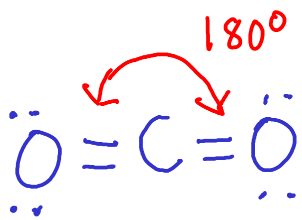
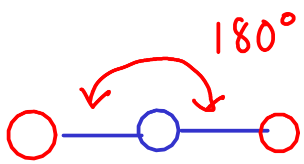
PREDICTING MOLECULAR SHAPE

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!

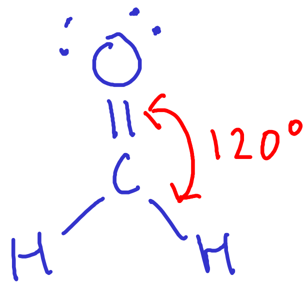


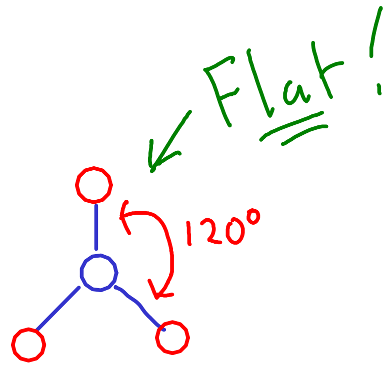


For the two red circles to be farthest apart, they must be 180 degrees apart

LINEAR MOLECULES

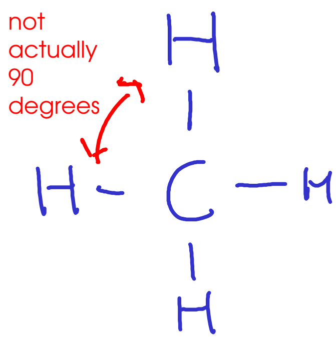
ANY diatomic (two-atom) molecule is linear, but only some three-atom molecules are!





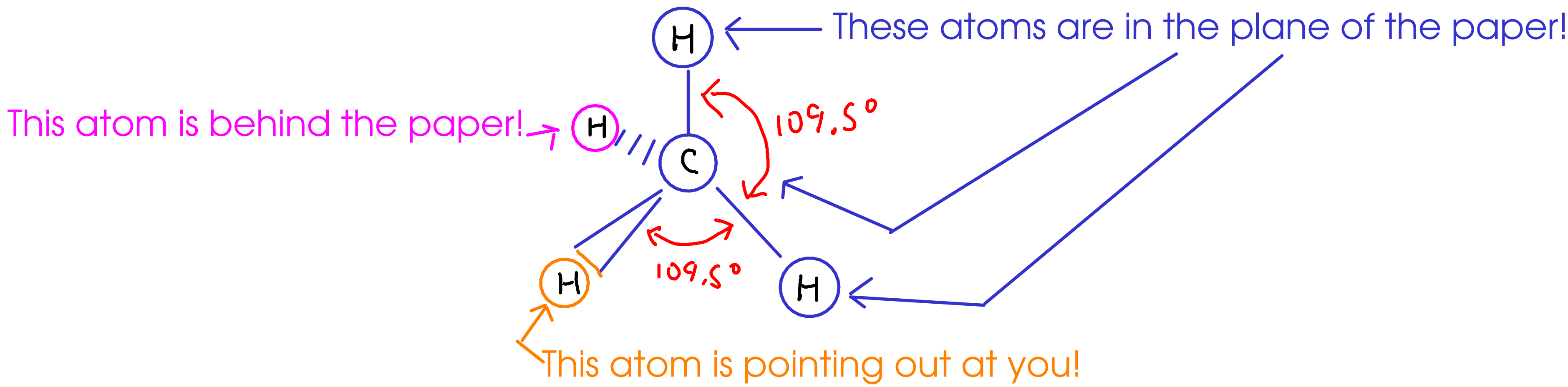
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

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.



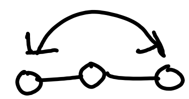
To see the tetrahedron in three dimensions WITHOUT buying a molecular model kit, just take four balloons, blow them up, and then tie them together. The knot will be the central atom, and the balloons will line themselves up to be 109.5 degrees apart.

