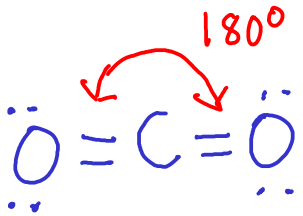
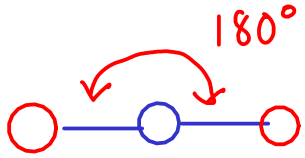
PREDICTING MOLECULAR SHAPE

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!

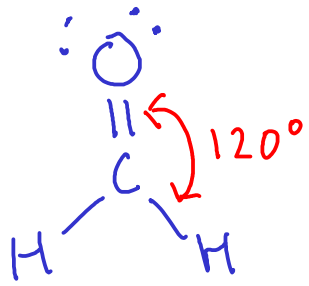


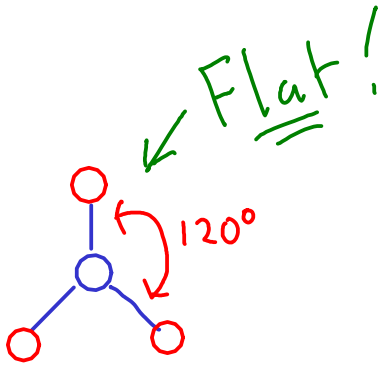


For the two red circles to be farthest apart, they must be 180 degrees apart

LINEAR MOLECULES

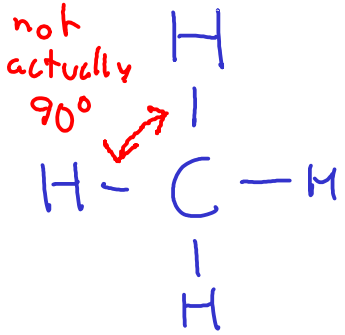
ANY diatomic (two-atom) molecule is linear, but only some three-atom molecules are!





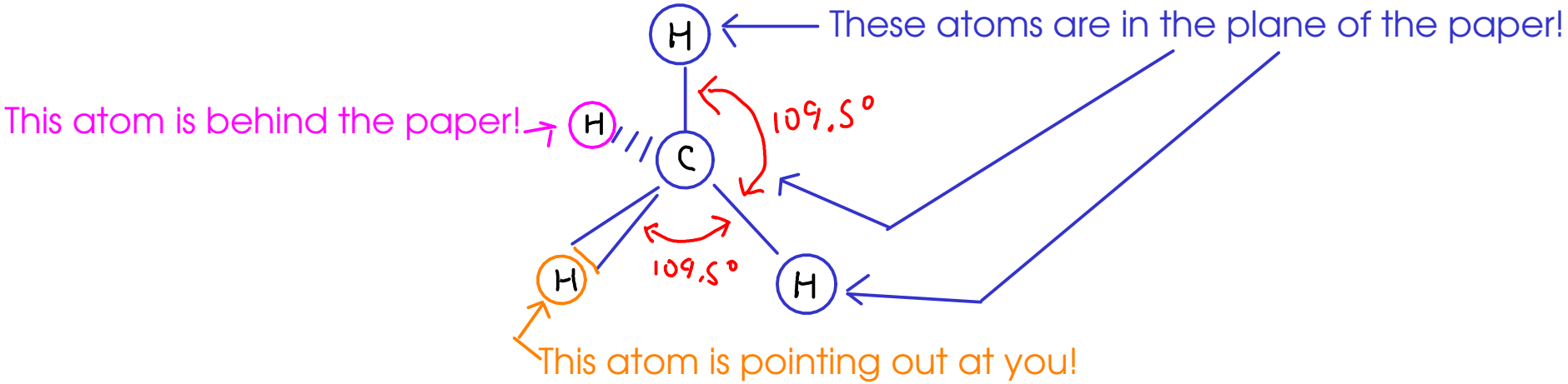
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

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.



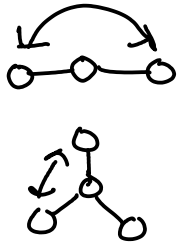
To see the tetrahedron in three dimensions WITHOUT buying a molecular model kit, just take four balloons, blow them up, and then tie them together. The knot will be the central atom, and the balloons will line themselves up to be 109.5 degrees apart.

