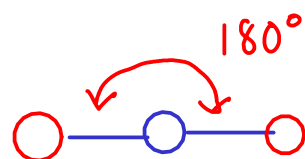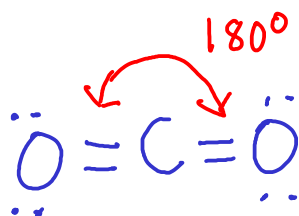# PREDICTING MOLECULAR SHAPE

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!

180°

$$\ddot{O} = C = \ddot{O}$$

180°

LINEAR MOLECULES

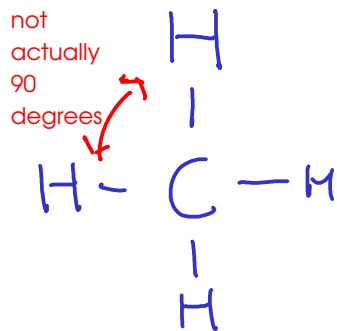For the two red circles to be farthest apart, they must be 180 degrees apart

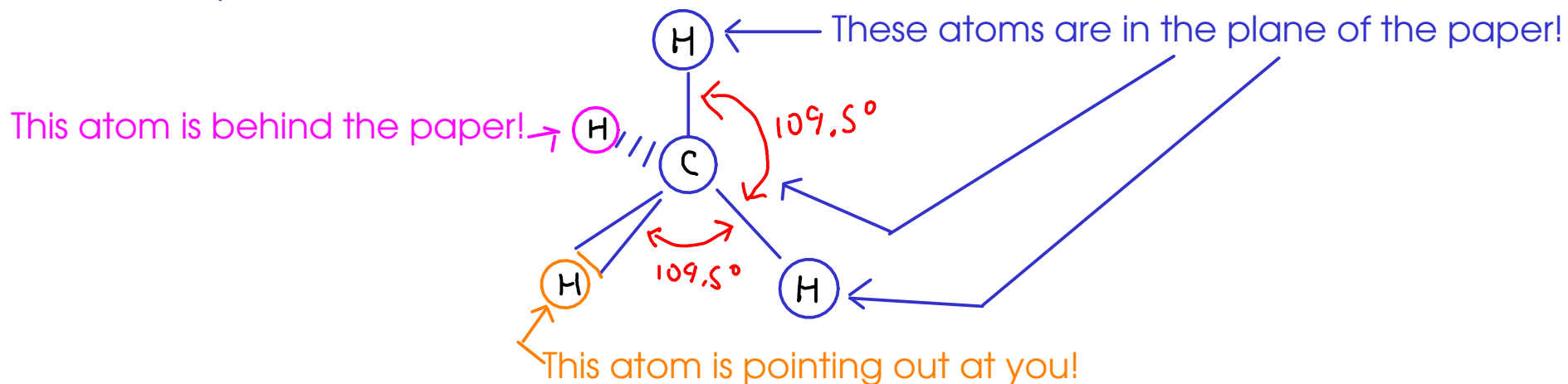ANY diatomic (two-atom) molecule is linear, but only some three-atom molecules are!

Flat!

120°

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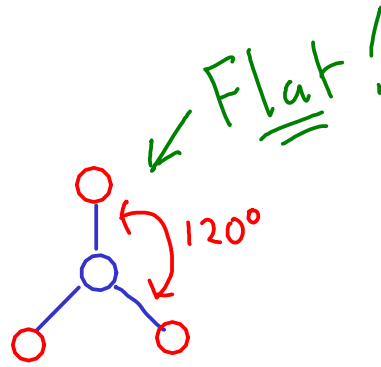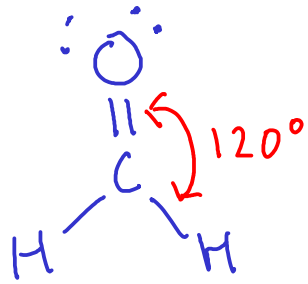
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

TRIGONAL PLANAR MOLECULES

not actually 90 degrees

H
|
H— C —H
|
H

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.

(H) ← These atoms are in the plane of the paper!

This atom is behind the paper! → (H)

(C)

109.5°

109.5°

(H)

(H)

This atom is pointing out at you!

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

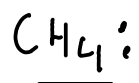✻ "Groups" can be either BONDS or LONE PAIRS!

VSEPR shapes:

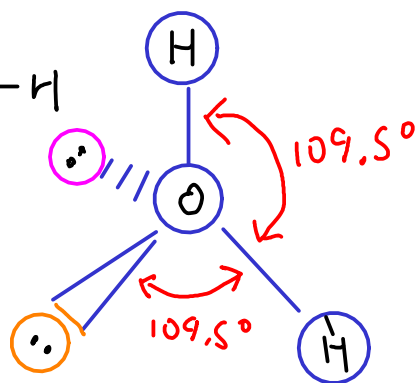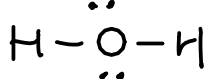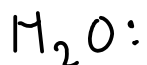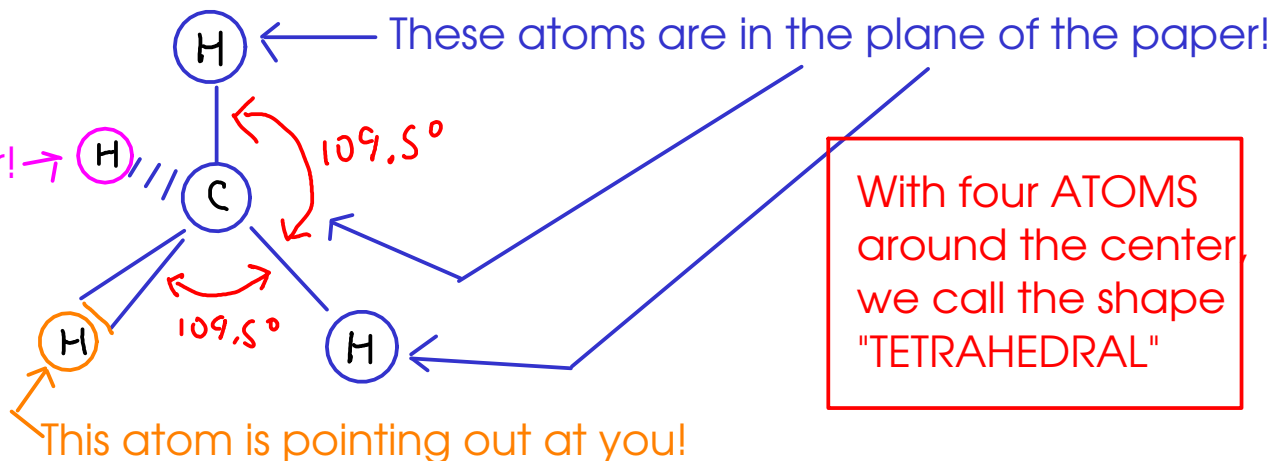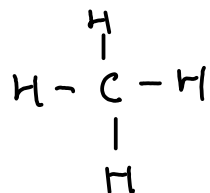| Groups* around central atom	Shape	Bond angle(s) in degrees
2	linear	180
3	trigonal planar	120
4	tetrahedral / pyramidal / bent	109.5
5	trigonal bipyramidal (and derivatives)	90 and 120
6	octahedral (and derivatives)	90
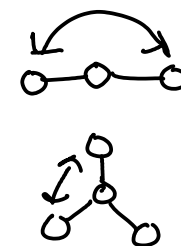
5 and 6 violate "octet rule"
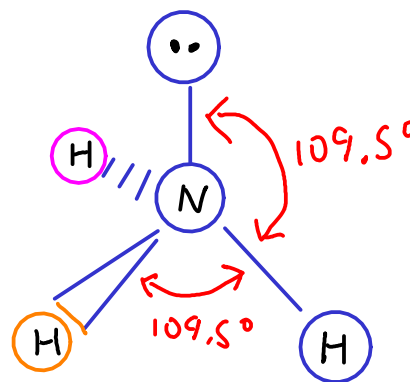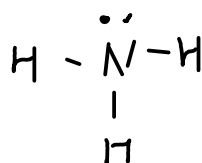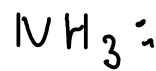
More on "4 things around a central atom":

- 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:

This atom is behind the paper! →

H - C - H (with H above and H below)

← These atoms are in the plane of the paper!

109.5°
109.5°

This atom is pointing out at you!

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

H_2O:

H - Ö - H

109.5°
109.5°

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

NH_3:

H - N̈ - H (with H below)

109.5°
109.5°

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