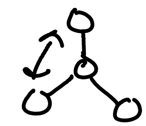
VSEPR shapes

* "Groups" can be either BONDS or LONE PAIRS!

VSEPR shapes:

Groups* around central atom	Shape	Bond angle(s) in degrees
2	linear	180
3	trigonal planar	120
4	tetrahedral / pyramidal / bent	109.5
5	trigonal bipyramidal (and derivatives)	90 and 120
6	octahedral (and derivatives)	90



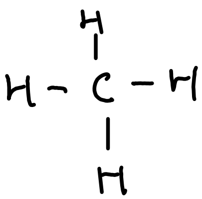


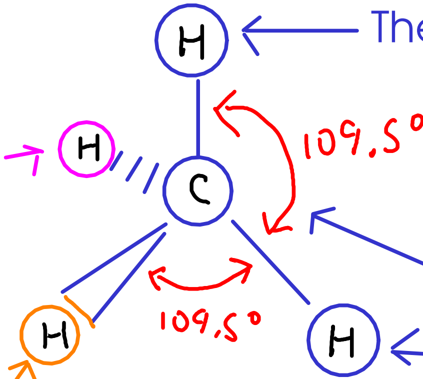
5 and 6 violate "octet rule"

More on "4 things around a central atom":

- A compound that obeys the octet rule can have a maximum of four groups around its central atom. But we describe the molecular shape based on how ATOMS are arrnaged around the center. What if some of those groups aren't atoms, but pairs of UNSHARED electrons?

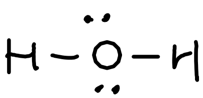
CH_4:

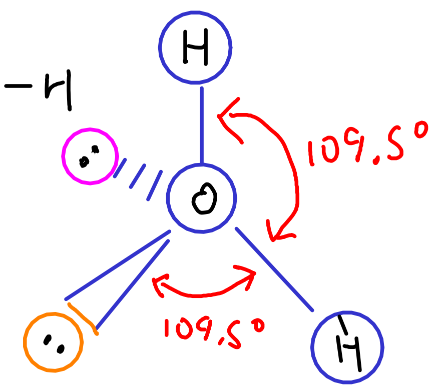




With four ATOMS around the center, we call the shape "TETRAHEDRAL"

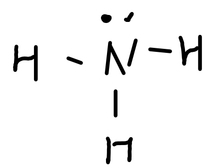
H_2O:

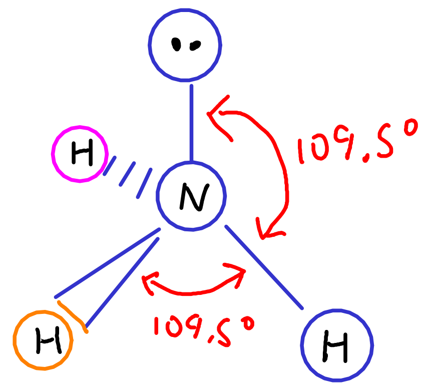


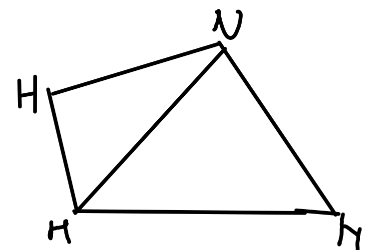


With two ATOMS and two LONE PAIRS, we call the shape "BENT"

NH_3:



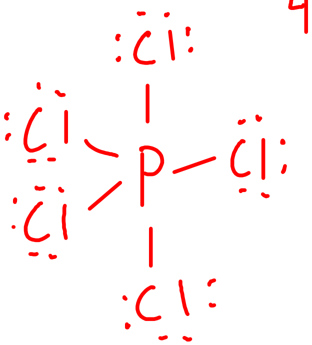




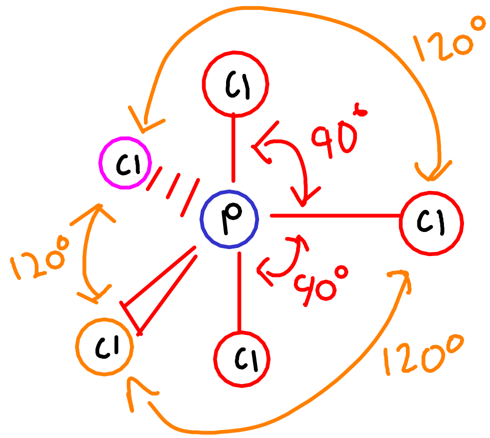
With three ATOMS and one LONE PAIR, we call the shape "PYRAMIDAL"

