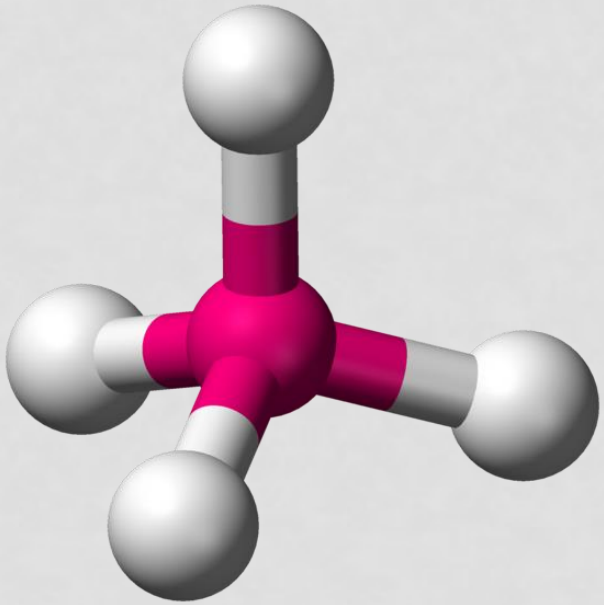
What is Molecular Geometry



The SHAPES of molecules

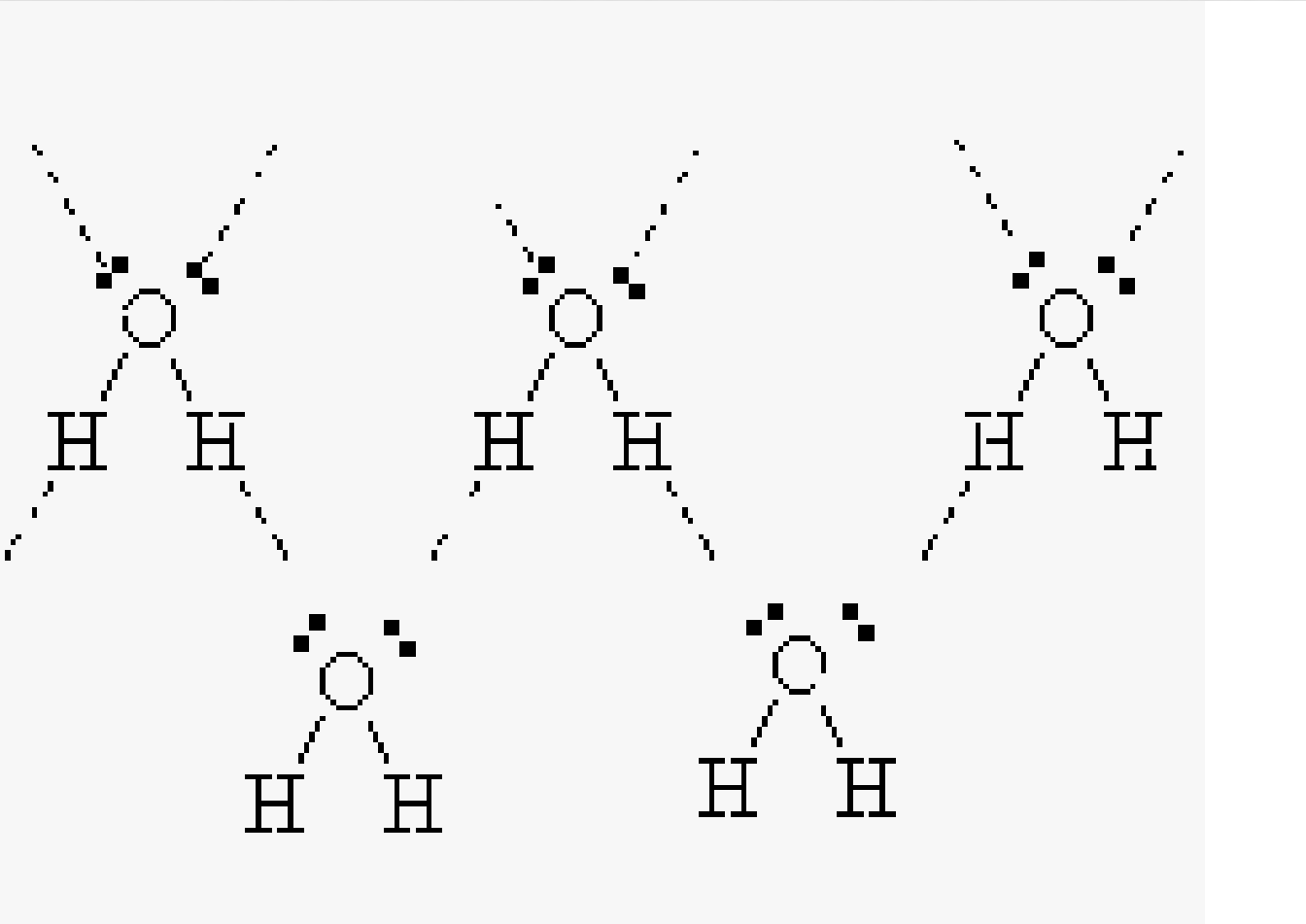
Why the shape of a molecule is important

Structure and function: the shape of a molecule determines its properties and uses

