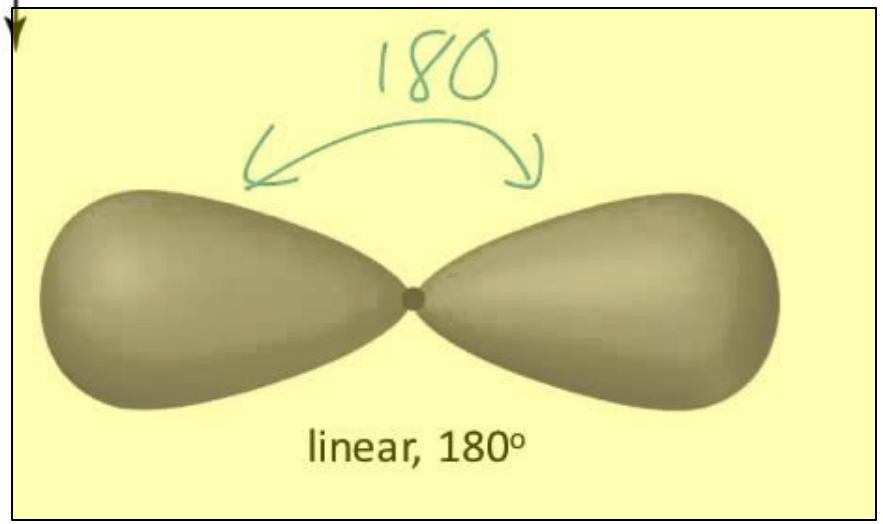
s orbital

p orbital

Hybridize



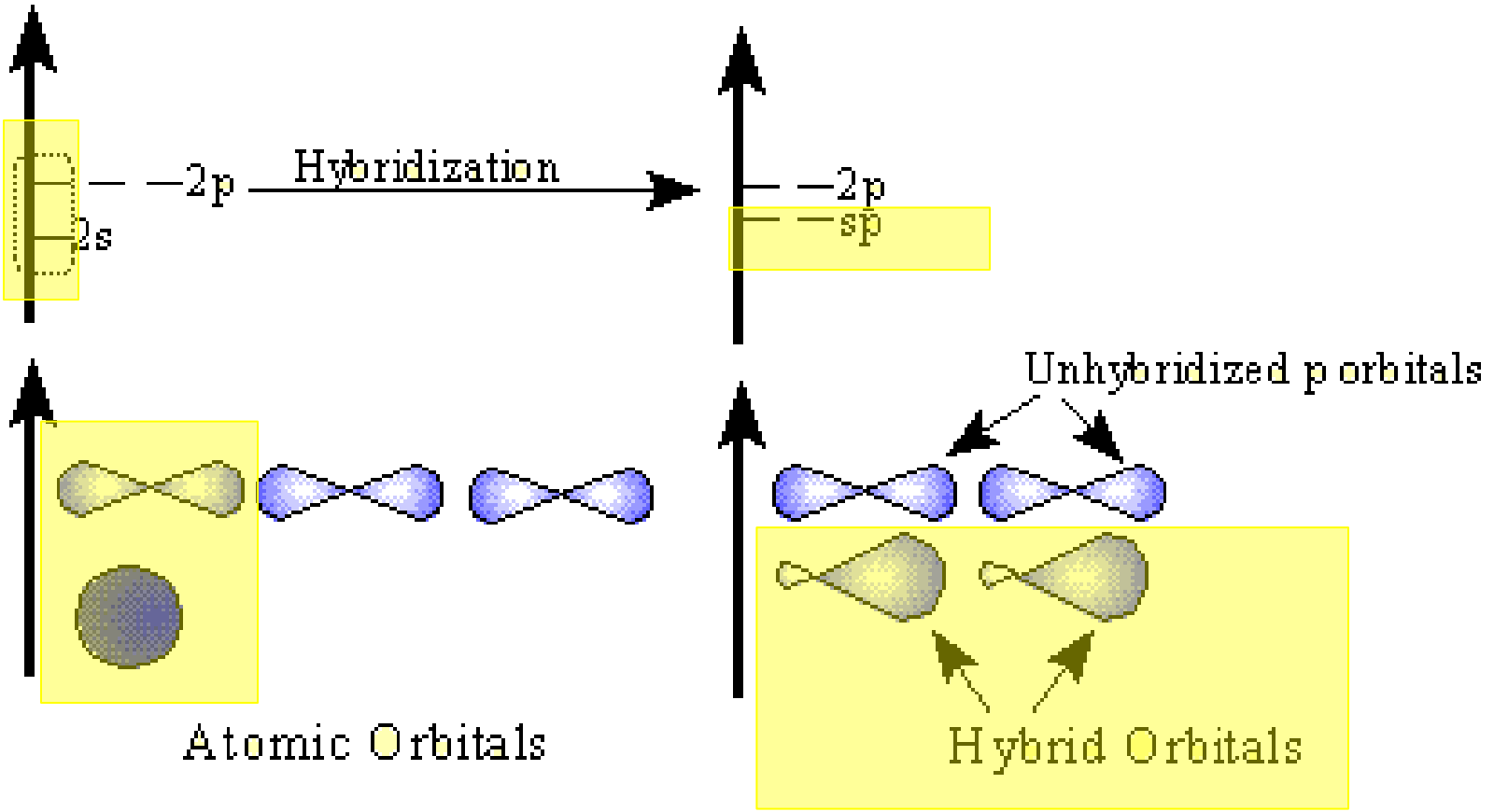
Two *sp* hybrid orbitals



sp hybrid orbitals shown together (large lobes only)

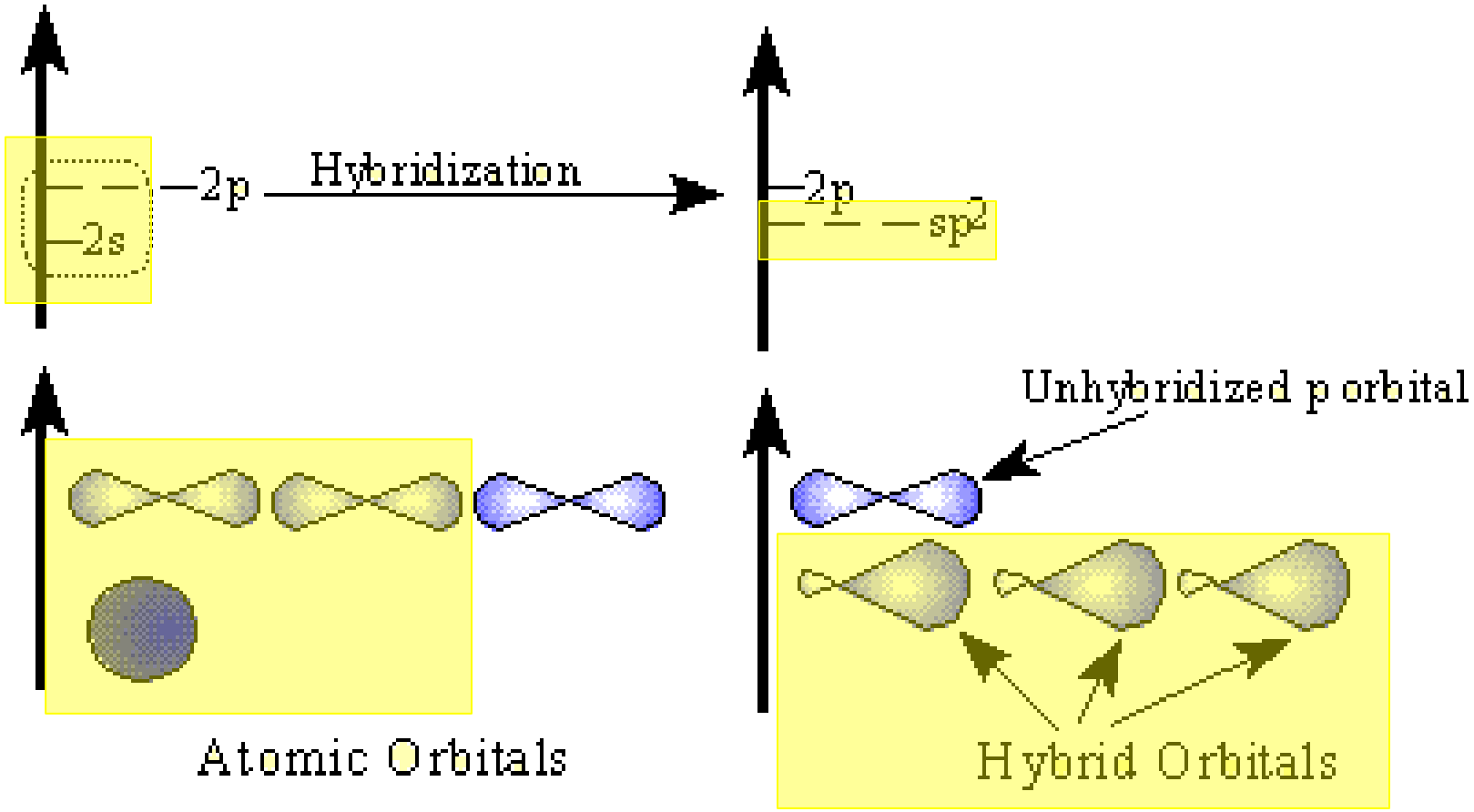
sp Hybrid Orbitals

One s orbital combines with one p orbital
Two p orbitals are left the same



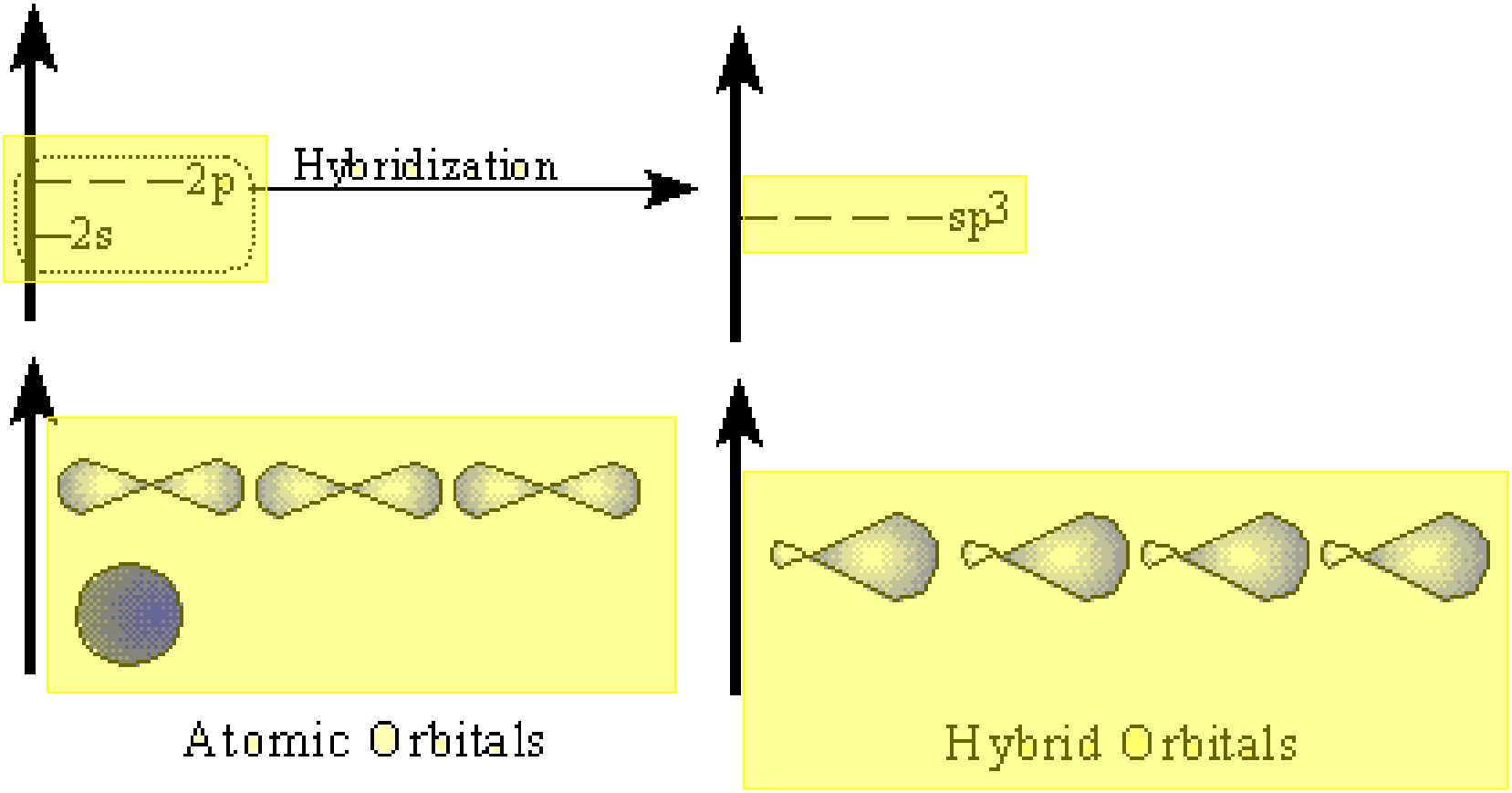
sp^2 Hybrid Orbitals

One s orbital combines with two p orbitals
One *p* orbital remains unchanged.



sp^3 Hybrid Orbitals

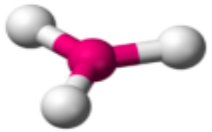
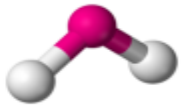
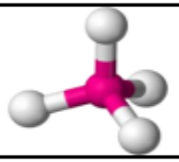
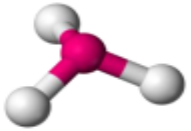
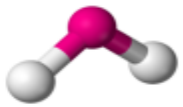
One s orbital combines with three p orbitals

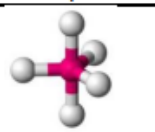
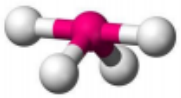
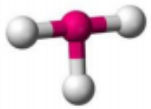
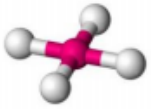
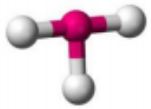


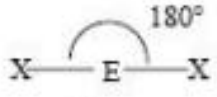
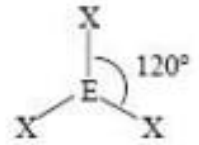
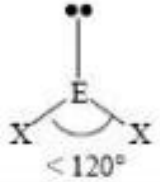
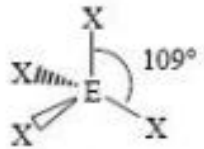
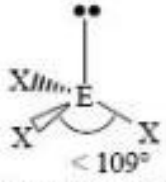
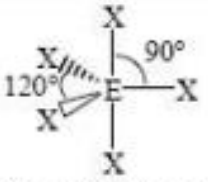
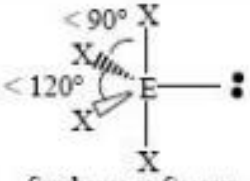
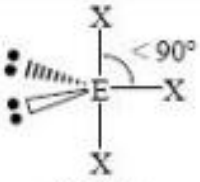
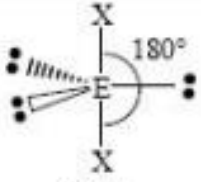
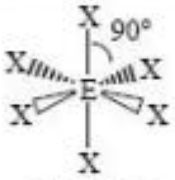
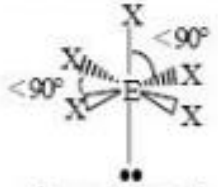
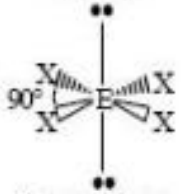
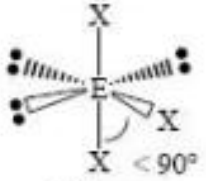
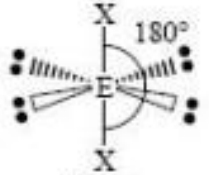
VSEPR – AXE Method

- The **A** represents the central atom.
- The **X** represents how many bonded atoms.
- The **E** represents the number of lone electron pairs present on the central atom.
- The sum of **X** and **E**, sometimes known as the **steric** number.

Steric # → X → E → "generic" shape → "specific" shape – Only looking at atoms

Electron Groups	Bonding Groups	Lone Pairs	Electron Geometry *(Hybridization)*	Molecular Geometry *(VSEPR class)*	Approximate Bond Angles	Geometry Examples
2	2	0	Linear *(sp)*	Linear *(AX_2)*	180	
3	3	0	Trigonal Planar *(sp^2)*	Trigonal Planar *(AX_3)*	120	
	2	1		Bent *(AX_2E)*		
4	4	0	Tetrahedral *(sp^3)*	Tetrahedral *(AX_4)*	109.5	
	3	1		Trigonal Pyramidal *(AX_3E)*		
	2	2		Bent *(AX_2E_2)*		

Electron Groups	Bonding Groups	Lone Pairs	Electron Geometry *(Hybridization)*	Molecular Geometry *(VSEPR class)*	Approximate Bond Angles	Geometry Examples
5	5	0	Trigonal Bipyramidal (sp^3d)	Trigonal Bipyramidal (AX_5)	120 (in plane) 90 (above and below)	
	4	1		Seesaw (AX_4E)		
	3	2		T-Shaped (AX_3E_2)		
	2	3		Linear (AX_2E_3)	180	
6	6	0	Octahedral (sp^3d^2)	Octahedral (AX_6)	90	
	5	1		Square Pyrimidal (AX_5E)		
	4	2		Square Planar (AX_4E_2)		
	3	3		T-Shaped (AX_3E_3)		
	2	4		Linear (AX_2E_4)		

VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 **Linear**				
3	 **Trigonal Planar**	 **Bent or Angular**			
4	 **Tetrahedral**	 **Trigonal Pyramid**	 **Bent or Angular**		
5	 **Trigonal Bipyramid**	 **Sawhorse or Seesaw**	 **T-shape**	 **Linear**	
6	 **Octahedral**	 **Square Pyramid**	 **Square Planar**	 **T-shape**	 **Linear**

Great Hybridization Video:

https://m.youtube.com/watch?feature=youtu.be&v=vHXViZTxLXo

Online 3D Shape Simulation:

https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html

Link to YouTube Presentation

https://youtu.be/zvTSm6kT7C0