SHAPES OF EXPANDED VALENCE MOLECULES

PCl_5: P : 5
Cl : 7 x 5
40

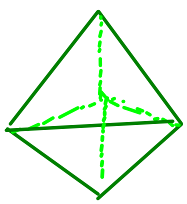


There are five atoms bonded to the central phosphorus atom, and they will attempt to get as far apart as possible from one another!



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.

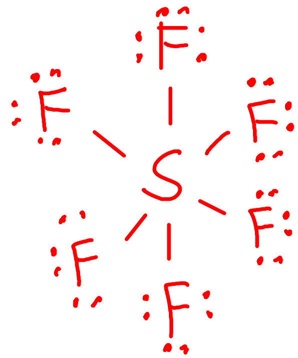


There are acually two DIFFERENT bond angles in this structure. It's called TRIGONAL BIPYRAMIDAL.

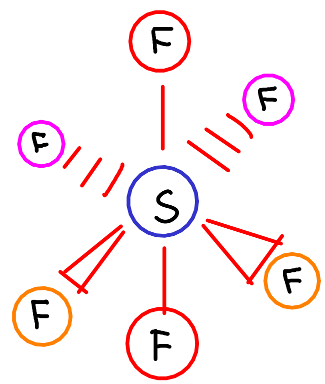
There are several derivatives of the trigonal bipyramidal shape (like the tetrahedral shape) - depending on how many things around the central atom are atoms!

SF_6:

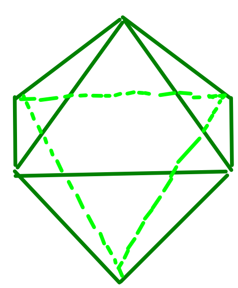
S: 6
F: 7x6
48



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!

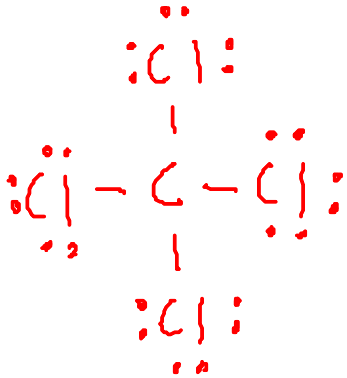
Examples:

CCl_4

$C: 1 \times 4$

$Cl: 4 \times 7$

$32\,e^-$



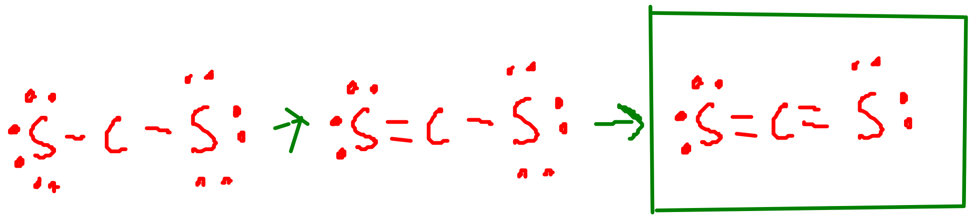
Geometry? 4 groups around central atom. TETRAHEDRAL.
Shape? All four are other atoms, so TETRAHEDRAL.

CS_2

$C: 1 \times 4$

$S: 2 \times 6$

$16\,e^-$



skeletal structure

final structure

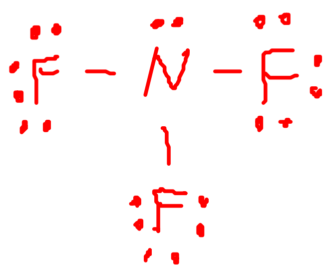
Geometry? Two groups around central atom, so LINEAR.
Shape? Both groups are atoms, also LINEAR.