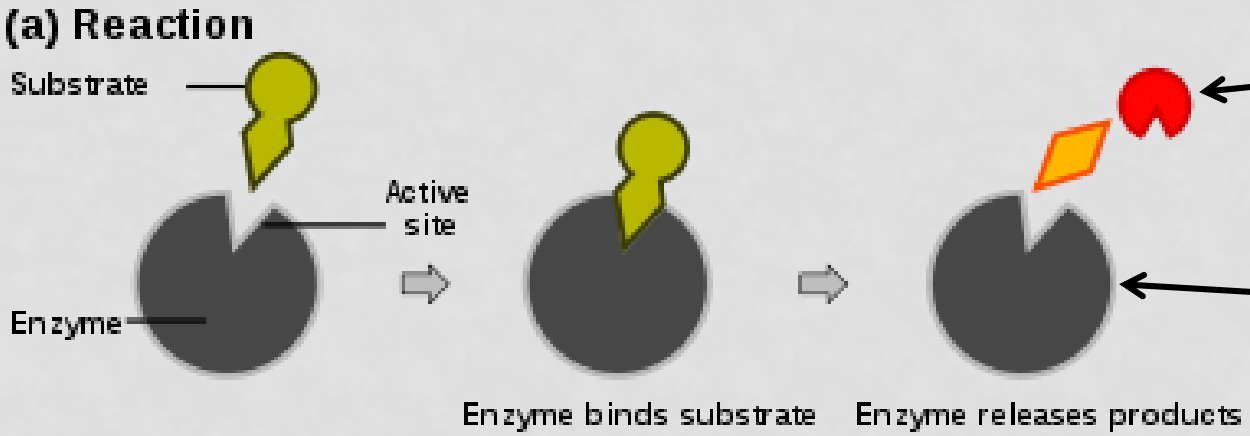
Properties such as melting and boiling point (temperatures), smell, taste, and drug reactions are all dependent on the shapes of molecules

WHY CAN YOU FLOAT ON WATER?

The Structure (shape) of water!



Aspirin works because of its shape!

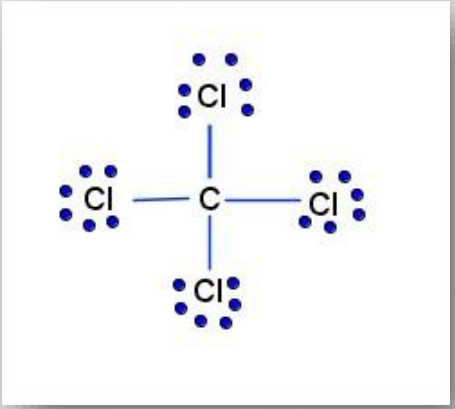


Prostaglandin which causes inflammation (swelling) is produced by the COX-1 and COX-2 enzymes

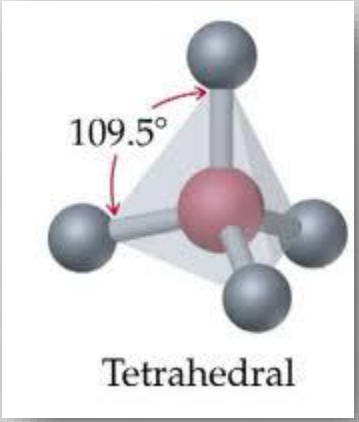
Aspirin can block the substrate from bonding to the COX-1 or COX-2 enzyme thus preventing the production of prostaglandin

Determining the Shape of a molecule

Lewis structures don't give us a 3-dimensional view of how the atoms are bonded together



The Lewis structure implies a cross shape with 90° angles



Actual Shape

So how do we find the shape of a molecule?

By using the VSEPR Theory

(pronounced Vess Purr)

VSEPR Theory

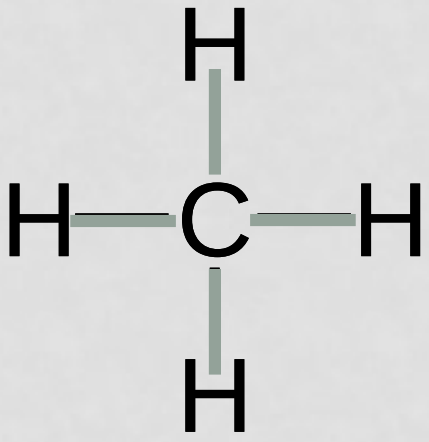
Valence Shell Electron Pair Repulsion Theory

Main Premise: Molecules will adopt a shape that is lowest in energy by minimizing the valence shell electron pair repulsion (VSEPR) between adjacent atoms

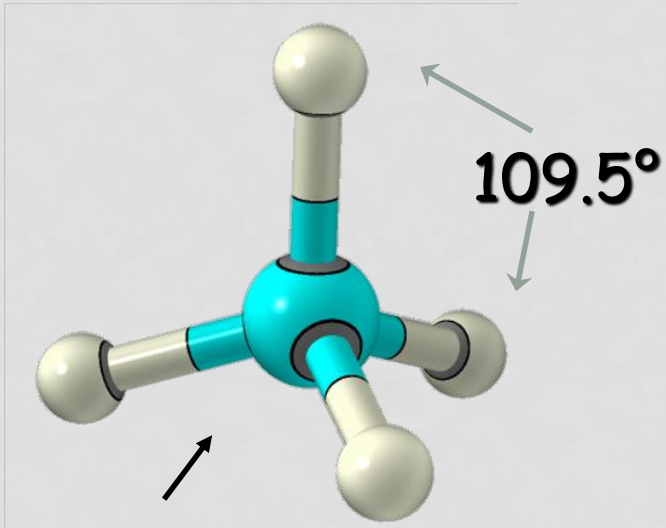
Huh???