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 pyramidal (and derivatives)	90 and 120
6	ocrahedral (and derivatives)	90

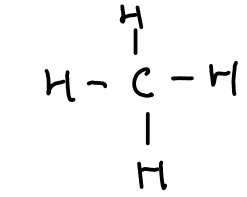


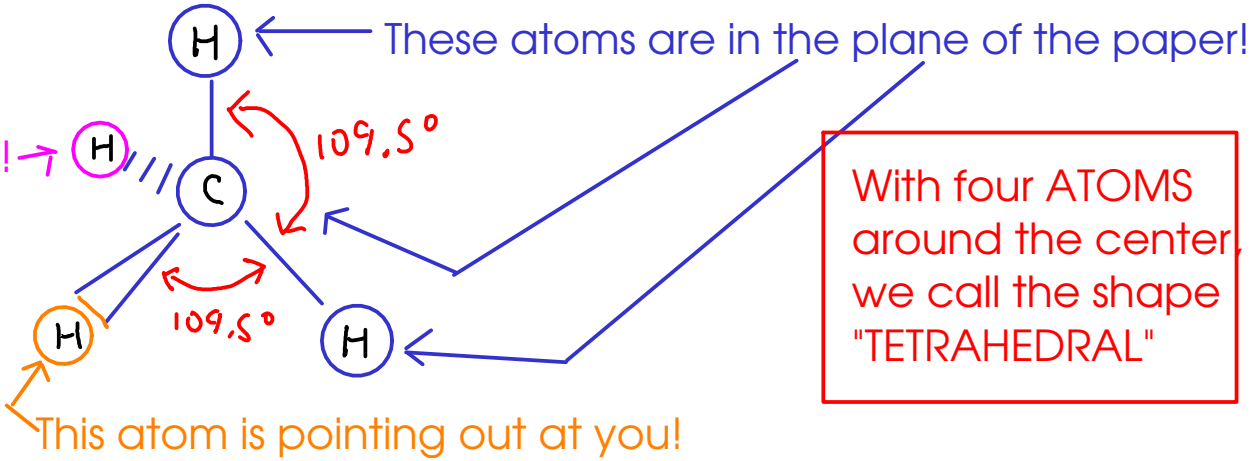
5 and 6 violate "octet rule"

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?

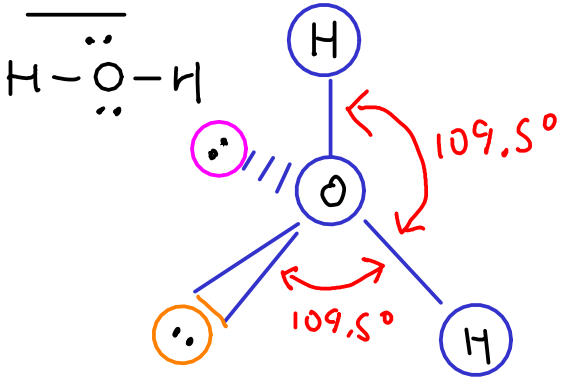
CH_4:





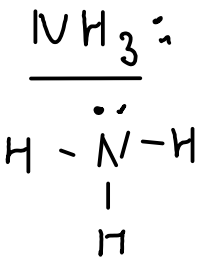
With four ATOMS around the center, we call the shape "TETRAHEDRAL"

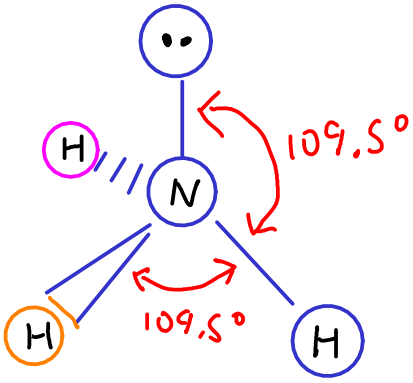
H_2O:

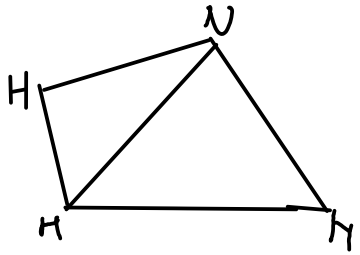


With two ATOMS and two LONE PAIRS, we call the shape "BENT"

NH_3:



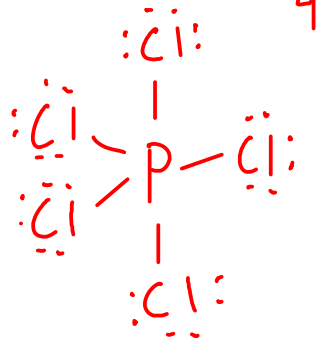




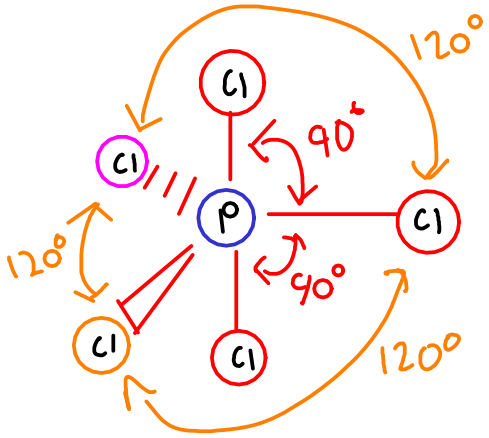
With three ATOMS and one LONE PAIR, we call the shape "PYRAMIDAL"

SHAPES OF EXPANDED VALENCE MOLECULES

PCl_5 : P : 5
Cl : 7 × 5
40

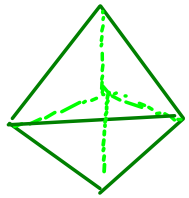


There are five atoms bonded to the central phosphorus atom, and they will attempt to get as far apart as possible from one another!



