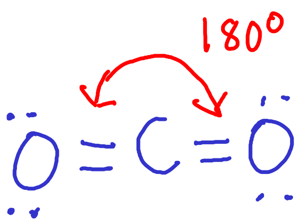
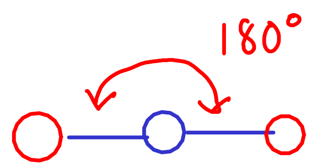
PREDICTING MOLECULAR SHAPE

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!

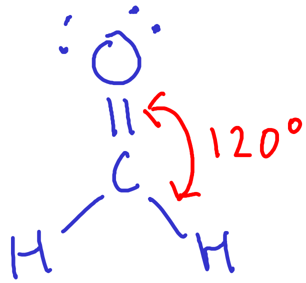


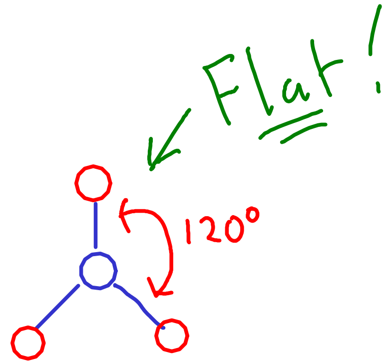


For the two red circles to be farthest apart, they must be 180 degrees apart

LINEAR MOLECULES

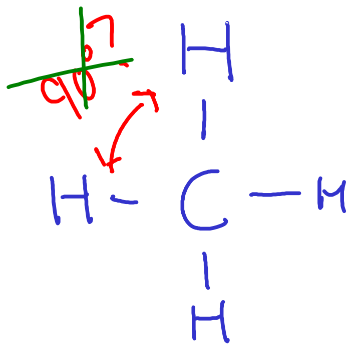
ANY diatomic (two-atom) molecule is linear, but only some three-atom molecules are!





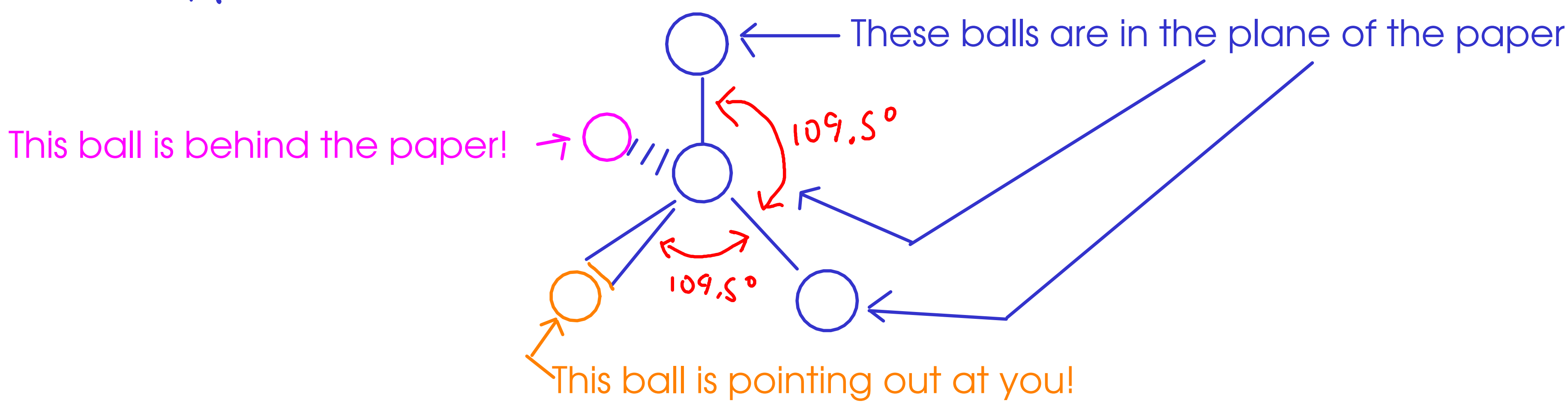
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