NF_3

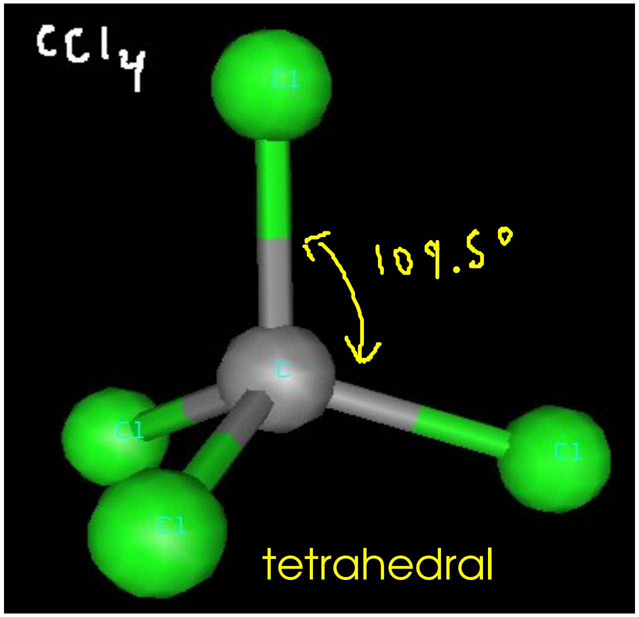
$N: 1 \times 5$

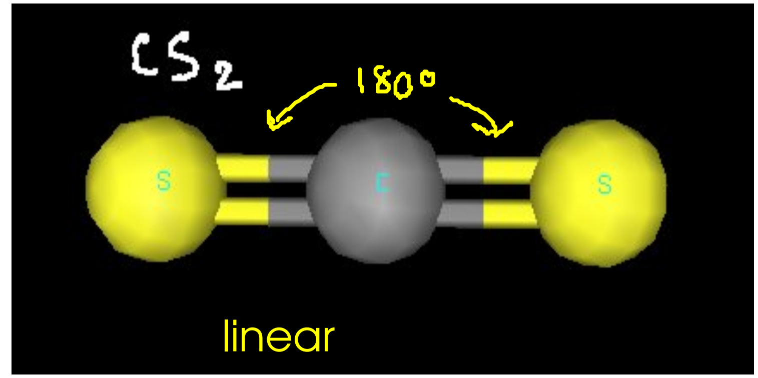
$F: 3 \times 7 = 21$

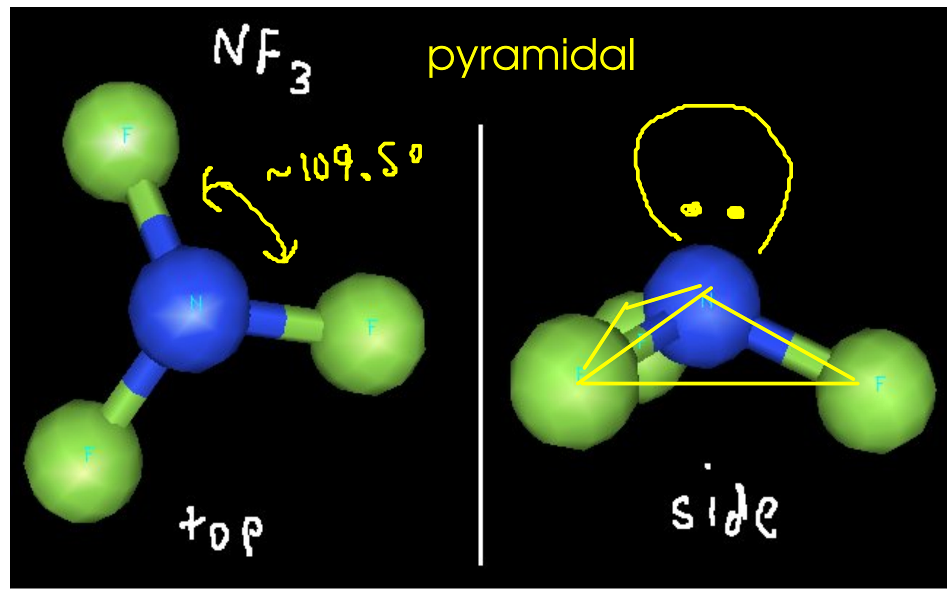
$26\,e^-$



Geometry? 4 groups around central atom. TETRAHEDRAL geometry.
Shape? Three of the four groups are atoms, and one is a lone pair. PYRAMIDAL.