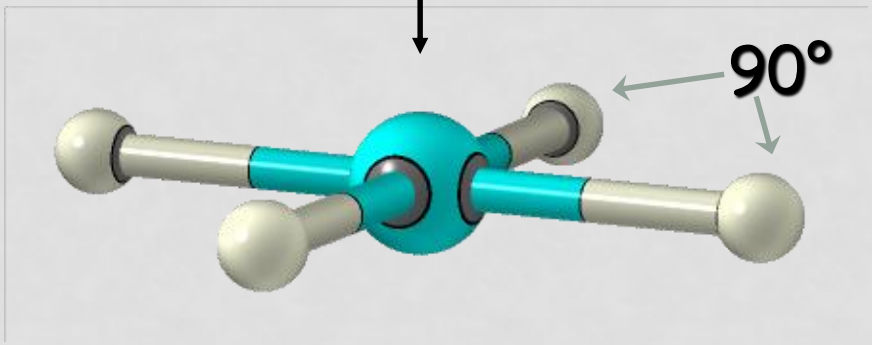
Atoms in a molecule try to spread out from one another as much as possible to reduce the "like charge repulsion" between their outer electrons

methane, CH_4



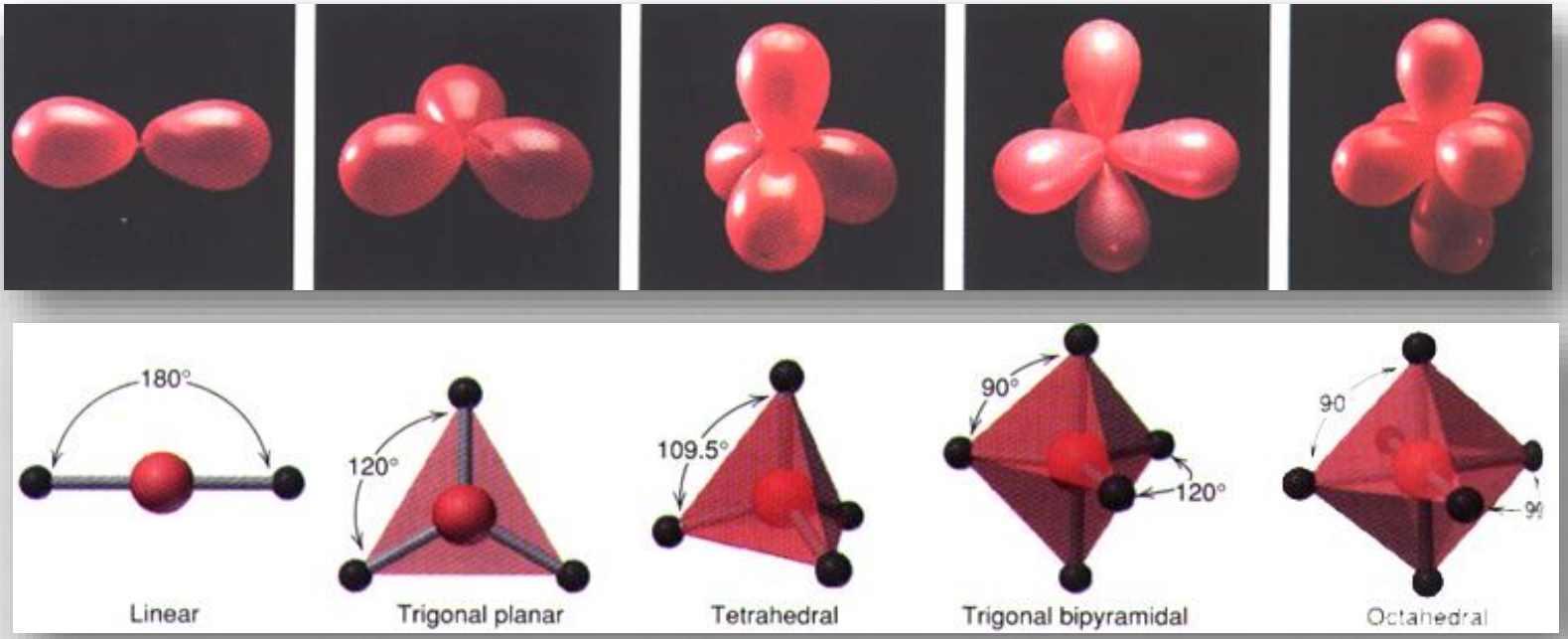
You might think this is the farthest that the hydrogens can get away from each other





But if you think in 3 dimensions, the hydrogens can actually get farther away from each other and minimize adjacent electron cloud repulsions

THE 5 MAIN VSEPR SHAPES



These shapes minimize the like charge repulsion between adjacent electron clouds

FROM LEWIS TO VSEPR SHAPE

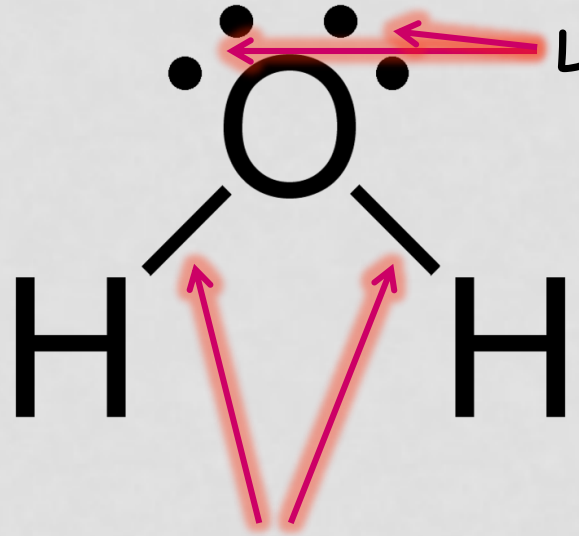
1. Draw a Lewis structure

2. Count the number of "electron groups" around the central atom
   - -Each single, double and triple bond counts as ONE Electron Group
   - -Each unshared pair of electrons (lone pair) counts as ONE Electron Group

3. Use VSEPR Chart to determine the shape based on how many bonds vs lone pair electron groups are around the central atom