TRIGONAL PLANAR MOLECULES



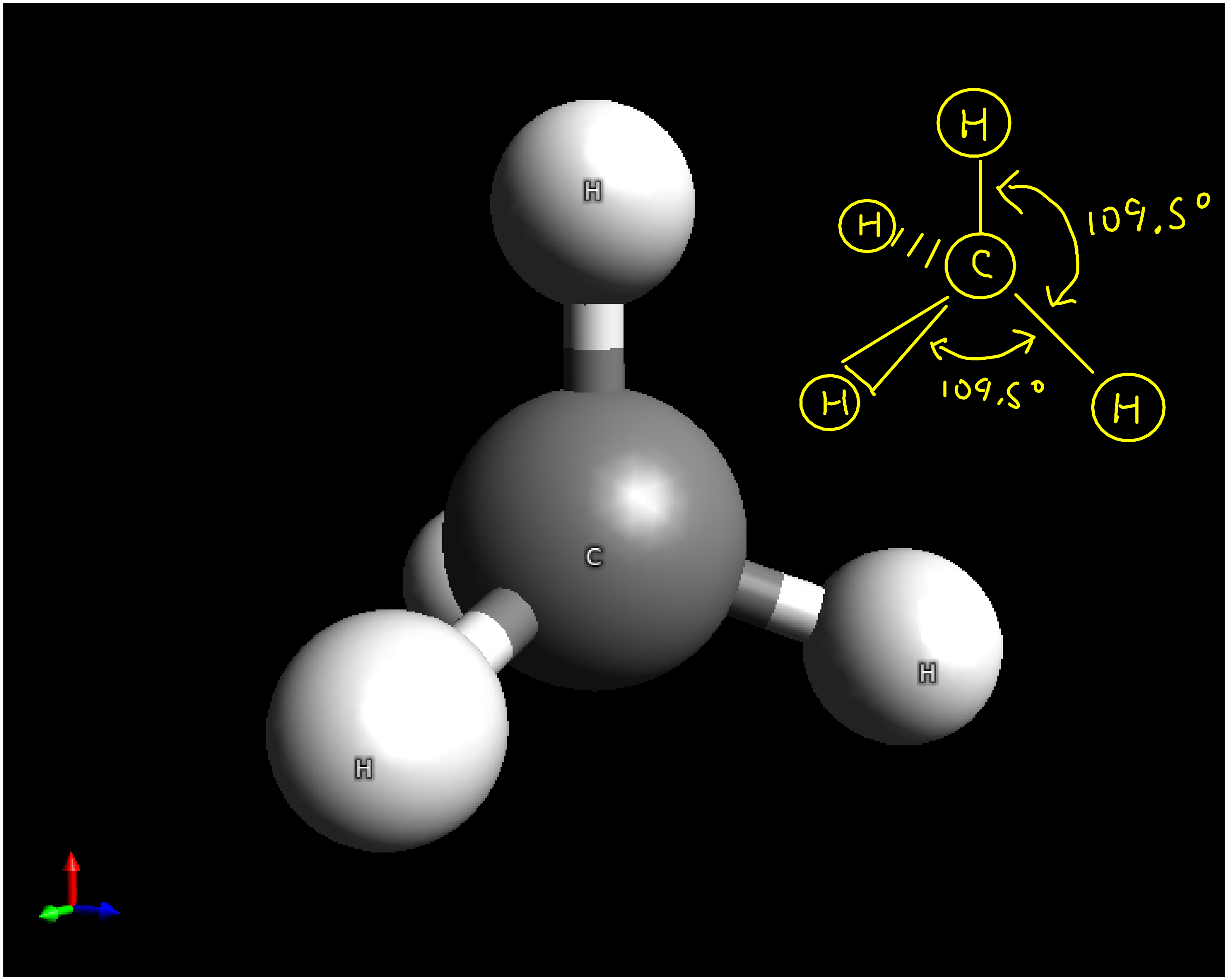
These hydrogen atoms might appear at first glance to be 90 degrees apart, but remember that molecules exist in THREE DIMENSIONS, not two!

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



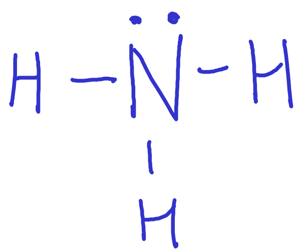
To see the tetrahedron in three dimensions WITHOUT buying a molecular model kit, just take four balloons, blow them up, and then tie them together. The knot will be the central atom, and the balloons will line themselves up to be 109.5 degrees apart.

Here's a computer ball-and-stick rendering of the methane molecule.



