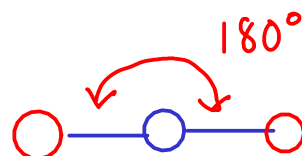
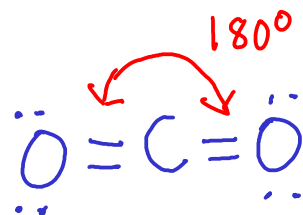


PREDICTING MOLECULAR SHAPE

The shape of simple molecules (and parts of larger molecules) can be easily predicted using the VSEPR model

VSEPR = Valence Shell Electron Pair Repulsion Model

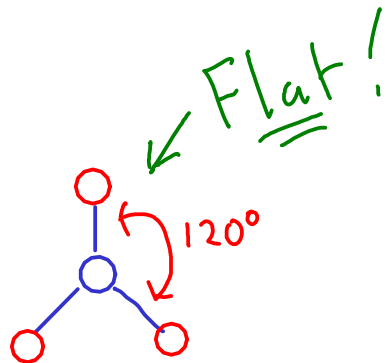
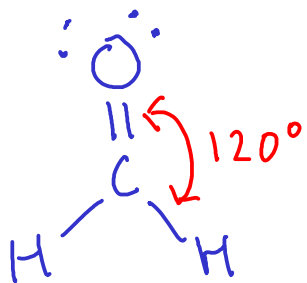
- Each BOND or LONE PAIR OF ELECTRONS around an atom will try to move itself as far away from other bonds or lone pairs as possible!



For the two red circles to be farthest apart, they must be 180 degrees apart

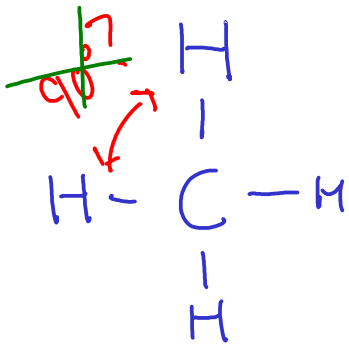
LINEAR MOLECULES

ANY diatomic (two-atom) molecule is linear, but only some three-atom molecules are!



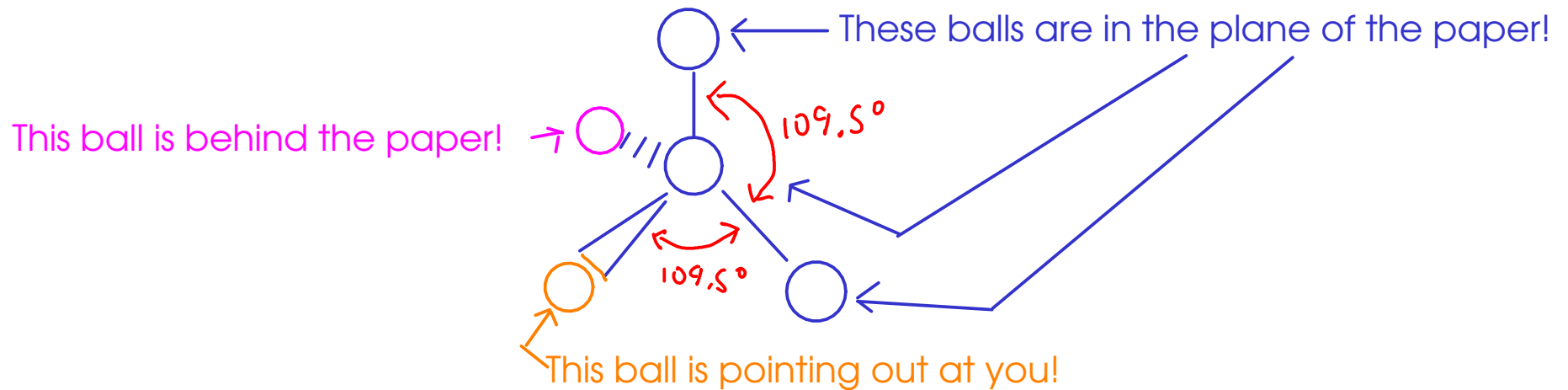
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

TRIGONAL
PLANAR
MOLECULES



These hydrogen atoms might appear at first glance to be 90 degrees apart, but remember that molecules exist in THREE DIMENSIONS, not two!

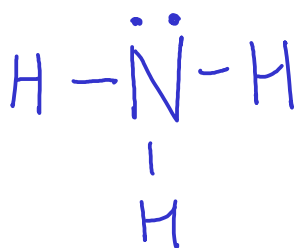
Each hydrogen atom is actually 109.5 degrees apart, forming a TETRAHEDRON.



To see the tetrahedron in three dimensions WITHOUT buying a molecular model kit, just take four balloons, blow them up, and then tie them together. The knot will be the central atom, and the balloons will line themselves up to be 109.5 degrees apart.

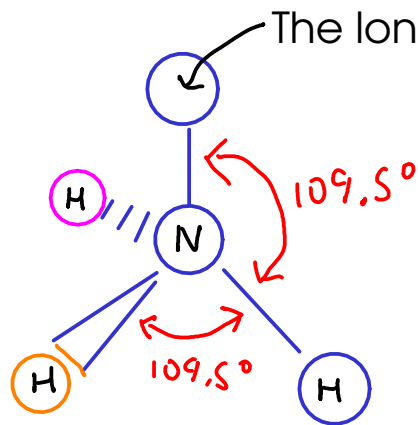
DERIVATIVES OF THE TETRAHEDRON

- What if there are lone pairs? The way the shape of a molecule is described depends on the ATOMS in the molecule, even though lone pairs play a role in the positions of the atoms.

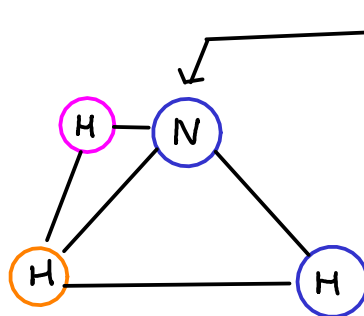


Since there are four "things" around the nitrogen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT ... only three of these things are atoms.

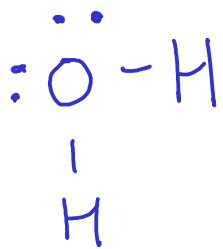
The atoms are arranged in a PYRAMID shape, so we call this molecule PYRAMIDAL!



The lone pair takes one position in the tetrahedron



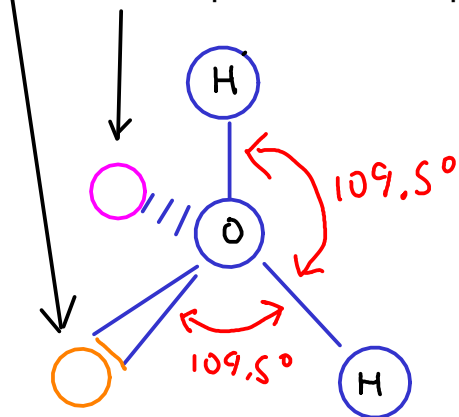
By just looking at the atoms, you can see the pyramid - with the central nitrogen atom as the top and the hydrogen atoms forming the base of the pyramid.



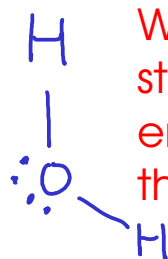
Since there are four "things" around the oxygen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT... only two of these things are atoms.

The atoms are all in a single plane, but they are not lined up in a straight line. We call this shape "BENT".

Lone pairs take up two positions in the tetrahedron

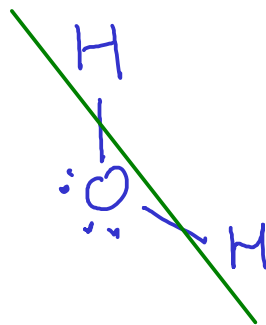


Atoms are in one plane like CO₂, but bent instead of linear!



We sometimes draw the Lewis structure of water this way to emphasize the "bent" nature of the molecule!

Notice that this molecule has two "sides", one with the oxygen atom and one with hydrogen atoms.



POLARITY

- When atoms share electrons, the electrons might not be EVENLY shared. Shared electrons may spend more time around one atomic nucleus than the other.
- When electrons are shared UNEVENLY, this results in a POLAR BOND.

... but how can we tell whether or not a bond will be POLAR? Use experimental data on ELECTRONEGATIVITY!

ELECTRONEGATIVITY:

- A measure of how closely to itself an atom will hold shared electrons
- A bond where there is a LARGE electronegativity difference between atoms will be either POLAR or (for very large differences) IONIC!
- A bond with little or no electronegativity difference between atoms will be NONPOLAR

ELECTRONEGATIVITY TRENDS

- You may look up electronegativity data in tables, but it helps to know trends!

(p344, text)

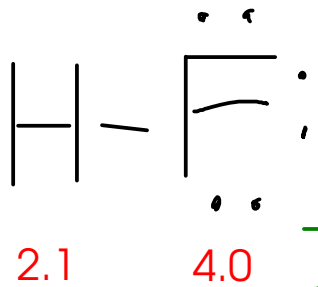
INCREASING
ELECTRO-
NEGATIVITY

	IA	IIA											IIIA	IVA	VA	VIA	VIIA
2	Li	Be											B	C	N	O	F
3	Na	Mg	IIIB	IVB	VB	VIB	VII B	VIII B	IB	IIB			Al	Si	P	S	Cl
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
6	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
7	Fr	Ra	Ac*	Rf	Db	Sg	Bh	Hs	Mt	*"inner" transition metals go here							

Notes:

- ① - FLUORINE is the most electronegative element, while FRANCIUM is the least!
- ② - All the METALS have low electronegativity
- ③ - HYDROGEN is similar in electronegativity to CARBON, so C-H bonds are considered NONPOLAR

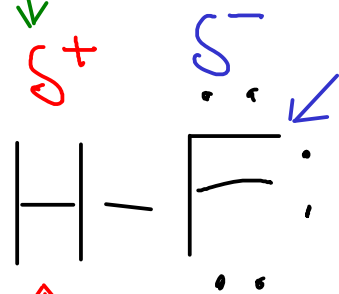
ELECTRONEGATIVITY EXAMPLE



Electronegativity values
Difference = 1.9

Fluorine is much more electronegative than hydrogen. This is a POLAR BOND, and the shared electrons will be held more closely to FLUORINE!

δ
means
"small"



This end of the molecule will have a slight NEGATIVE charge, since the shared electrons are closer to FLUORINE!

This end of the molecule will have a slight POSITIVE charge, since the shared electrons are pulled away from HYDROGEN!

POLARITY OF MOLECULES

So what can a molecule's LEWIS STRUCTURE, SHAPE, and the POLARITY of its bonds tell us?

... the POLARITY of the overall molecule, which will tell us (among other things) what a given molecule will mix with or dissolve in!

POLAR MOLECULES

- Will dissolve in or dissolve other polar molecules
- Will dissolve some ionic compounds
- Will NOT easily dissolve nonpolar molecules

Example:
WATER

NONPOLAR MOLECULES

- Will dissolve in or dissolve other nonpolar molecules
- Will NOT easily dissolve polar molecules or ionic compounds

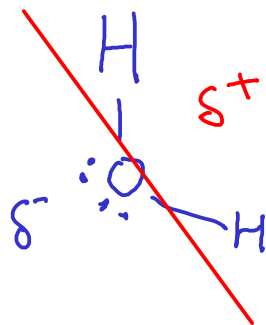
Example:
OILS

For a molecule to be polar, it must ...

- ① Have polar bonds! (Any molecule that contains no polar bonds must be nonpolar!)
- ② Have polar bonds arranged in such a way that they don't balance each other out! (This is why you need to know the structure and shape of the molecule)

EXAMPLES

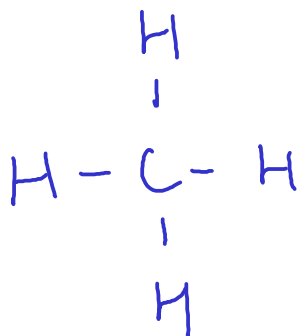
Water, H_2O



O-H bond is polar (O more electronegative than H)!

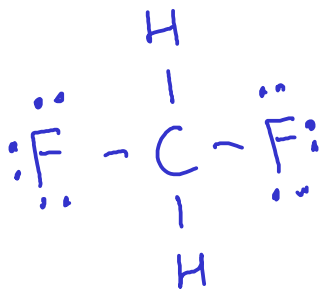
Molecule is polar, since the hydrogen "side" is going to have a slight positive charge (electrons are pulled towards OXYGEN!)

methane, CH_4

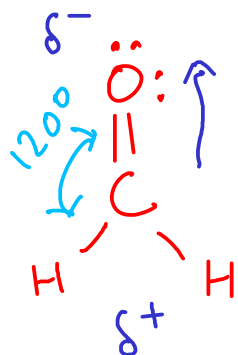
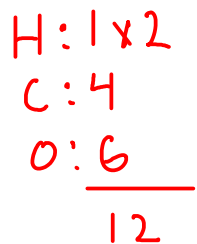


Methane is NONPOLAR, since all the bonds in methane are nonpolar.

CH_2F_2

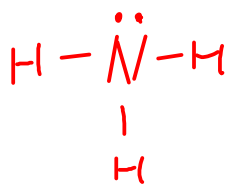
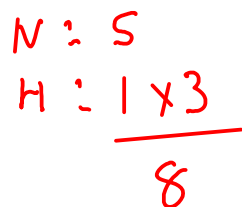


This molecule (in 3D) has two sides - one with the fluorine atoms and one with the hydrogen atoms. Since C-F bonds are polar, electrons are pulled towards the fluorine end - and this molecule is POLAR.



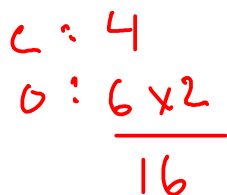
What about shape? TRIGONAL PLANAR. There are three things (=O, 2 -H) around the central carbon, so they will spread out as far as possible - 120 degrees.

Polarity? The C=O bond is a polar bond, and it is not "canceled" out by other bonds. The molecule is POLAR.



Shape? There are FOUR groups around the central nitrogen atom - 109.5 degrees apart. (same as tetrahedral). The ATOMS in the molecule form a PYRAMID - we call the structure PYRAMIDAL.

Polarity? N-H bonds are polar, and they are arranged in such a way that electrons can be pulled towards the nitrogen "top" of the pyramid. So the nitrogen end of the pyramid will be slightly negative and the bottom hydrogens will be slightly positive. A POLAR MOLECULE!



Shape? LINEAR. The oxygen atoms can move 180 degrees apart.

Polarity? C=O bonds are polar. BUT, they are 180 degrees apart, so they cancel each other out. Carbon dioxide is NONPOLAR.