ELECTRON GROUPS

Regions in a molecule where there are high concentrations of electrons

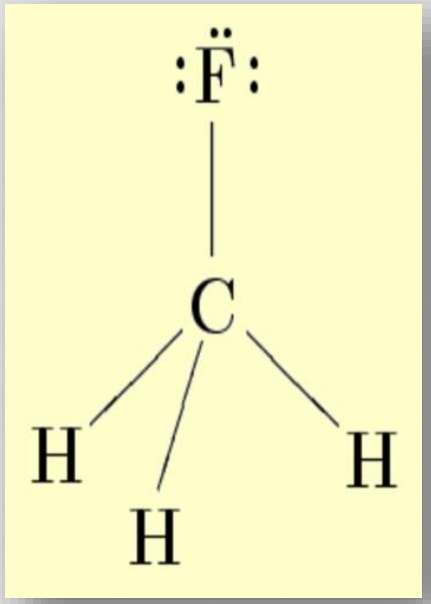


Lone pairs= (unshared pairs of electrons)

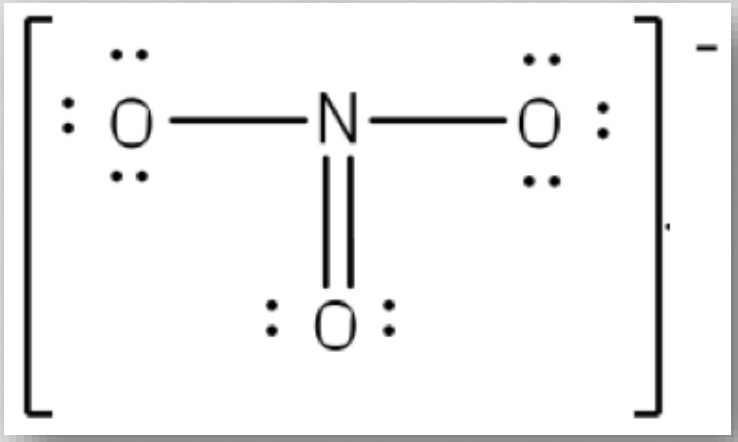
Bonds = (bonding groups)

This Lewis structure shows
2 bonding groups
and
2 non bonding groups (lone pairs)

HOW MANY "ELECTRON GROUPS" AROUND THE CENTRAL ATOM?

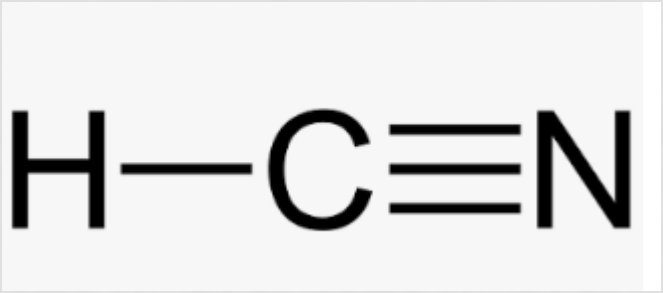


4 around C



3 around N

Remember: single, double and triple bonds count as ONE domain



2 around C

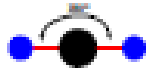
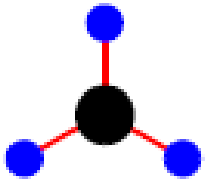
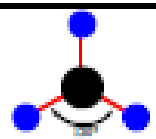
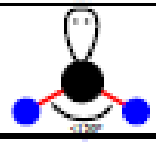
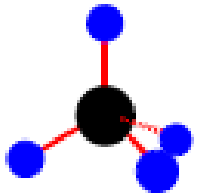
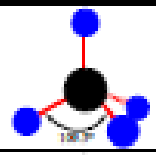
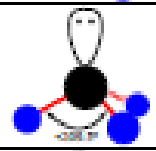
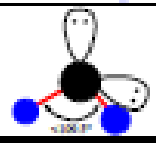
REMEMBER THE BIG PICTURE?

Electron groups are all negatively charged so they want to spread out from each other as much as possible to minimize like-charge-repulsion within a molecule

Doing this allows the molecule to be more stable (low energy)

THE VSEPR CHART

Using VSEPR to Predict the Shapes of Molecules

Electron Groups on central atom[1]	Electron-Group Shape	Bonds[2]	Lone Pairs	AX_mE_n[3]	Molecular Shape	Bond angles	Polarity	Hybrid-ization	Appearance
2	 Linear	2	0	AX_2	linear	180°	nonpolar[4]	sp	
3	 Trigonal Planar	3	0	AX_3	trigonal planar	120°	nonpolar[4]	sp^2	
		2	1	AX_2E	bent	<120°[5]	polar	sp^2	
4	 Tetrahedral	4	0	AX_4	tetrahedral	109.5°	nonpolar[4]	sp^3	
		3	1	AX_3E	trigonal pyramidal	<109.5°	polar	sp^3	
		2	2	AX_2E_2	bent	<109.5°	polar	sp^3	

THE VSEPR CHART

Electron shape
how the
electron groups
are arranged
around the central
atom

Molecular shape
how the atoms
bonded to the
central atom are
arranged.