DERIVATIVES OF THE TETRAHEDRON

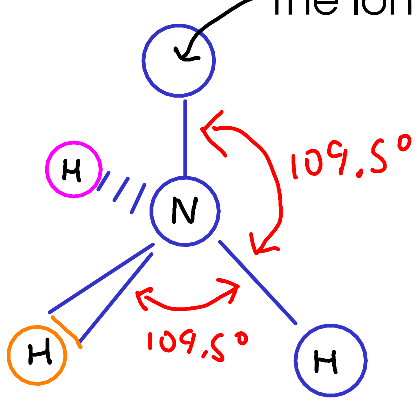
- What if there are lone pairs? The way the shape of a molecule is described depends on the ATOMS in the molecule, even though lone pairs play a role in the positions of the atoms.

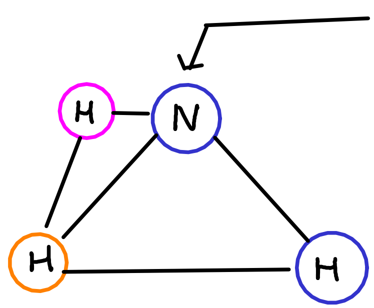


Since there are four "things" around the nitrogen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT ... only three of these things are atoms.

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

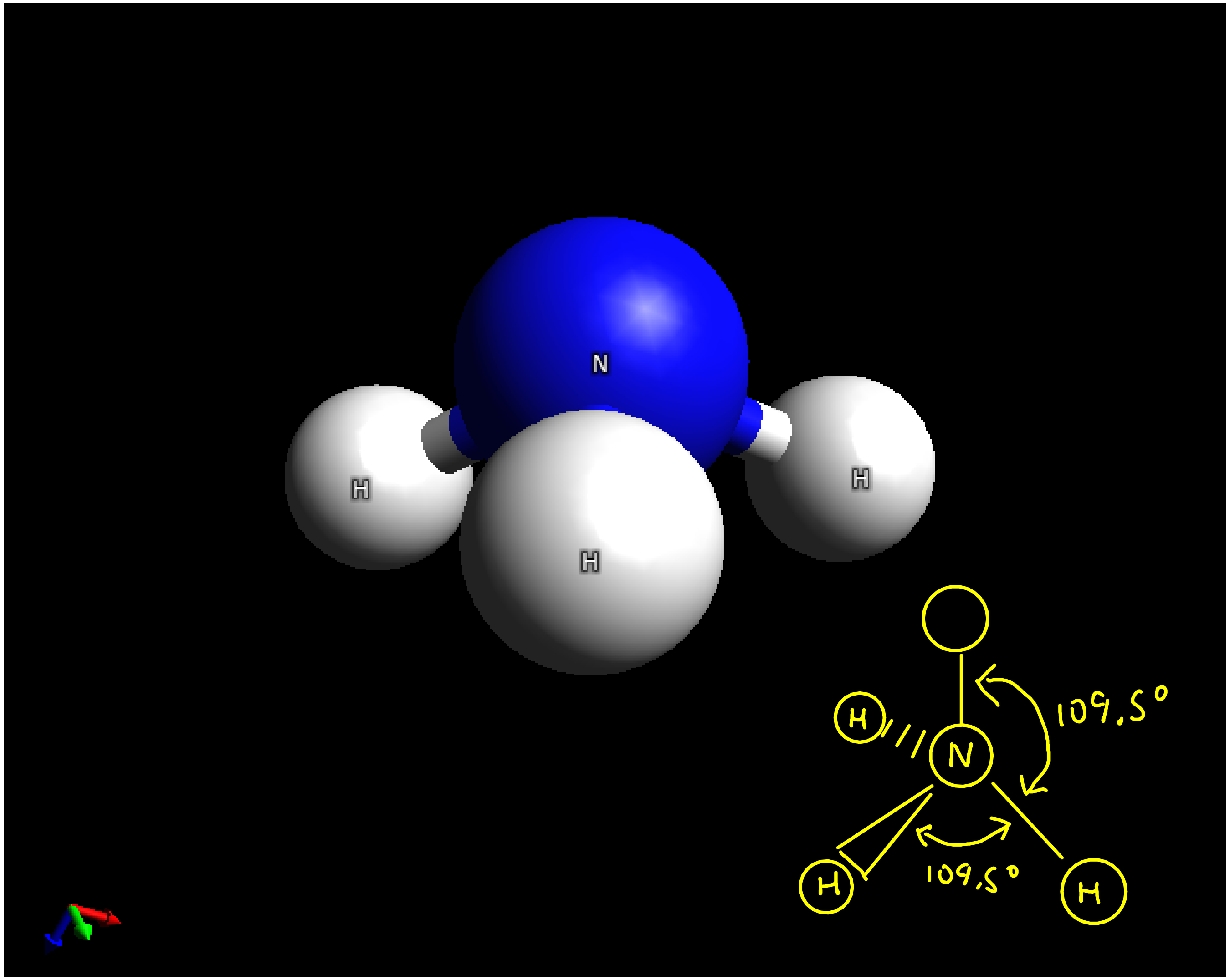
The lone pair takes one position in the tetrahedron

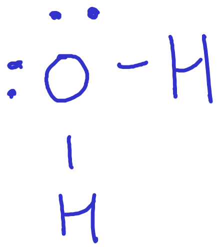




By just looking at the atoms, you can see the pyramid - with the central nitrogen atom as the top and the hydrogen atoms forming the base of the pyramid.

NH_3

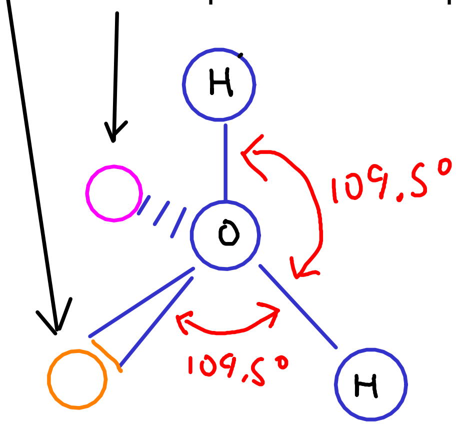




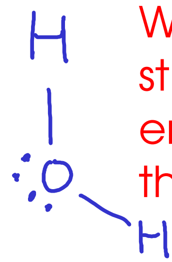
Since there are four "things" around the oxygen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT... only two of these things are atoms.

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

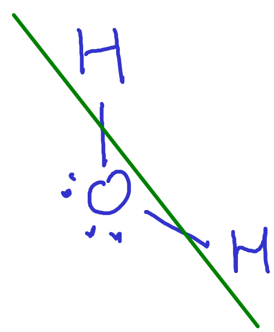


* Atoms are in one plane like CO_2, but bent instead of linear!

