Molecular Shapes
(VSEPR model)

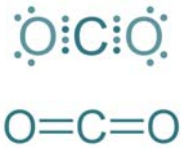
VSEPR Model

- **V**alence **S**hell **E**lectron **P**air **R**epulsion
- used to predict structures of molecules

Main idea:
Electron groups around a central atom will naturally **spread out** – they **maximize the distance between them,** because this minimizes repulsion

Electron Groups?

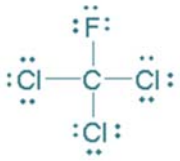
1. **Bonding domains** (bonded atoms)
   Single, double, triple bond = ONE bonding domain (all equivalent)
2. **Lone (un-bonded) pairs**



Carbon dioxide, CO_2
Central atom: Carbon
- Bonding domains = 2
- Lone pairs = 0

In each molecule, identify the number of electron groups around **carbon**

Lone pairs: ____
Bonding domains: ____



Lone pairs: ____
Bonding domains: ____

Lone pairs: ____
Bonding domains: ____

Steric number

Steric number = # of bonded atoms + # of lone pairs

Examples:

NH_3 

Bonded atoms	3
Lone pairs	
Steric number	

H_2O 

Bonded atoms	2
Lone pairs	
Steric number	

AXE Notation for Electron Counting

Letter	Represents
A	Central atom
X	Atoms bonded to central atom
E	Lone pairs

X + E = Steric number

Examples:

Molecule	VSEPR notation	Steric number
NH_3	AX_3E	
H_2O		

Basic Molecular Shapes

When NO lone pairs are present, all bonded atoms spread out equally around the central atom.

Steric number	VSEPR notation	Shape name	Geometry	Bond angles
1	AX	linear	A--X	180°
2	AX_2	linear	X—A—X	180°
3	AX_3	trigonal planar	 	120°

Steric number	VSEPR notation	Shape name	Geometry	Bond angles
4	AX_4	tetrahedral	 	109.5°
5	AX_5	trigonal bipyramid	 	90°, 120°
6	AX_6	octahedral	 	90°

Expanded VSEPR Geometry

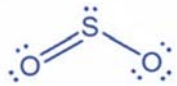
- Lone pairs are "bulkier" than bonding domains.
- They repel bonding domains away from them.
  - modifies molecular geometry from basic symmetrical 3-D shape

Steric Number 3: Electron Geometry = Trigonal Planar

Steric number	Lone pairs	VSEPR notation	Shape name	Geometry	Bond angles
3	0	AX_3	trigonal planar	 	120°
3	1	AX_2E	bent (V-shaped)	 	< 120°

When lone pairs are present, the actual bond angle will depend on the specific molecule.

generic AX_2E bent shape: predicted bond angle is **<120°**



Steric Number 4: Electron Geometry = Tetrahedral

Steric number	Lone pairs	VSEPR notation	Molecule shape	Geometry	Bond angles
4	0	AX_4	tetrahedral	 	109.5°
4	1	AX_3E	trigonal pyramid	 	<109.5°
4	2	AX_2E_2	bent	 	<<109.5°

Steric #

Other VSEPR shapes...

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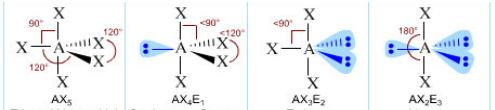

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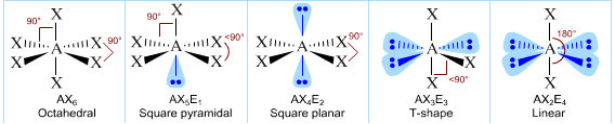
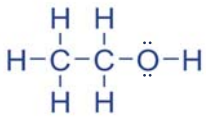
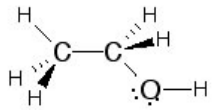


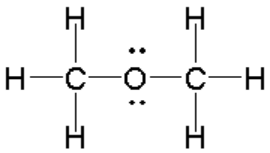
VSEPR Theory can be applied to molecules with more than one central atom.



Each Carbon: AX_4

Oxygen: AX_2E_2





Homework

Complete worksheet *Molecular Shapes*

- For each molecule,
  - Draw the Lewis structure, with bond angles
  - Write the VSEPR AXE notation
  - Write the steric number
  - Name the shape