Using VSEPR to Predict the Shapes of Molecules

Electron Groups on central atom[1]	Electron-Group Shape	Bonds[2]	Lone Pairs	AX_mE_n[3]	Molecular Shape	Bond angles	Polarity	Hybrid -ization	Appearance
2	Linear	2	0	AX_2	linear	180°	nonpolar[4]	sp	
3	Trigonal Planar	3	0	AX_3	trigonal planar	120°	nonpolar[4]	sp^2	
		2	1	AX_2E	bent	<120°[5]	polar	sp^2	
4	Tetrahedral	4	0	AX_4	tetrahedral	109.5°	nonpolar[4]	sp^3	
		3	1	AX_3E	trigonal pyramidal	<109.5°	polar	sp^3	
		2	2	AX_2E_2	bent	<109.5°	polar	sp^3	

THE VSEPR CHART

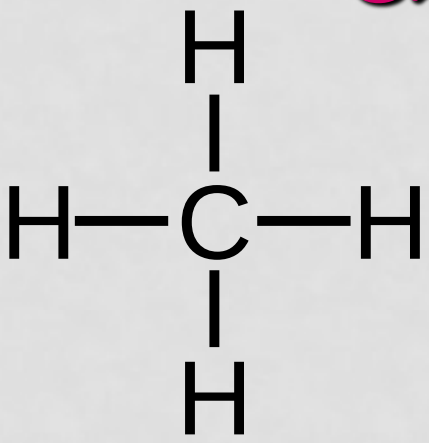
Bond Angle
Distance
between electron groups

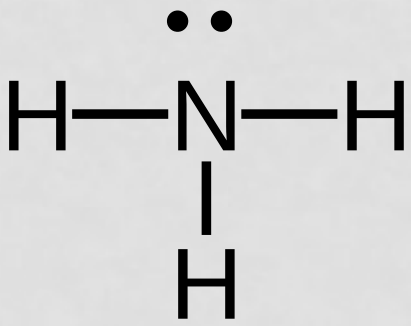
Polarity
Polarity of the molecule when all **outer atoms** are the same.

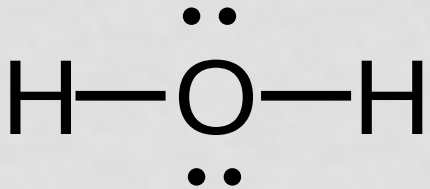
Using VSEPR to Predict the Shapes of Molecules

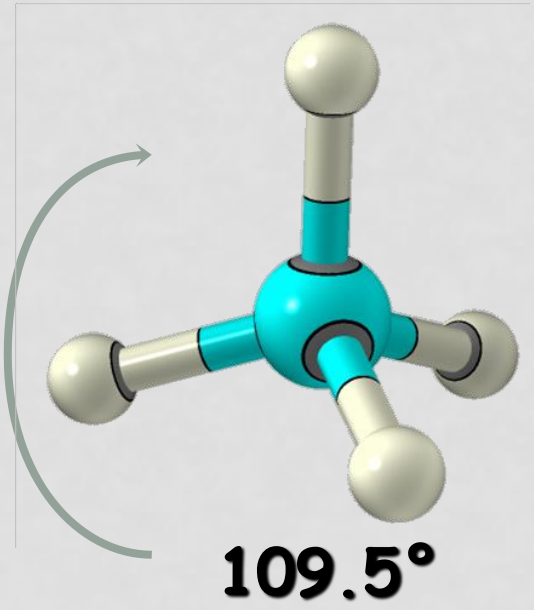
Electron Groups on central atom[1]	Electron-Group Shape	Bonds[2]	Lone Pairs	AX_mE_n[3]	Molecular Shape	Bond Angles	Polarity	Hybrid-ization	Appearance
2	Linear	2	0	AX_2	linear	180°	nonpolar[4]	sp	
3	Trigonal Planar	3	0	AX_3	trigonal planar	120°	nonpolar[4]	sp^2	
		2	1	AX_2E	bent	<120°[5]	polar	sp^2	
4	Tetrahedral	4	0	AX_4	tetrahedral	109.5°	nonpolar[4]	sp^3	
		3	1	AX_3E	trigonal pyramidal	<109.5°	polar	sp^3	
		2	2	AX_2E_2	bent	<109.5°	polar	sp^3	

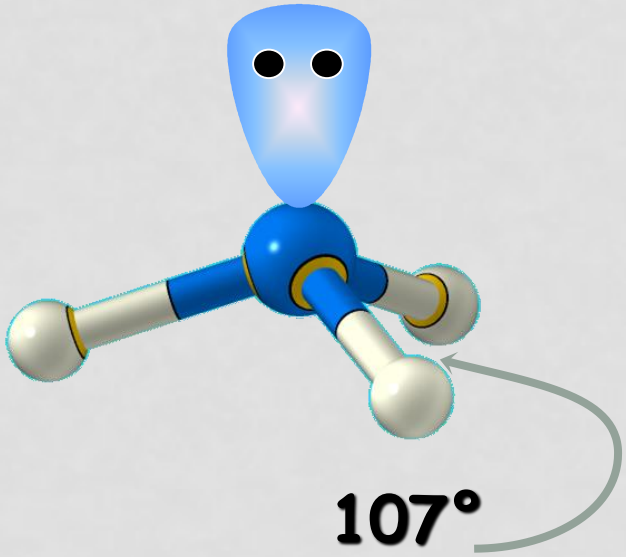
Lone pairs decrease the expected bond angle