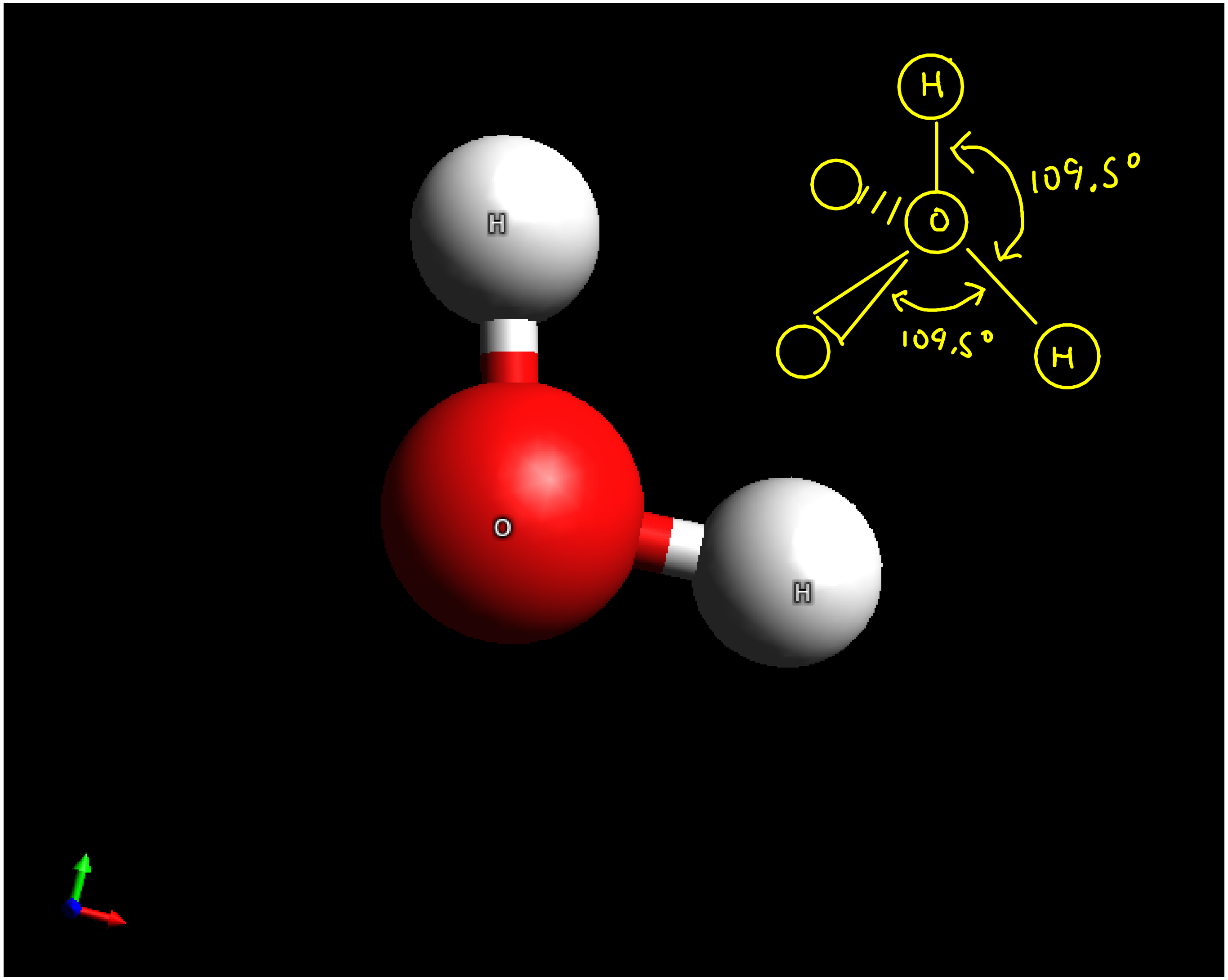


We sometimes draw the Lewis structure of water this way to emphasize the "bent" nature of the molecule!

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



H_2O



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 elecronegativity data in tables, but it helps to know trends!

↰ (p362, text) Fig 12.3

→ INCREASING ELECTRO-NEGATIVITY ↑

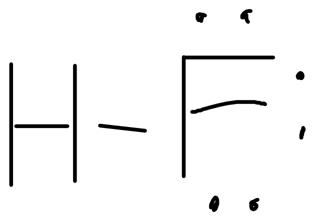
	IA	IIA	IIIB	IVB	VB	VIB	VIIB	VIIIB			IB	IIB	IIIA	IVA	VA	VIA	VIIA
2	Li	Be											B	C	N	O	F
3	Na	Mg											Al	Si	P	S	Cl
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I
6	Cs	Ba	La*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At
7	Fr	Ra	Ac*	Rf	Db	Sg	Bh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

*"inner" transition metals go here

Notes:

1. - FLUORINE is the most elecronegative 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

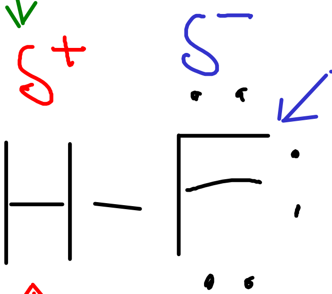


2.1 4.0 – Electronegativity values

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"



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!

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

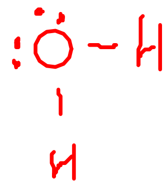
For a molecule to be polar, it must ...

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

H: 2 x 1
O: 1 x 6
———
8

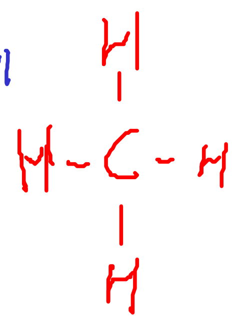


Polar bonds? YES! O-H bonds should be polar since oxygen is more electronegative than hydrogen

This molecule is BENT, and electrons will be pulled towards the oxygen end of the molecule - making the overall molecule POLAR.

methane, CH_4

C: 1 x 4
H: 4 x 1
———
8

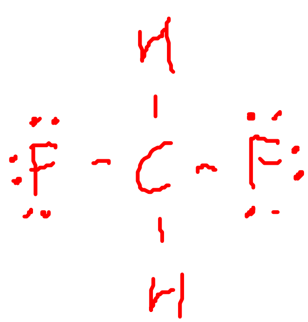


Polar bonds? NO! C-H bonds are nonpolar, since carbon and hydrogen are similar in electronegativity./

