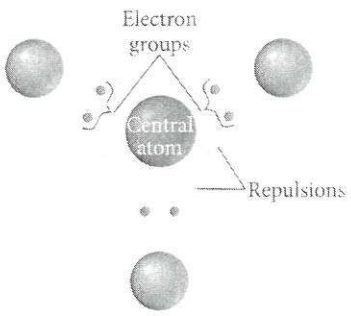
VSEPR Theory: Valence Shell Electron Pair Repulsion

VSEPR Theory: (Valence Shell Electron Pair Repulsion) predicts the geometry (shape) of molecules.

- Electrons surrounding an atom tend to repulse (repel) each other.

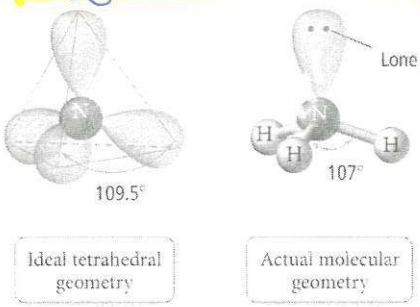


- Electrons (bonds and lone pairs) surrounding an atom will adopt a shape to minimize this repulsion, by arranging themselves as far as possible from each other.
- Double and triple bonds are treated the same as a SINGLE bond in terms of ability to repel electrons.

Magnitude of repulsion:

more repulsive

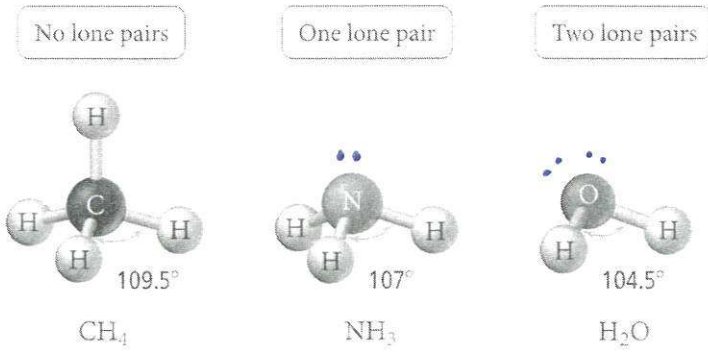
Lone pair > bonding pair(s)



But why?

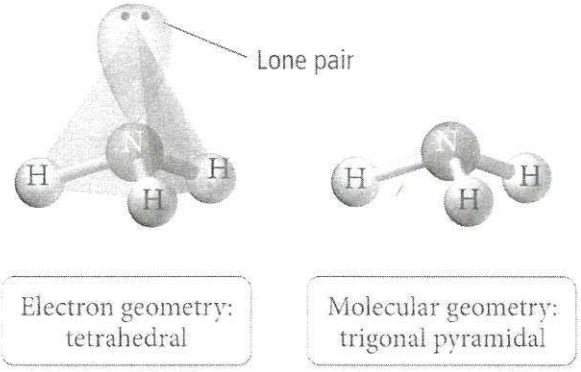
- Since lone pairs experience an attraction (or pull) from only 1 nucleus (as opposed to 2 nuclei for bonding electron pairs), lone pairs have a more concentrated electron density and thus a GREATER repulsive effect: they take up more space around an atom!

Effect of Lone Pairs on Molecular Geometry



Key Definitions

Electron Domains	Bonding Domains
Regions of electron density about a central atom.	Regions of bonding electron density about a central atom.
Used to determine electron geometry: • bond angles!	Used to determine molecular geometry: • VSEPR shape!
One electron domain equals: • One lone pair, or • One single bond, or • One double bond, or • One triple bond Yep, you read that right → a single, double, or triple bond only counts as **ONE** electron domain!	**One bonding domain** equals: • One single bond, or • One double bond, or • One triple bond Yep, you read that right → a single, double, or triple bond only counts as **ONE** bonding domain!



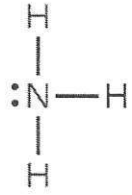
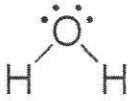
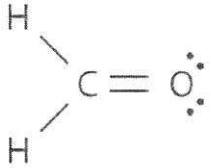
Electron geometry: tetrahedral

Molecular geometry: trigonal pyramidal

Important things to know about Molecular and Electron Geometry:

1. When lone pairs are not present on the central atom, molecular and electron geometries are the same!
2. In expanded octets, lone pairs can be in two possible locations: axial (top and bottom) or equatorial (around the center). **Place lone pairs wherever they'll be farthest apart (maximum possible angle)!**

Let's Practice! How many electron domains and bonding domains are around the central atom for each of the following molecules?

1)	2)	3)
		
# electron domains? 4 # bonding domains? 3	# electron domains? 4 # bonding domains? 2	# electron domains? 3 # bonding domains? 3

<u>You MUST be able to identify VSEPR shapes</u> of Lewis structures by their correct names!

- Count electron groups around the central atom
- Each of the following is considered one electron group
  - A lone pair, a single bond, a double bond, a triple bond
- Electron groups repel each other to get as far apart as possible

A = central atom, **X** = terminal atom, **E** = a lone pair of electrons

Only 2 atoms = Linear

# of e⁻ groups	2	3		4		
General Formula	AX_2	AX_3	AX_2E	AX_4	AX_3E	AX_2E_2
Electron Geometry	Linear	Trigonal planar	Trigonal planar	Tetrahedral	Tetrahedral	Tetrahedral
Molecular Geometry (VSEPR Shape)	Linear	Trigonal planar	Bent	Tetrahedral	Trigonal pyramidal	Bent
Bond Angle	180°	120°	< 120°	109.5°	< 109.5°	<< 109.5°
Example	$\ddot{O}=C=\ddot{O}$	BF_3	SO_2	CH_4	NH_3	H_2O

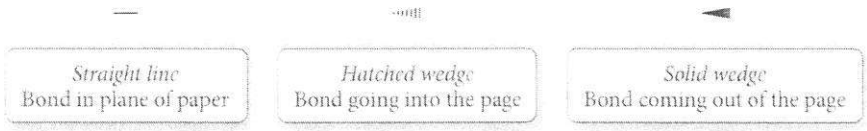
More e- repulsion = smaller angle

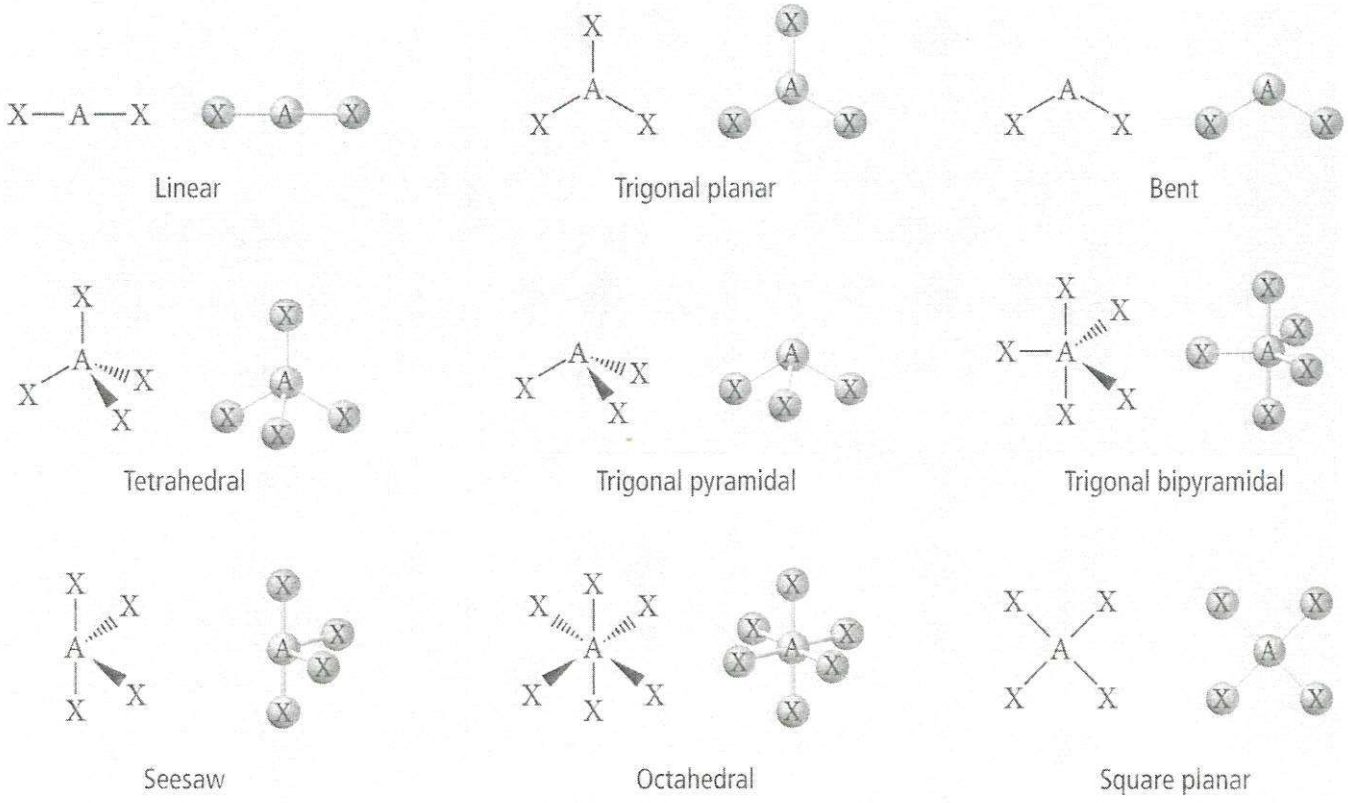
More e- repulsion = smaller angle

# of e⁻ groups	5				6		
General Formula	AX_5	AX_4E	AX_3E_2	AX_2E_3	AX_6	AX_5E	AX_4E_2
Electron Geometry	Trigonal bipyramidal	Trigonal bipyramidal	Trigonal bipyramidal	Trigonal bipyramidal	Octahedral	Octahedral	Octahedral
Molecular Geometry (VSEPR Shape)	Trigonal bipyramidal	See-saw	T-shaped	Linear	Octahedral	Square pyramidal	Square planar
Bond Angle	120 ° (equatorial) 90° (axial)	< 120° equatorial) < 90° (axial)	< 90°	180°	90°	< 90°	90°
Example							

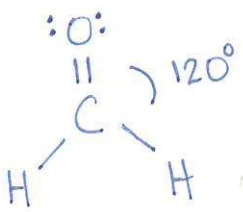
How to Draw 3-D Shapes on Paper

You won't be expected to use this 3-D drawing strategy, but you have to know what it means when you see it with an example molecule!





Let's Practice! Complete the table below.

	Lewis Dot Structure (2D) (w/ predicted bond angles)	**Electron geometry**	**Molecular geometry**
CH_2O		# electron domains: 3 e⁻ geometry: trigonal planar	# bonding domains: 3 VSEPR shape: trigonal planar