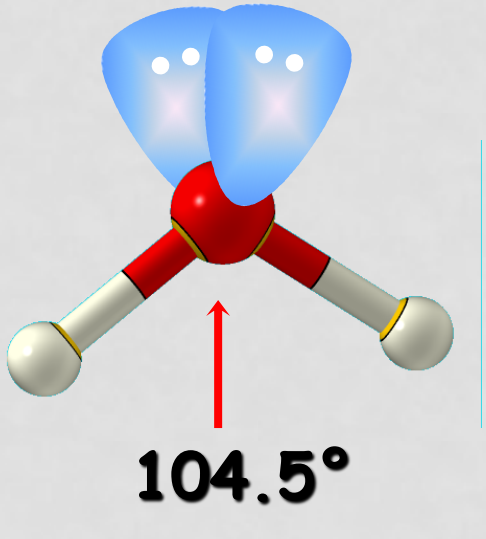




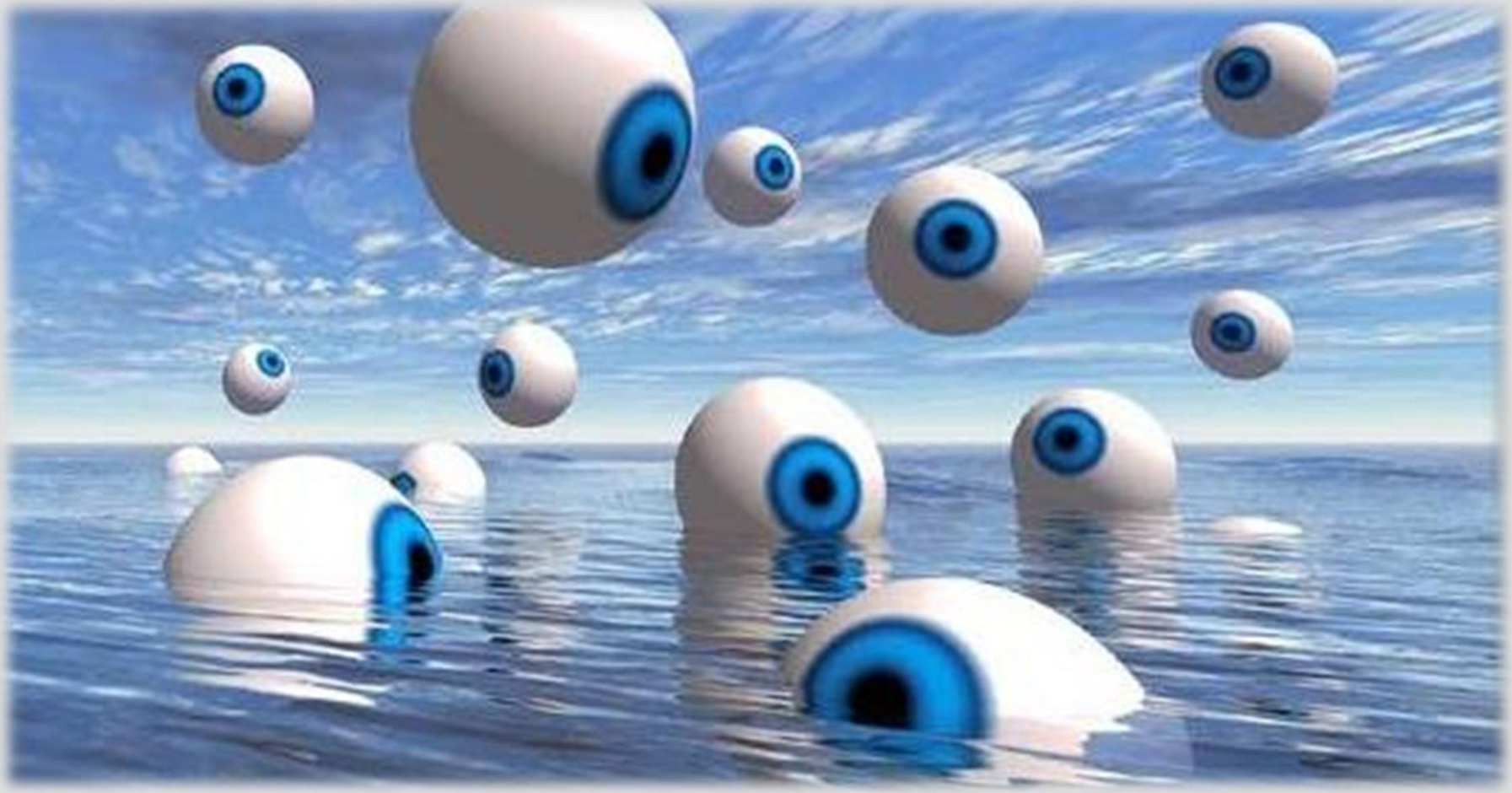








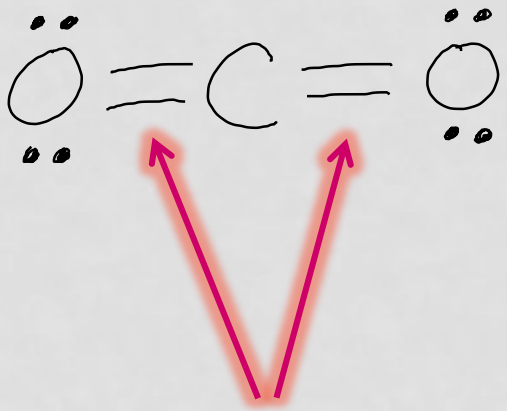
LET'S LOOK AT SOME EXAMPLES



VSEPR EXAMPLE 1

CO_2

$4 + 6(2) = 16$ valence e⁻



2 Electron Groups

Electron shape is **linear**

2 Bonds **0** Lone Pairs

Molecular shape is **linear**

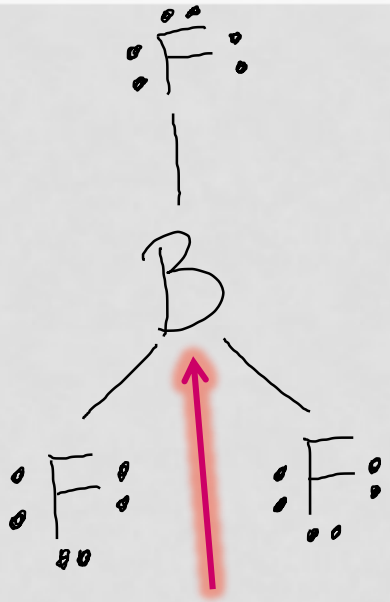
Bond angle is **180°** Polarity is **nonpolar**

VSEPR EXAMPLE 2

BF_3

$3 + 7(3) = 24$ valence e⁻

*Boron is an exception to the octet rule and is only surrounded by 6 electrons



3 Electron Groups

Electron shape is trigonal planar

3 Bonds 0 Lone Pairs

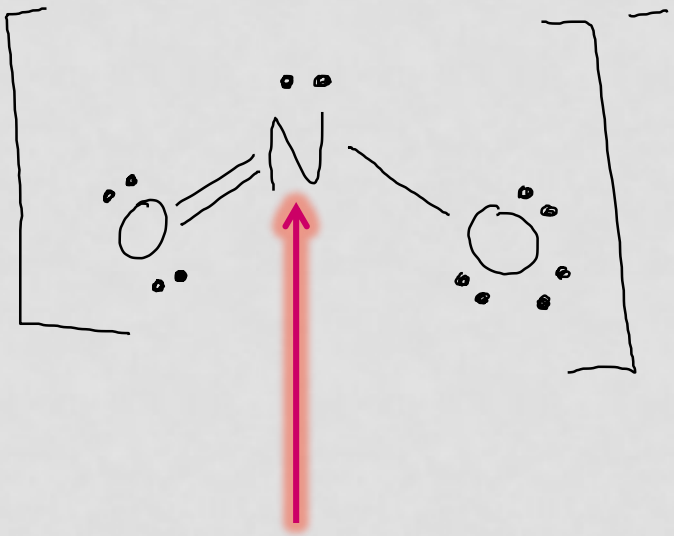
Molecular shape is trigonal planar

Bond angle is 120° Polarity is nonpolar

VSEPR EXAMPLE 3

NO_2^-

$5 + 6(2) + 1 = 18$ valence e⁻



3 Electron Groups

Electron shape is trigonal planar

2 Bonds 1 Lone Pairs

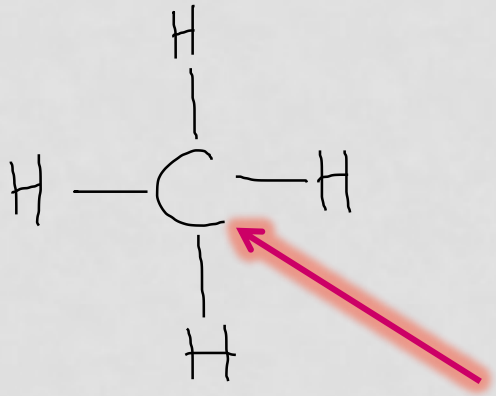
Molecular shape is bent

Bond angle is <120° Polarity is Polar

VSEPR EXAMPLE 4

CH_4

$4 + 1(4) = 8$ valence e⁻



4 Electron Groups

Electron shape is **Tetrahedral**

4 Bonds **0** Lone Pairs:

Molecular shape is **Tetrahedral**

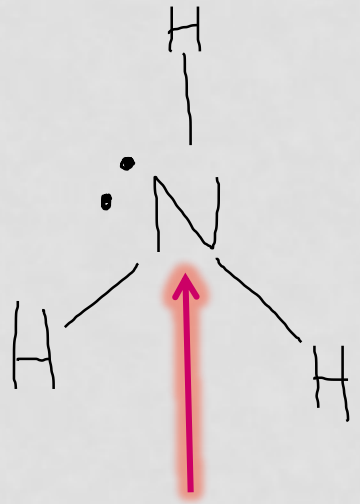
Bond angle is **109.5°**

Polarity is **nonpolar**

VSEPR EXAMPLE 5

NH_3

$5 + 1(3) = 8$ valence e⁻



4 Electron Groups

Electron shape is **tetrahedral**

3 Bonds **1** Lone Pairs

Molecular shape is **trigonal pyramidal**

Bond angle is **<109.5°** Polarity is **Polar**

VSEPR NOTATION

Also known as "**AXE**" notation

It is just a shorthand way to communicate VSEPR information

EXAMPLES OF USING AXE NOTATION

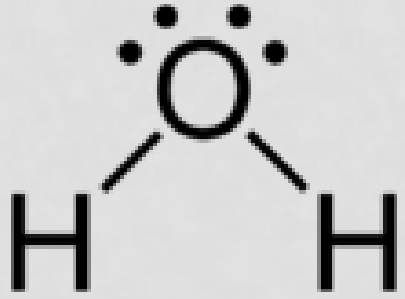
AX_3E_1

This subscript tells how many atoms are bonded to the central atom

This subscript tells how many lone pairs are on the central atom

AX_3E_1 is always trigonal pyramidal

EXAMPLES OF USING AXE NOTATION



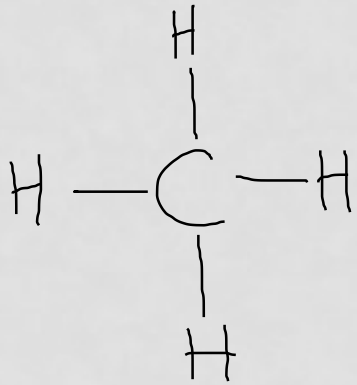
AX_2E_2

This subscript tells how many atoms are bonded to the central atom

This subscript tells how many lone pairs are on the central atom

AX_2E_2 is always bent

EXAMPLES OF USING AXE NOTATION



AX_4

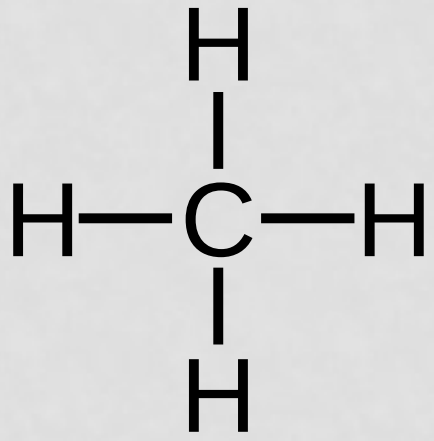
This subscript tells how many atoms are bonded to the central atom

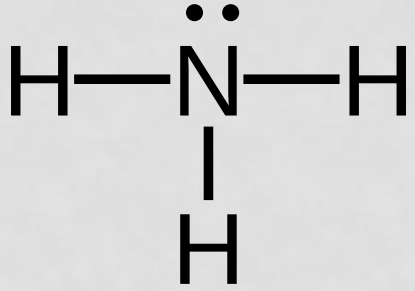
Don't put the "E" if there aren't any lone pairs

AX_4 is always tetrahedral

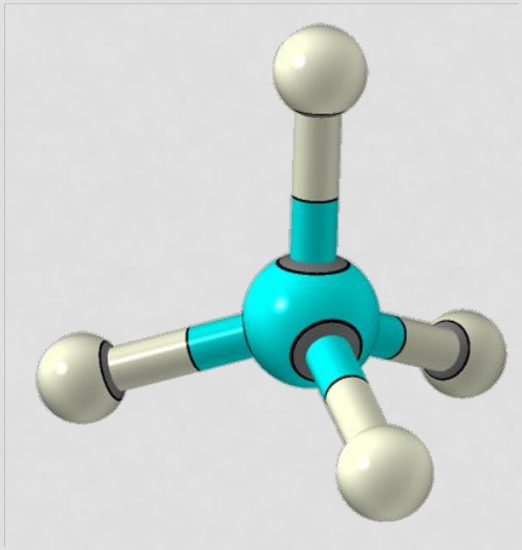
FISHER PROJECTIONS

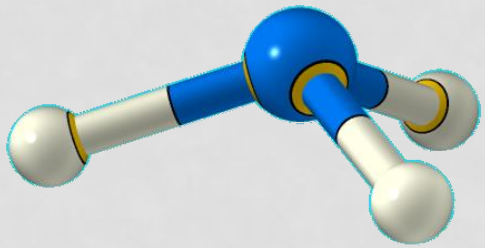
A way to make your Lewis structures indicate their three dimensional VSEPR shape on paper

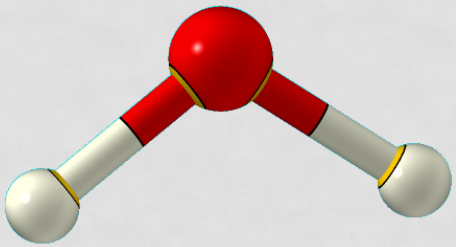

H
H
C
H
H

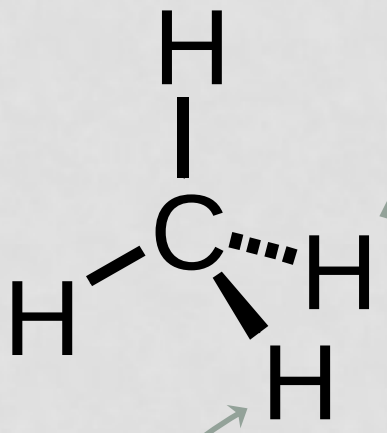

H
N
H
H

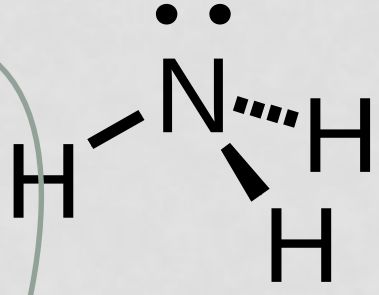

H
O
H

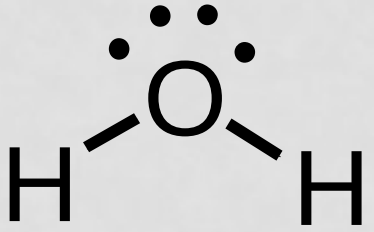


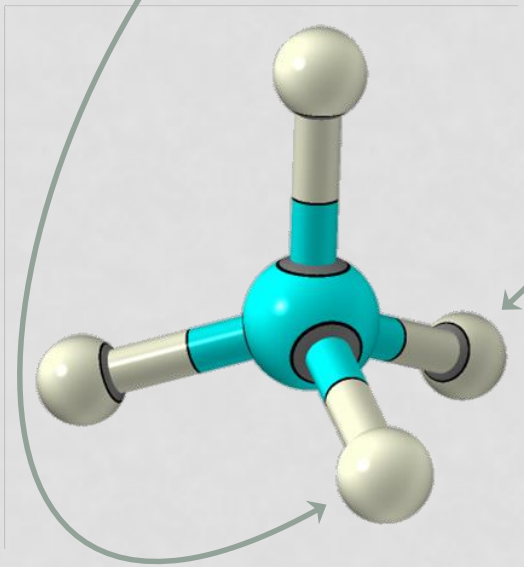


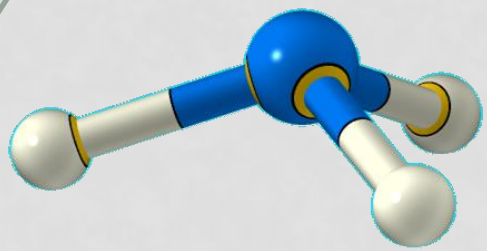


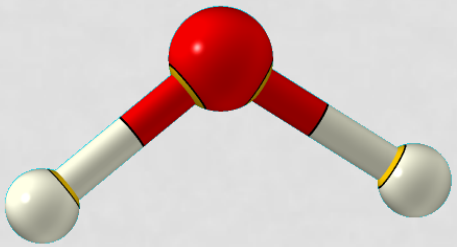

H
C
H
H
H


N
H
H
H


O
H
H







FISHER PROJECTIONS

Bonds in the plane of the paper are shown as lines

Bonds projecting in front of the plane of the paper are shown as triangles

Bonds projecting behind the plane of the paper are shown as stacked lines