This molecule is TETRAHEDRAL, but this doesn't affect polarity. The molecule has no polar bonds, so it's NONPOLAR

CH_2F_2

C: 1 x 4
H: 2 x 1
F: 2 x 7
———
20

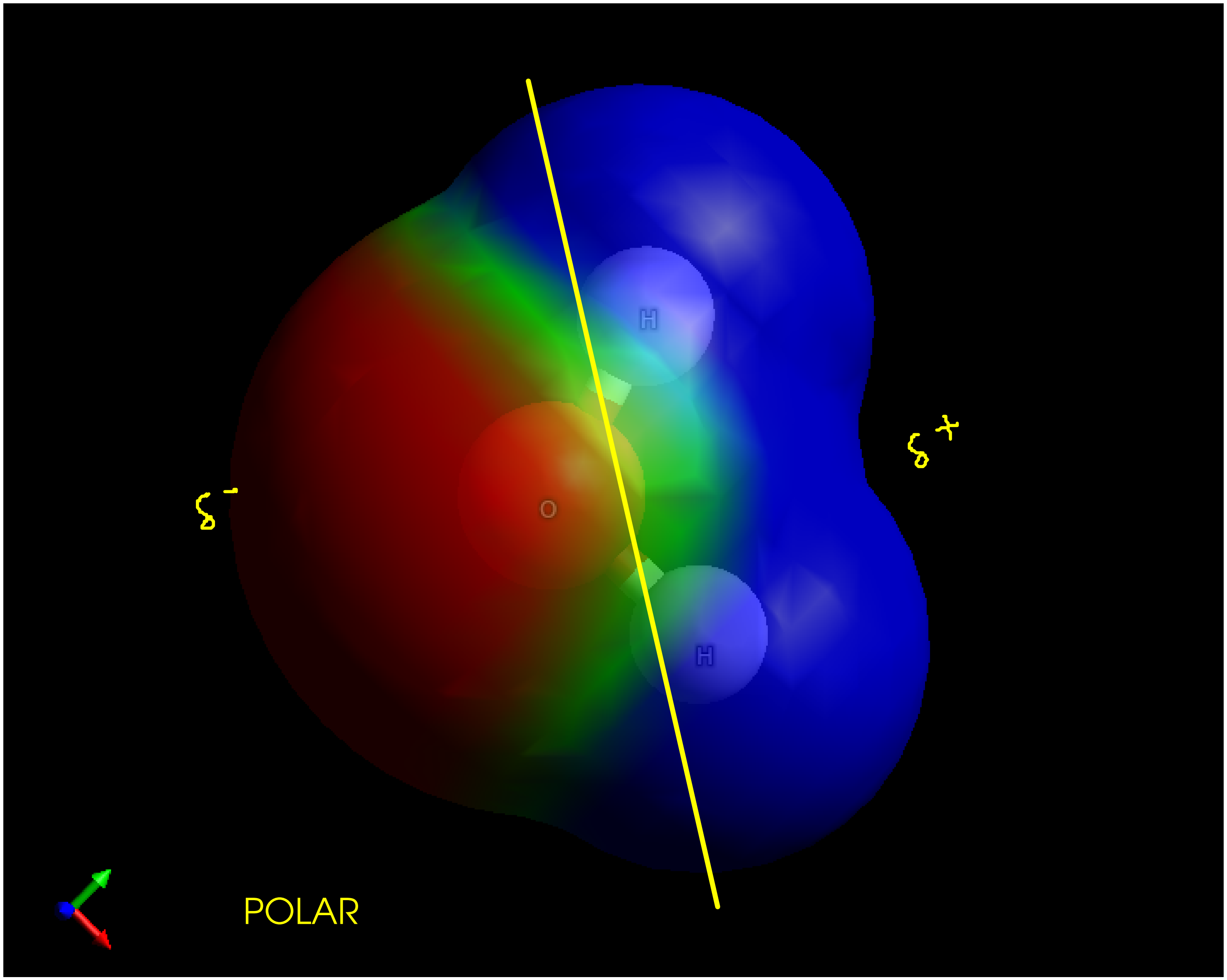


Like methane, this molecule is TETRAHEDRAL. UNLIKE methane, this molecule has some polar bonds (C-F).

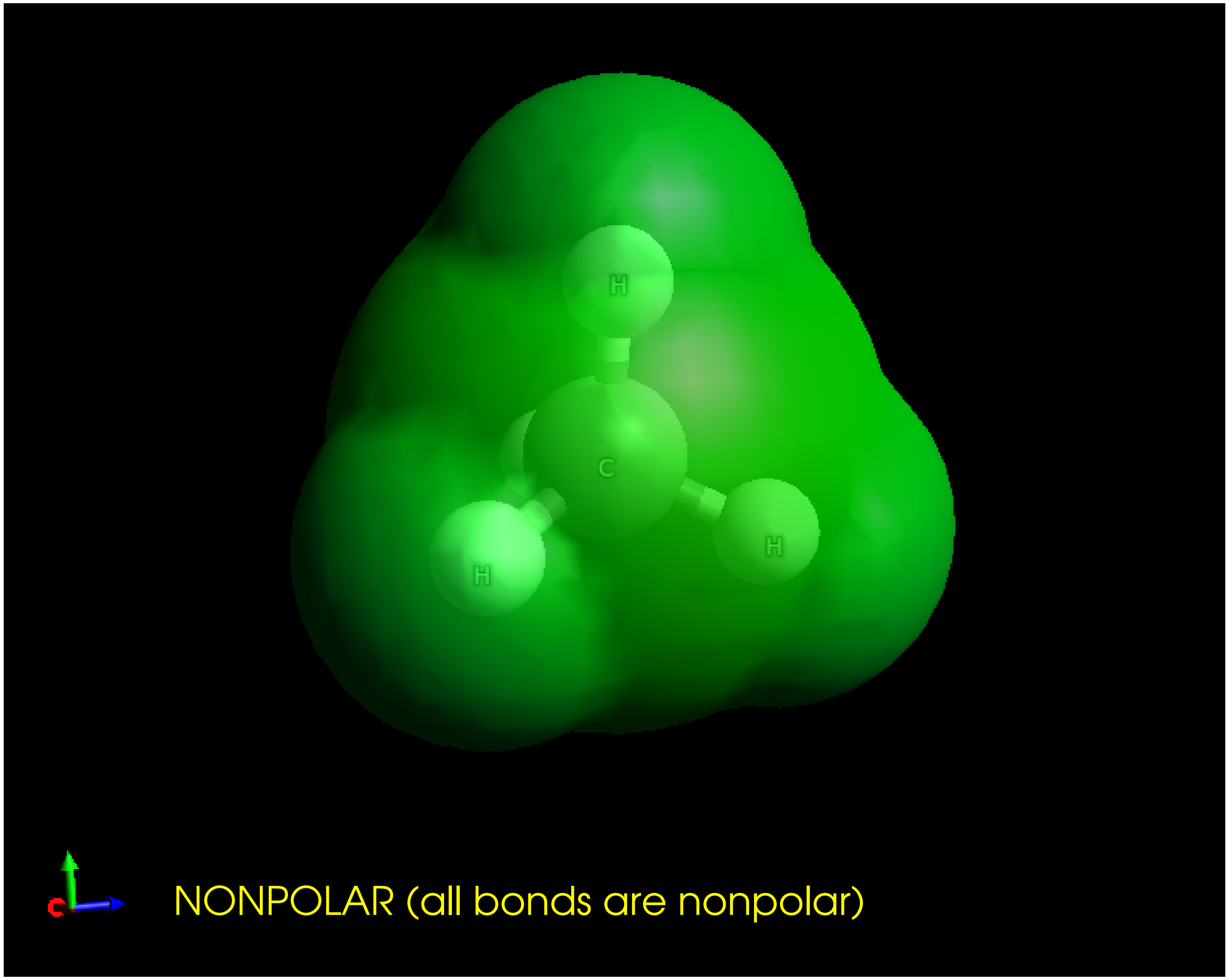
This molecule is POLAR, since fluorine atoms will pull electrons to the fluorine "side" of the moelcule. (The Lewisi structure doesn't show the 3D arrangement - in 3D, the fluorines are NOT on opposite sides of the molecule!)

H_2O

This ball-and-stick model shows electrostatic potential - red for more negative and blue for more positive



CH_4



CH_2F_2