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

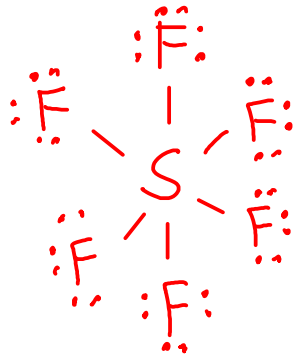
The atoms around the center are 120 degrees apart from each other.



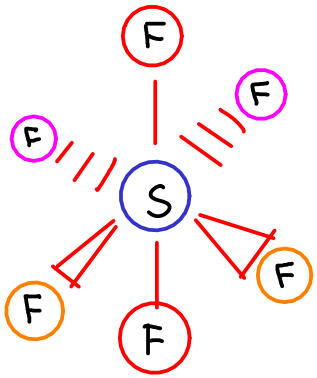
There are acually two DIFFERENT bond angles in this structure. It's called TRIGONAL BIPYRAMIDAL.

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

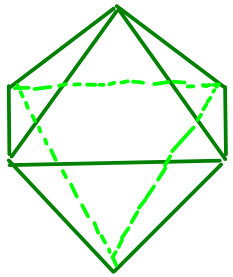
SF_6 : S : 6
F : 7 x 6
48



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!

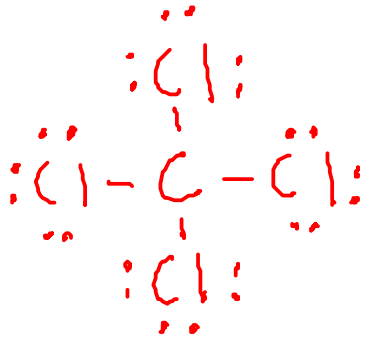
Examples:

CCl_4

C: 4

Cl: 7 x 4 = 28

32



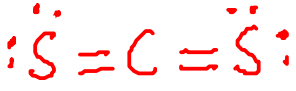
Molecular shape? There are FOUR atoms bonded to the central carbon atom (no lone pairs on the carbon). This gives a TETRAHEDRAL molecule.

CS_2

C: 4

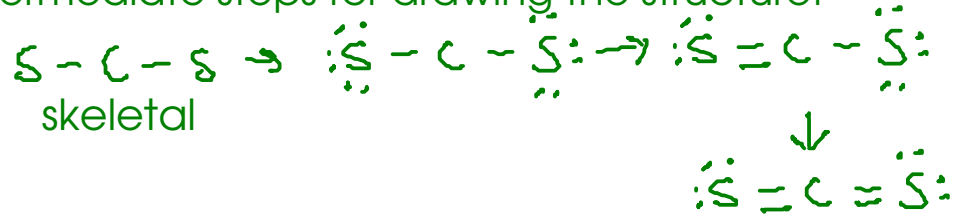
S: 6 x 2 = 12

16



Molecular shape? There are TWO sulfur atoms bonded to the central carbon (no lone pairs on carbon). This is a LINEAR molecule.

Intermediate steps for drawing the structure:

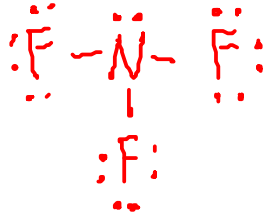


NF_3

N: 5

F: 7 x 3 = 21

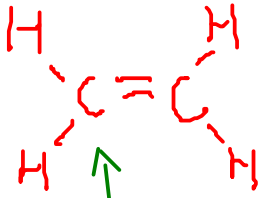
26



Molecular shape? There are FOUR GROUPS around the central atom, but only THREE atoms. (one lone pair on nitrogen). This is a PYRAMIDAL structure - the lone pair pushes the fluorine atoms out of the plane.

C_2H_4

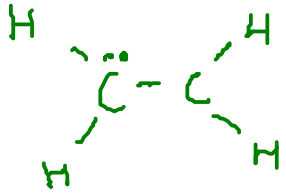
C : 4 x 2 = 8
H : 1 x 4 = 4
12



Shape? This molecule has TWO central atoms, so let's describe the shape of the molecule around each one. Each carbon center is TRIGONAL PLANAR.

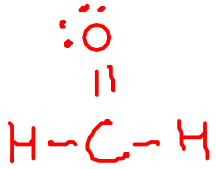
3 groups: H–, H–, =C

Intermediate step for this structure:



H_2CO

H : 1 x 2 = 2
C : 4
O : 6
12



Shape? This molecule has three atoms (and no lone pairs) around the central carbon atoms. It's TRIGONAL PLANAR.

Intermediate step for this structure: