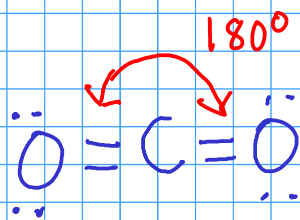
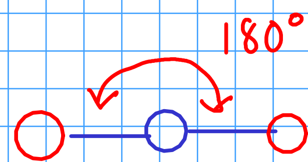
PREDICTING MOLECULAR SHAPE

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!

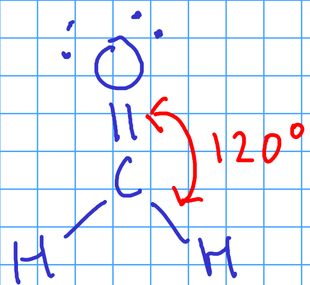


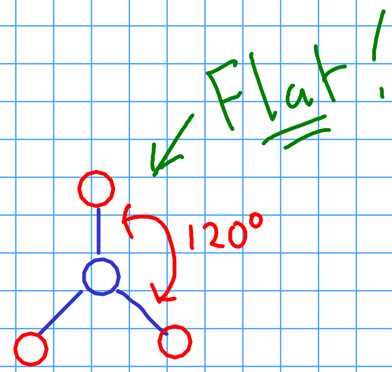


For the two red circles to be farthest apart, they must be 180 degrees apart

LINEAR MOLECULES

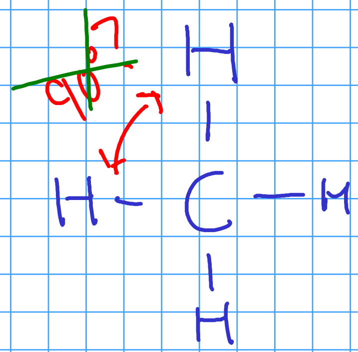
ANY diatomic (two-atom) molecule is linear, but only some three-atom molecules are!





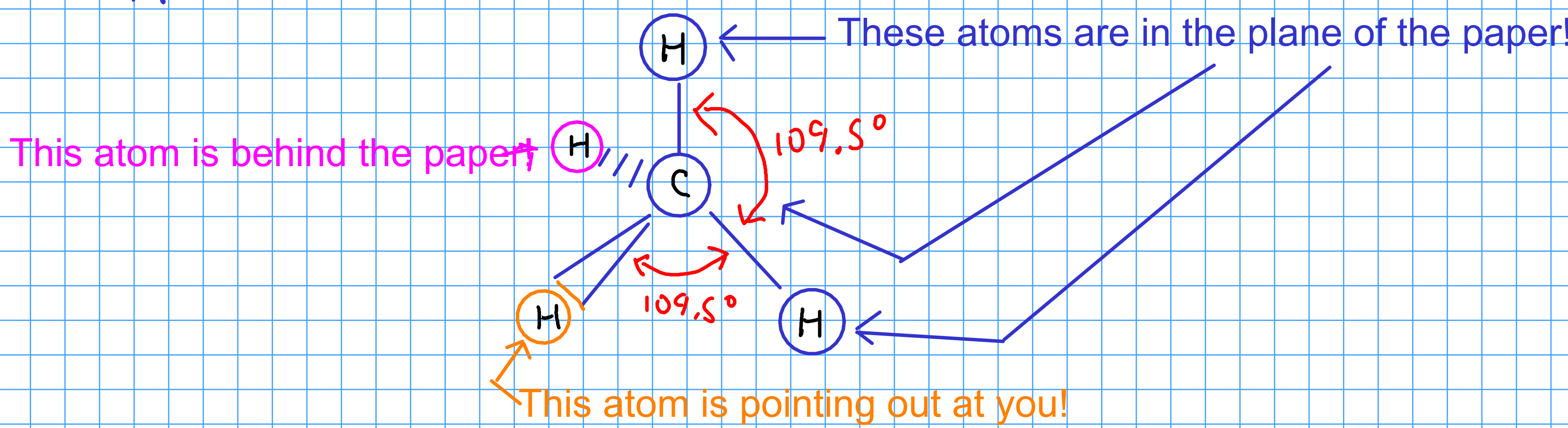
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

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!

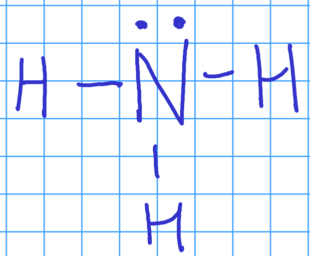
Each hydrogen atom is actually 109.5 degrees apart, forming a TETRAHEDRON.



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

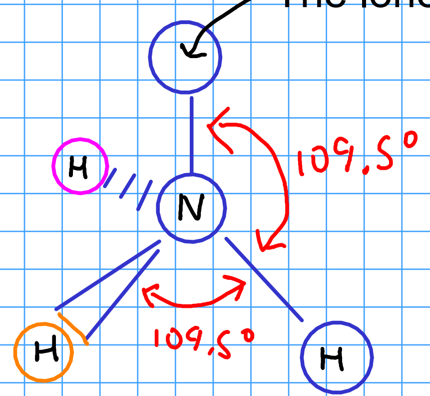
- What if there are lone pairs? The way the shape of a molecule is described depends on the ATOMS in the molecule, even though lone pairs play a role in the positions of the atoms.

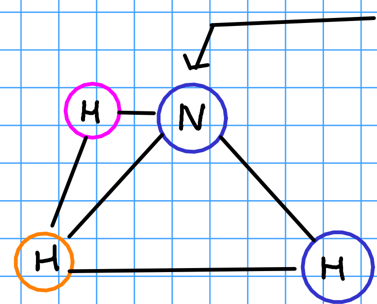


Since there are four "things" around the nitrogen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT ... only three of these things are atoms.

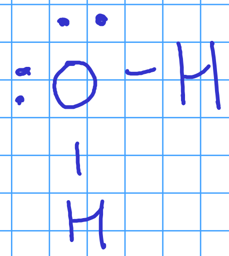
The atoms are arranged in a PYRAMID shape, so we call this molecule PYRAMIDAL!

The lone pair takes one position in the tetrahedron





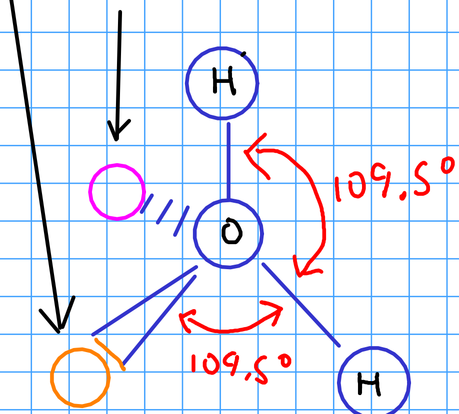
By just looking at the atoms, you can see the pyramid - with the central nitrogen atom as the top and the hydrogen atoms forming the base of the pyramid.



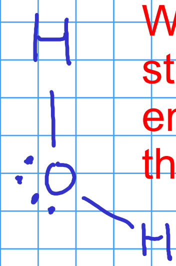
Since there are four "things" around the oxygen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT... only two of these things are atoms.

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

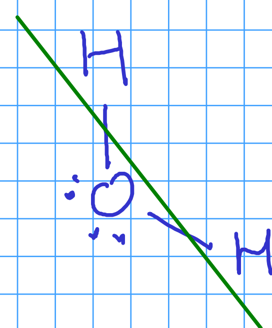


* These atoms are in the same plane, like carbon dioxide. But they are not arranged linearly!



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

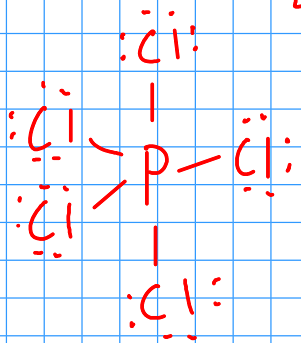
Notice that this molecule has two "sides", one with the oxygen atom and one with hydrogen atoms.



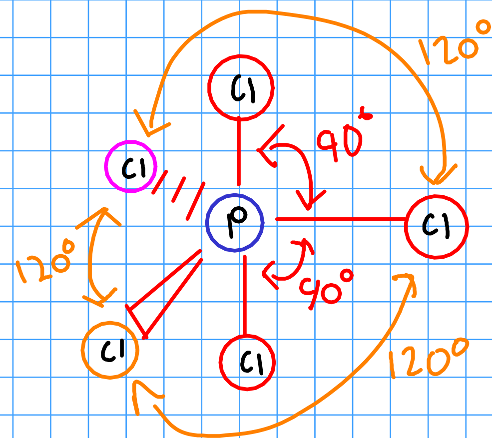
SHAPES OF EXPANDED VALENCE MOLECULES

PCl_5:

P : 5
Cl : 7 x 5
40

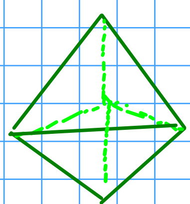


There are five atoms bonded to the central phosphorus atom, and they will attempt to get as far apart as possible from one another!



The top and bottom atoms are 90 degrees apart from the atoms around the center.

The atoms around the center are 120 degrees apart from each other.

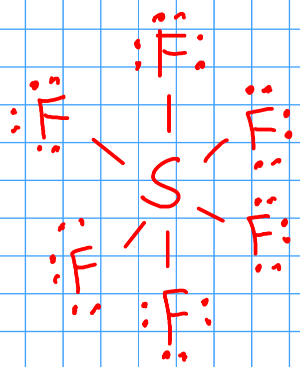


There are acually two DIFFERENT bond angles in this structure. It's called TRIGONAL BIPYRAMIDAL.

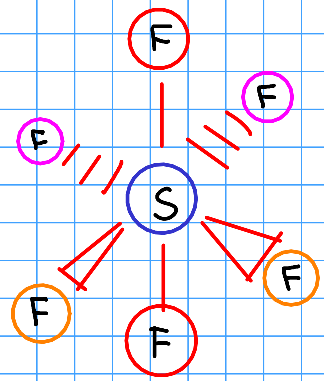
There are several derivatives of the trigonal bipyramidal shape (like the tetrahedral shape) - depending on how many things around the central atom are atoms!

SF_6:

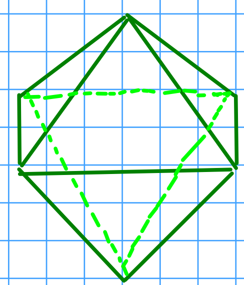
S: 6
F: 7x6
48



There are six atoms bonded to the central sulfur atom, and they will attempt to get as far apart as possible from one another!



All bond angles in this arrangement are 90 degrees!



This shape is called OCTAHEDRAL, since it has eight sides.

Like the tetrahedral and trigonal bipyramidal arrangements, there are several derivatives of the octahedron - depending on how many of the six things around the center are 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 (AGAIN!)

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

INCREASING ELECTRO-NEGATIVITY

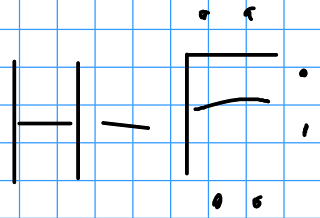
	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA
2	Li	Be											B	C	N	O	F
3	Na	Mg											Al	Si	P	S	Cl
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
6	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
7	Fr	Ra	Ac*	Rf	Db	Sg	Bh	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, and metal/nonmetal combinations form IONIC bonds
3. - HYDROGEN is similar in electronegativity to CARBON, so C-H bonds are considered NONPOLAR

ELECTRONEGATIVITY EXAMPLE

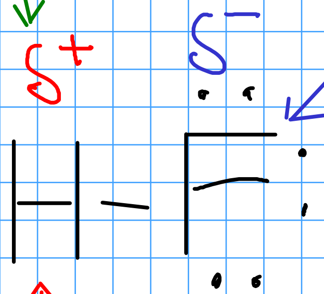


2.1 4.0]— Electronegativity values

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" here



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 nonpolar molecules or ionic compounds

Example: OILS

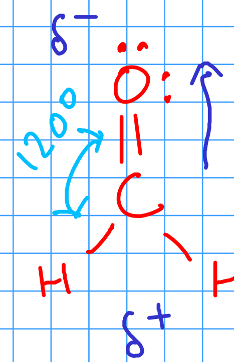
For a molecule to be polar, it must ...

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:

H_2CO

H : 1 x 2
C : 4
O : 6
———
12



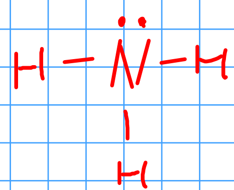
What about shape? TRIGONAL PLANAR. There are three things (=O, 2 -H) around the central carbon, so they will spread out as far as possible - 120 degrees.

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

NH_3

N : 5
H : 1 x 3
———
8

Shape? There are FOUR things around the central nitrogen atom - forcing the bond angles to be 109.5, or tetrahedral. BUT, only three of the things are atoms, and we describe shape based on ATOMS. We call this one PYRAMIDAL.



Polarity? N-H bonds are polar, and they're arranged so that the "top" of the pyramid (N) will be slightly negative, while the "bottom" H atoms will be slightly positive. So the overall molecule is POLAR.

CO_2

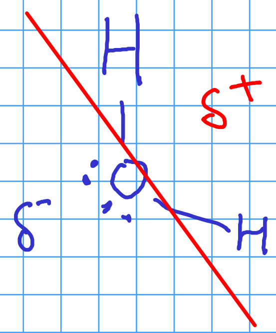
C : 4
O : 6 x 2
———
16

Shape? Only two things (=O) around the carbon center, and they will spread out as far as possible. LINEAR!

Polarity? C=O bonds should be polar, but they are arranged so that they will cancel each other out. This molecule is NONPOLAR.

EXAMPLES

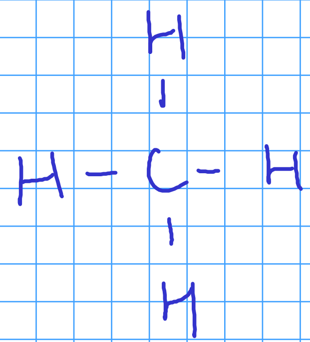
Water, H_2O



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

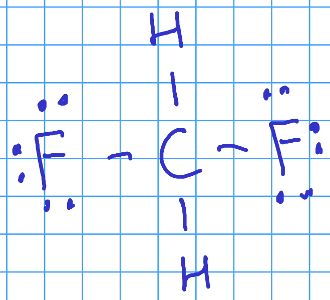
Molecule is polar, since the hydrogen "side" is going to have a slight positive charge (electrons are pulled towards OXYGEN!)

methane, CH_4



NONPOLAR, since all the bonds are nonpolar!

CH_2F_2



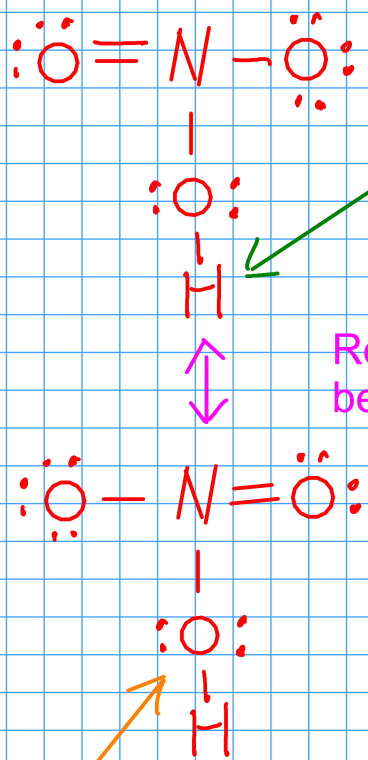
Molecule is POLAR. In three dimensions, the fluorine atoms are on one side of the molecule, while the hydrogen atoms are on the other. The flat structure drawn here is deceiving!

HNO_3

H : 1
N : 5
O : 6 x 3

24

Start drawing skeleton by recognizing that this compound is an OXYACID .... hydrogen attached to a polyatomic ion.



In an OXYACID, the acidic hydrogen atoms are always attached to an OXYGEN atom.

Resonance structures. The "double bond" electrons are really shared between all three atoms (O-N-O)

Shape? Since this molecule has two centers, give the shape around each center! Around NITROGEN, the shape is TRIGONAL PLANAR (3 things around N). Around the bottom oxygen, there are four things but only two atoms: BENT

Polarity? We expect electrons to be pulled away from H, and that the H end would end up slightly positive. POLAR.

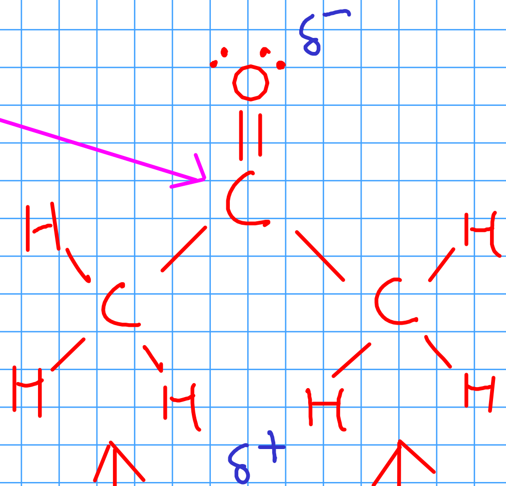
In water, the bottom oxygen atom is able to TAKE the electrons it is sharing with H, forming IONS! (H+ and nitrate)!

CH_3COCH_3 (acetone)

C: 4x3
H: 1x6
O: 6
24

The formula provides a clue to the skeletal structure of the molecule. There are three carbon centers in this molecule!

Shape? we need to describe the shape of the molecule around each of the carbon centers!



These two carbon centers are TETRAHEDRAL, since they are surrounded by four other atoms and no lone pairs.

This carbon center is TRIGONAL PLANAR. It is surrounded by THREE other atoms and no lone pairs.

Polarity? The C=O bond is polar, and electrons are pulled towards the oxygen "side" of the molecule. Experimentally, we observe that water (another polar molecule) and acetone mix very well with each other,