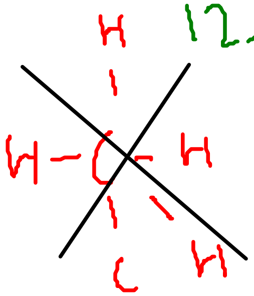

CCl4
109.5°
tetrahedral


CS2
180°
S
C
S
linear

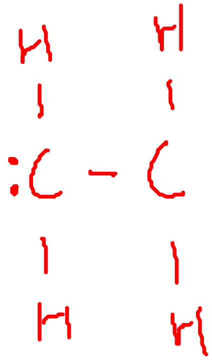

NF3
pyramidal
~109.5°
F
N
F
F
top
side

C_2H_4

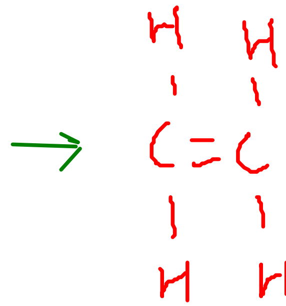
C: 2 x 4
H: 4 x 1
12 e⁻



Structure tip: Multiple carbon atoms mean multiple "central atoms"

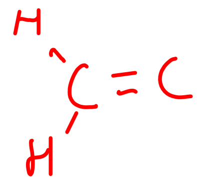


skeletal structure



final structure

For larger molecules, describe geometry and shape around each center.

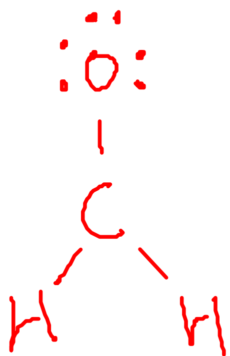


The carbon on the left has TRIGONAL PLANAR gemoetry (3 groups). Also, TRIGONAL PLANAR shape!

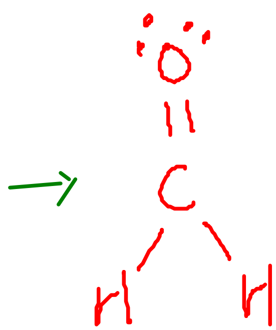
The other carbon is the same. This molecule has two TRIGONAL PLANAR carbon centers.

H_2CO

H : 2 x 1
C : 1 x 4
O : 1 x 6
12 e⁻

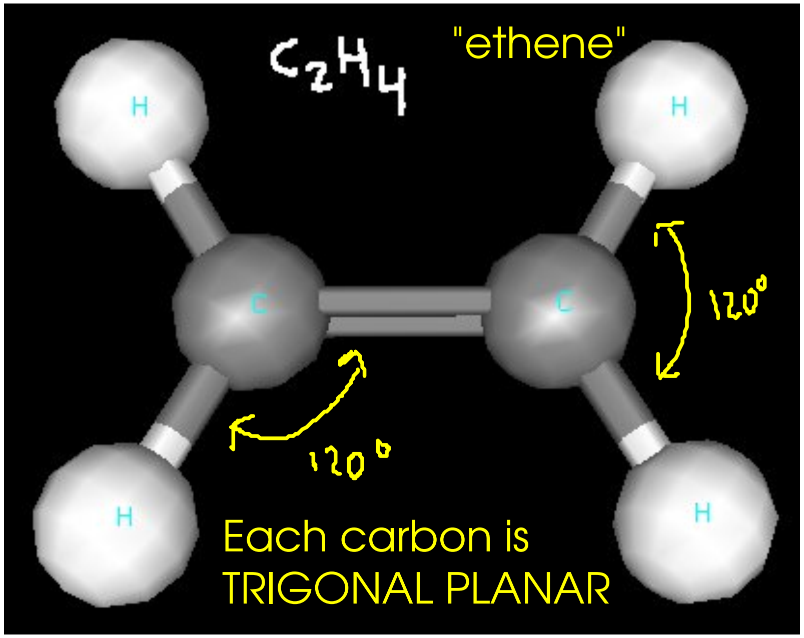


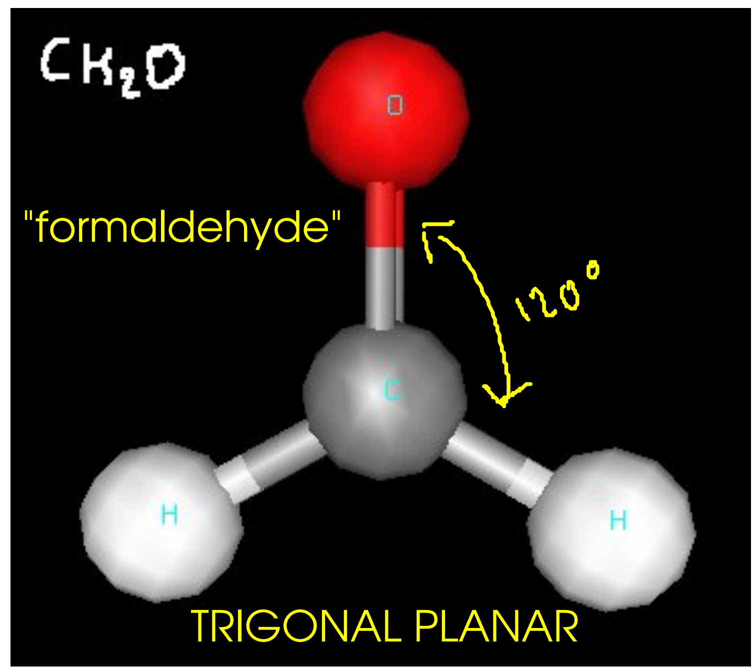
skeletal structure



final structure

Geometry? Three groups bonded to central carbon - TRIGONAL PLANAR
Shape? All three are atoms, so also TRIGONAL PLANAR.


C_2H_4
"ethene"
H
H
C
C
120°
120°
H
H
Each carbon is
TRIGONAL PLANAR

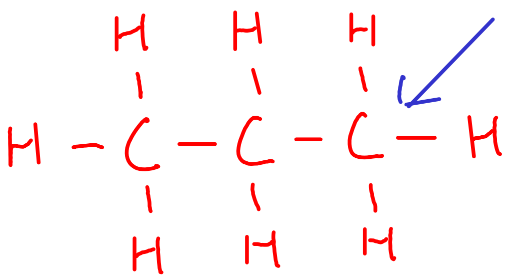

CH_2O
O
"formaldehyde"
120°
C
H
H
TRIGONAL PLANAR

VSEPR and large molecules

- Large molecules have more than one "center" atom

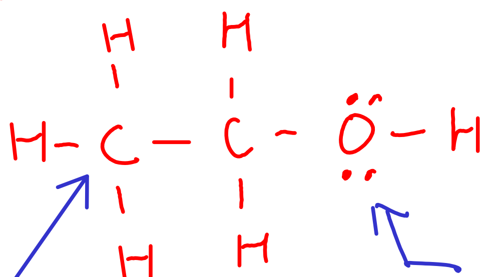
- Describe the molecule by describing the shape around each "center".

C_3H_8:



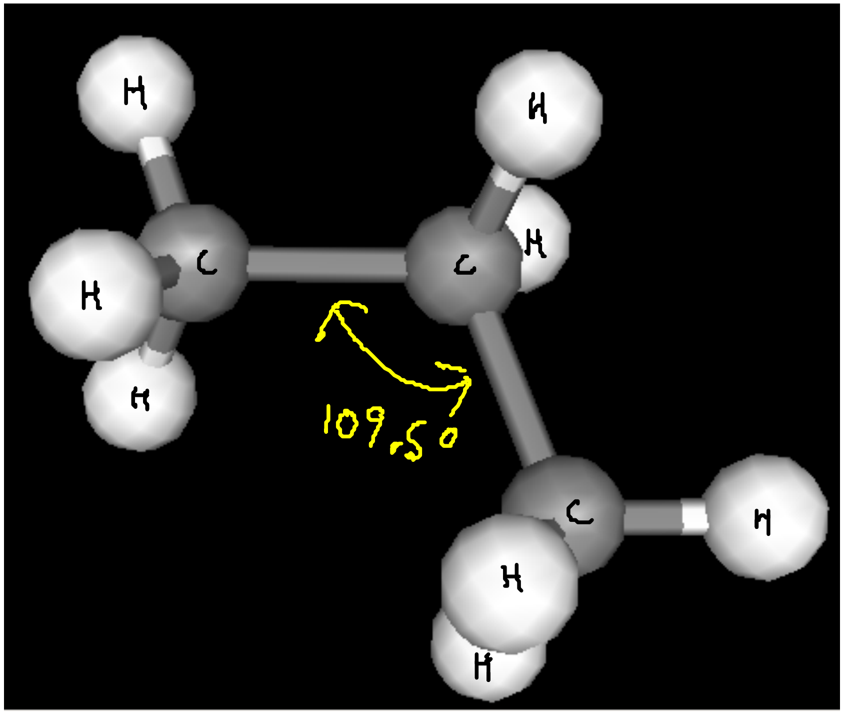
Each of the three carbon centers is TETRAHEDRAL, since each are surrounded by four groups.

CH_3CH_2OH:



The shape around this oxygen atom is BENT.

These carbon atoms have TETRAHEDRAL geometry.

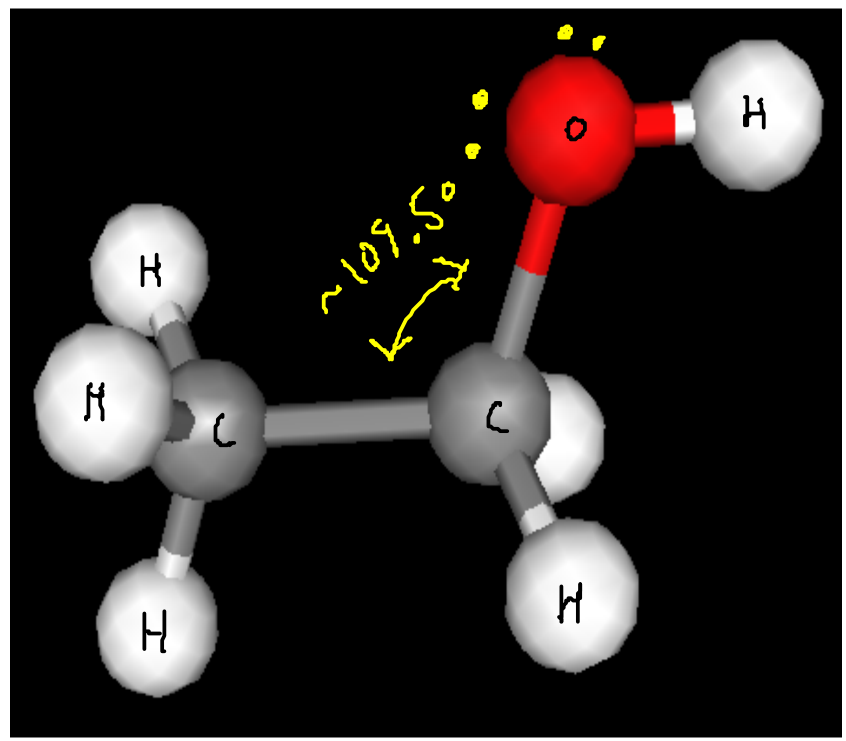


C_3H_8

All bond angles in the propane molecule are 109.5 degrees

CH_3CH_2OH

Like propane, the bond angles in ethanol are also close to 109.5 degrees.



POLARITY and shape:

- A polar molecule has an uneven distribution of electron density, making it have ends (poles) that are slightly charged.

POLARITY influences several easily observable properties.

- Melting point. (Polar substances have higher melting points than nonpolar substances of similar molecular weight.)
- Boiling point. (Polar substances have higher boiling points than nonpolar substances of similar molecular weight.)
- Solubility. (Polar substances tend to dissolve in other polar substances, while being insoluble in nonpolar substances. Nonpolar substances dissove other nonpolar substances, and generally have poor solubility in polar solvents.)

- Polar molecules contain POLAR BONDS arranged in such a way that they do not cancel each other out.

... 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! (chart, p 352)

- A bond with little or no electronegativity difference between atoms will be NONPOLAR