VSEPR Theory

- The **Valence Shell Electron-Pair Repulsion (VSEPR) theory** allows you to predict the 3-dimensional shape of a molecular compound

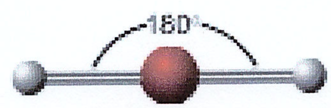
- The VSEPR theory states that molecules adjust their shapes so that valence electrons are as far away from each other as possible
  - This electron pair repulsion is not always equal; it is greatest between two lone pairs (LP), less between a lone pair and a bonding pair (BP), and lowest between two bonding pairs.

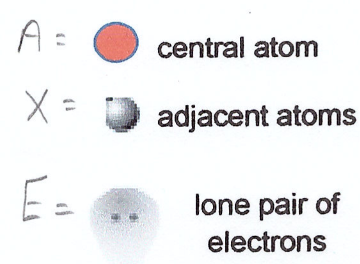
LP---LP > LP---BP > BP---BP electron repulsion!

greatest … lowest

- The shape of the molecule is determined around the central atom and there are five categories of shapes
  - To predict the shape of a molecule, it is important to start with a Lewis structure first

1. **Linear:** central atom is bonded to two other atoms and has no lone pairs around it OR there is only two atoms in the molecule.
   - VSEPR group AX_2
   - The angle between the two bonds (the **bond angle**) is 180°
   - Examples include $HCl_{(g)}$, $CO_{2(g)}$



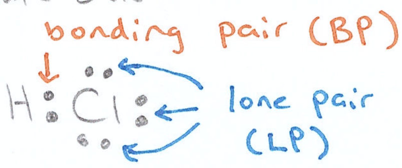


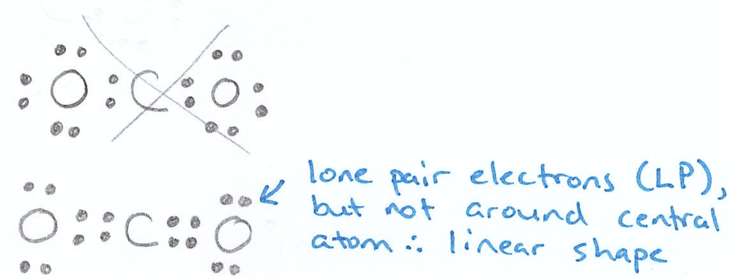
HCl

H = 1 v.e⁻
Cl = 7 v.e⁻
total = 8 v.e⁻

CO_2

C = 4 v.e⁻ ← central atom
O = 6 v.e⁻ (x2)
total = 16 v.e⁻



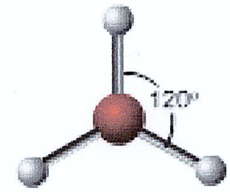


H — Cl

O = C = O

both linear VSEPR diagrams

2. **Trigonal Planar:** central atom is bonded to three other atoms and has no lone pairs around it
   - VSEPR group AX_3
   - An example would be $CH_2O_{(l)}$

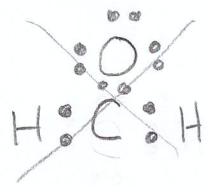


$C = 4\ v.e^-$ ← central atom

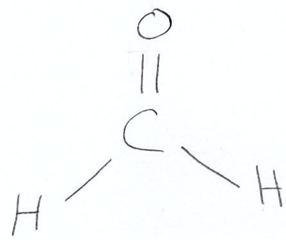
$H = 1\ v.e\ (x2)$

$O = 6\ v.e^-$

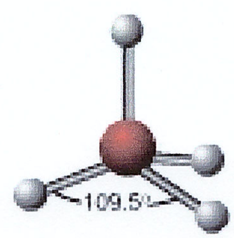
total = $12\ v.e^-$



∗ no lone pair electrons around central atom!



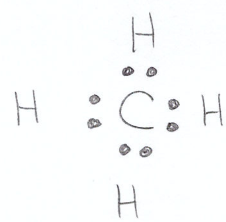
3. **Tetrahedral:** central atom is bonded to four other atoms and has no lone pairs around it
   - VSEPR group AX_4
   - An example would be $CH_{4(g)}$

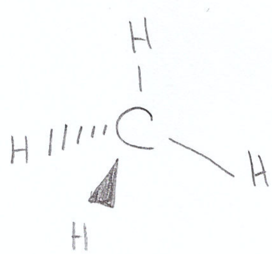


$C = 4\ v.e^-$ ← central atom

$H = 1\ v.e^-\ (x4)$

total = $8\ v.e^-$

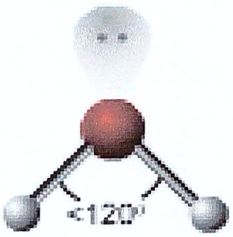




 represents bond coming out of the plane of page

 represents bond pointing into the plane of page

4. **Bent:** central atom is bonded to two other atoms and has either one or two lone pairs around it
   - VSEPR group AX_2E (trigonal planar electron group) or AX_2E_2 (tetrahedral electron group)
   - Examples include $HNO_{(g)}$ and $H_2O_{(l)}$



HNO

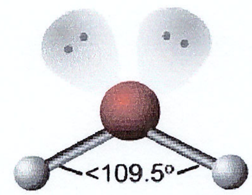
H = 1 v.e$^-$
N = 5 v.e$^-$ ← central atom
O = 6 v.e$^-$

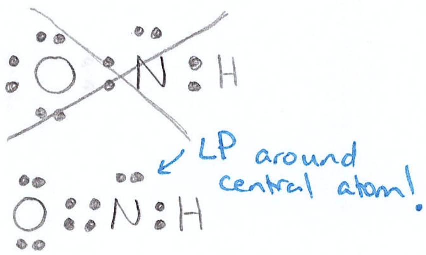
total = 12 v.e$^-$

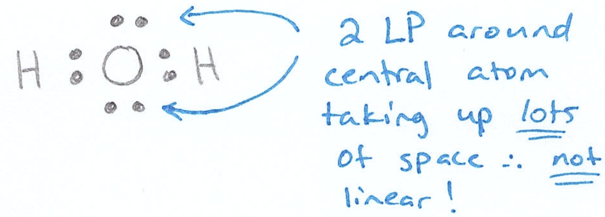
H₂O

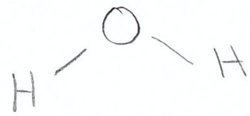
H = 1 v.e$^-$ (x2)
O = 6 v.e$^-$ ← central atom

total = 8 v.e$^-$

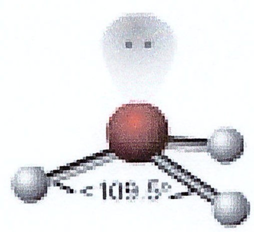






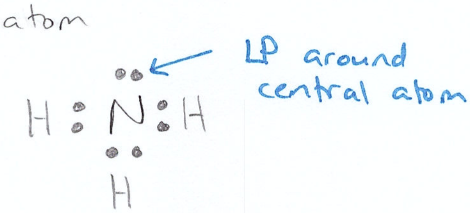


5. **Trigonal Pyramidal:** central atom is bonded to three other atoms and has one lone pair around it
   - VSEPR group AX_3E
   - An example would be $NH_{3(g)}$



N = 5 v.e$^-$ ← central atom
H = 1 v.e$^-$ (x3)

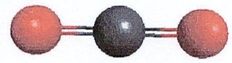
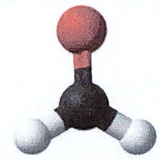
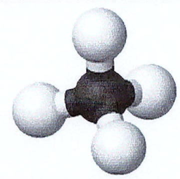
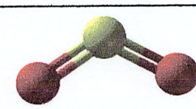
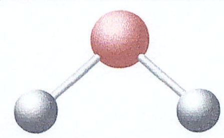
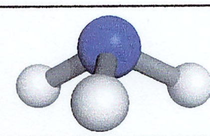
total = 8 v.e$^-$



*****Now try Practice Problem #1*****

only around central atom!

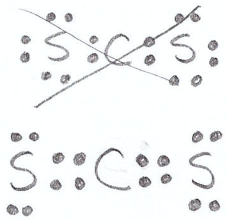
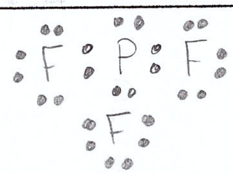
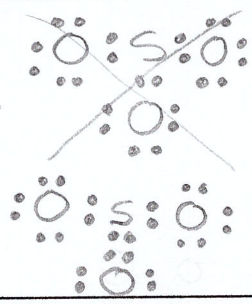
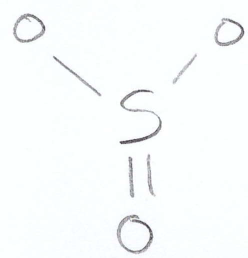
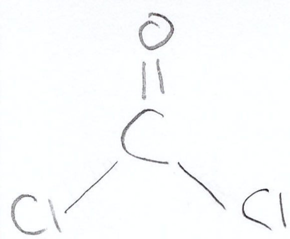
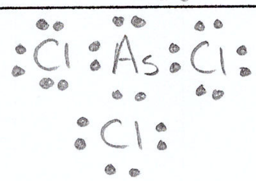
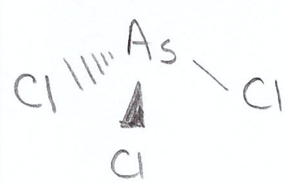
SUMMARY OF MOLECULAR SHAPES

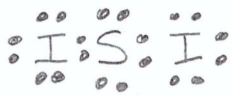
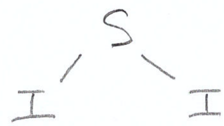
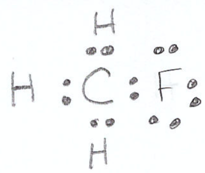
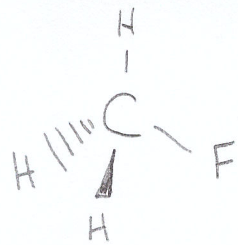
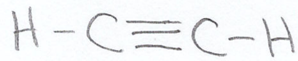
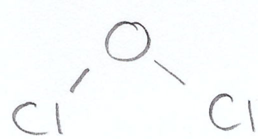
VSEPR Class	Name of Molecular Shape	Number of Bond Pairs (BP)	Number of Lone Pairs (LP)	Shape	Example
AX_2	Linear	2	0		CO_2
AX_3	Trigonal Planar	3	0		CH_2O
AX_4	Tetrahedral	4	0		CH_4
AX_2E	Bent	2	1		SO_2
AX_2E_2	Bent	2	2		H_2O
AX_3E	Trigonal Pyramidal	3	1		NH_3

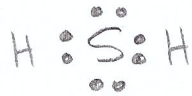
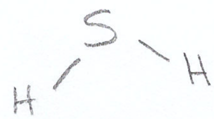
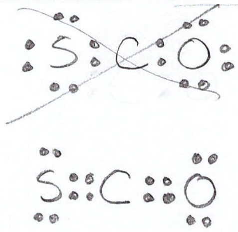
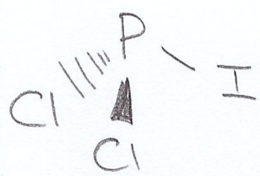
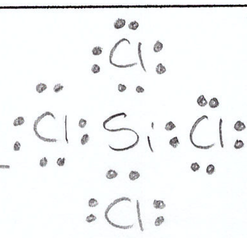
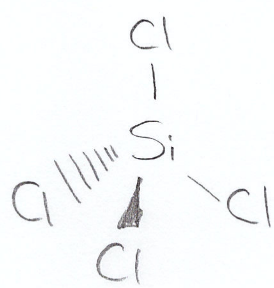
Practice Problems

only around central atom!

1. Complete the following chart. LP = Lone pair BP = Bonding pair

Formula	Lewis Diagram	VSEPR Shape Diagram	VSEPR Shape Name	Electrons #of LP	Electrons #of BP
$CS_{2(l)}$	C = 4 v.e⁻ S = 6 v.e⁻ (x2) total = 16 v.e⁻ 	S=C=S	linear	0	4
$PF_{3(g)}$	P = 5 v.e⁻ F = 7 v.e⁻ (x3) total = 26 v.e⁻ 		trigonal pyramidal	1	3
$SO_{3(g)}$	S = 6 v.e⁻ O = 6 v.e⁻ (x3) total = 24 v.e⁻ 		trigonal planar	0	4
$COCl_{2(aq)}$	C = 4 v.e⁻ O = 6 v.e⁻ Cl = 7 v.e⁻ (x2) total = 24 v.e⁻ 		trigonal planar	0	4
$AsCl_{3(l)}$	As = 5 v.e⁻ Cl = 7 v.e⁻ (x3) total = 26 v.e⁻ 		trigonal pyramidal	1	3

Formula	Lewis Diagram	VSEPR Shape Diagram	VSEPR Shape Name	Electrons	
				#of LP	#of BP
$SI_{2(g)}$	S = 6 v.e⁻ I = 7 v.e⁻ (x2) total = 20 v.e⁻ 		bent	2	2
$CH_3F_{(g)}$	C = 4 v.e⁻ H = 1 v.e⁻ (x3) F = 7 v.e⁻ total = 14 v.e⁻ 		tetrahedral	0	4
$CH_2F_{2(g)}$	C = 4 v.e⁻ H = 1 v.e⁻ (x2) F = 7 v.e⁻ (x2) total = 20 v.e⁻ 		tetrahedral	0	4
$C_2H_{2(g)}$	C = 4 v.e⁻ (x2) H = 1 v.e⁻ (x2) total = 10 v.e⁻ 		linear	0	4
$Cl_2O_{(g)}$	O = 6 v.e⁻ Cl = 7 v.e⁻ (x2) total = 20 v.e⁻ 		bent	2	2

Formula	Lewis Diagram	VSEPR Shape Diagram	VSEPR Shape Name	Electrons #of LP	Electrons #of BP
$H_2S_{(g)}$	H = 1v.e⁻ (x2) S = 6v.e⁻ total = 8 v.e⁻ 		bent	2	2
$COS_{(s)}$	C = 4 v.e⁻ O = 6v.e⁻ S = 6v.e⁻ total = 16 v.e⁻ 	S=C=O	linear	0	4
$PICl_{2(g)}$	P = 5v.e⁻ I = 7v.e⁻ Cl = 7v.e⁻ (x2) total = 26 v.e⁻ 		trigonal pryamidal	1	3
$SiCl_{4(g)}$	Si = 4 v.e⁻ Cl = 7v.e⁻ (x4) total = 32 v.e⁻ 		tetrahedral	0	4
$O_{2(g)}$	O = 6v.e⁻ (x2) total = 12 v.e⁻ 	O=O	linear	—	—