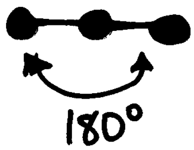
Step by step: Drawing Molecular Structures / Lewis Structures

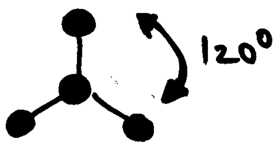
Molecular Shapes and Names

The names refer to where the <u>atoms are located</u>, not where the electrons are located!

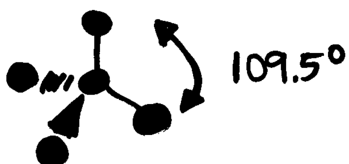
← **Linear**



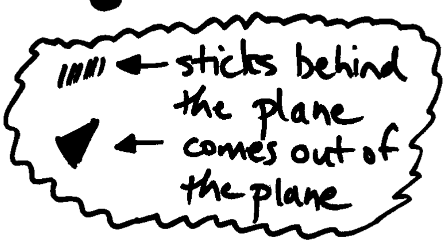
← **Linear**
(2 atoms around central atom)

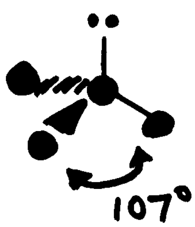


← **Trigonal Planar**
(3 atoms around central atom)

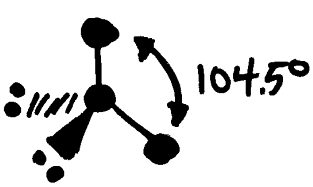


← **Tetrahedral** (pyramid has 4 faces)
(4 atoms around central atom)

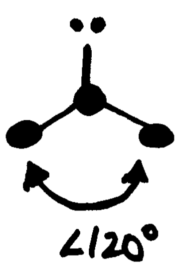




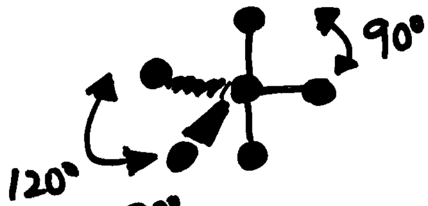
← **Trigonal Pyramidal**
(3 atoms & 1 pair of electrons around central atom)
*e^- can go anywhere



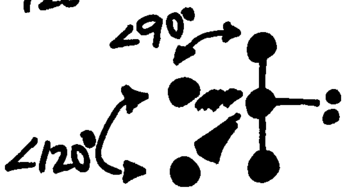
← **Bent**
(2 atoms & 2 pairs of electrons around central atom)
*e^- can go anywhere



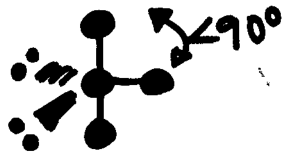
← **Bent**
(2 atoms & 1 pair of electrons around central atom)
*e^- can go anywhere



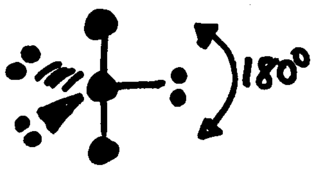
← **Trigonal Bipyramidal**
(5 atoms around central atom)



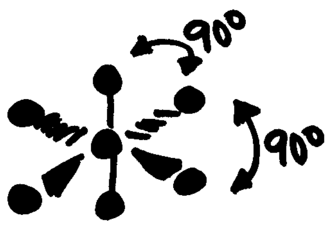
← **Seesaw, Irregular Tetrahedran, or Bi-sphenoid**
(4 atoms & 1 pair of electrons around central atom)
e^- must be around the middle, not top/bottom



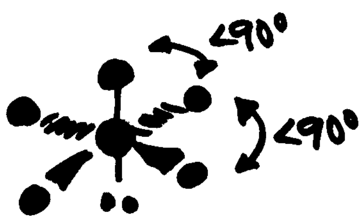
← **T- shaped (officially: T- shaped planar)**
(3 atoms & 2 pairs of electrons around central atom)
e^- must be around the middle, not top/bottom



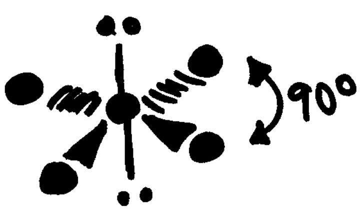
← **Linear**
(2 atoms & 3 pairs of electrons around central atom)
e^- must be around the middle, not top/bottom



← **Octahedral** (pyramids have 8 faces)
(6 atoms around central atom)



← **Square Pyramidal**
(5 atoms & 1 pair of electrons around central atom)



← **Square Planar**
(4 atoms & 2 pairs of electrons around central atom)
e^- must be opposite each other

****Notice that whenever there are 4 "sticks" around the central atom, the 4 "sticks" are always drawn the same way. Whenever there are 5 "sticks" around the central atom, the 5 "sticks" are always drawn the same way. Whenever there are 6 "sticks" around the central atom, the 6 "sticks" are always drawn the same way**.

VSEPR Model (Valence Shell Electron Pair Repulsion)

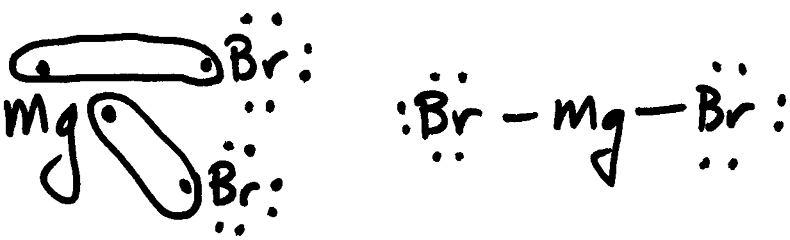
The structure around an atom is determined principally by minimizing electron pair repulsions.

Ex. 1) NaCl

linear, 180°

Na has one electron in the s, so one dot. (Row #3 of periodic table.)
Cl has 2 electrons in the s and 5 in the p, so 7 dots. (Row #3 of periodic table.)
(We are only counting the **outer layer** electrons, the ones in the same row as the element.)
2 electrons will make a bond. Join the one Na electron with one electron from Cl to make a bond. **The bond is drawn as a line or dash. (The line or dash equals 2 electrons.)** For the shape, the atoms are in a linear shape. (Two points in space will make a line.)
Each atom likes having 8 electrons around it, since all noble gases have 8 electrons around them (octet rule). Na has two electrons in the bond. This appears to be unhappy, but Na really loses its' original one electron to chlorine, since it is ionic. If Na loses its' original one electron to chlorine, its' second layer has 8 electrons, having 2 in the s and 6 in the p ($2s^2$ $2p^6$), so it is happy.
Chlorine has the two electrons in the bond and 6 extra electrons around it, to make a total of 8, so it is happy. The electrons **not** in bonds (extra electrons) are in lone pairs of electrons.

Ex. 2) $MgBr_2$

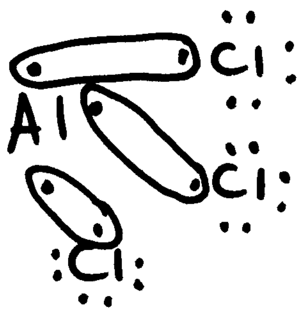


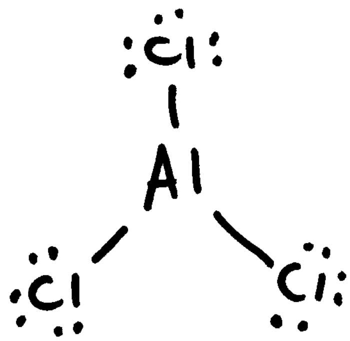
linear, 180°

Mg has 2 electrons in the s, so 2 dots.
Each Br has 2 electrons in the s and 5 electrons in the p, so 7 dots.
We do not count Br's electrons in the "d" orbital, since these are the 3d electrons. We only want the electrons in its' outer layer, the 4s and the 4p.
The 2 electrons of Mg will join with 2 electrons from the 2 bromines (one electron from each bromine) to make 2 bonds. Again each atom wants 8 electrons (octet rule). Again Mg appears unhappy with only 2 bonds, containing 2 electrons each, for a total of 4 electrons. But if Mg loses its' original 2 electrons to Br (ionic bonds), its' 2^{nd} layer is full, having 2 in the s and 6 in the p, for a total of 8 electrons ($2s^2$ $2p^6$). Each Br has 2 electrons in the bond plus 6 extra electrons for a total of 8 electrons. These extra electrons are in lone pairs of

electrons. The Br hate each other, since their lone pair electrons in their outer shells repel each other, so the Br will move away from each other to opposite sides. The 3 atoms are in a line, so linear.

Ex. 3) $AlCl_3$

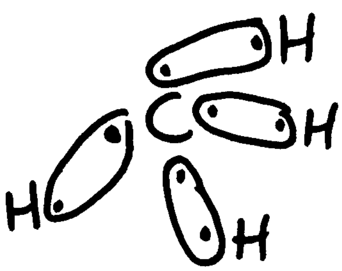


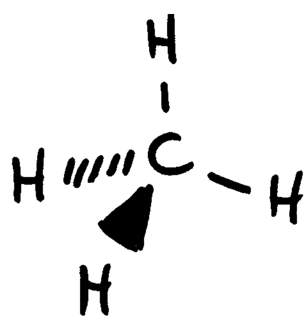


trigonal planar, 120^o

Al has 2 electrons in the s and 1 in the p, for a total of 3 electrons, so 3 dots.
Each Cl has 2 electrons in the s and 5 in the p, for a total of 7 electrons, so 7 dots.
The 3 electrons of Al will join with 3 electrons from the 3 chlorines (one electron from each chlorine) to make 3 bonds. Again Al appears unhappy, since it has 3 bonds of 2 electrons each around it, for a total of 6 electrons. But if Al loses its' original 3 electrons, it will have a full 2^{nd} layer with 2 electrons in the s and 6 in the p, for a total of 8 electrons ($2s^2$ $2p^6$). The chlorines have 2 electrons in each bond and 6 extra electrons, for a total of 8 electrons. Again the chlorines hate each other, since the electrons in the outer layers repel each other, so the Cl's will move as far away from each other as possible. Notice they are in a trigonal shape that is in one plane, so trigonal planar. Also a full circle divided by 3, equals 120^o. (360^o /3 = 120^o)

Ex. 4) CH_4



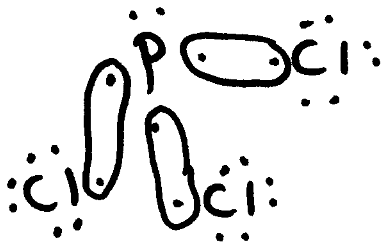


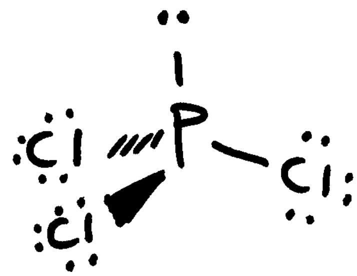
tetrahedral, 109.5^o

C has 2 electrons in the s and 2 in the p, for a total of 4 electrons, so 4 dots.
Each H has 1 electron in the s, so 1 dot.
Each H has 1 electron that can bond with 1 electron of C, for a total of 4 bonds. H now has 2 electrons in the bond, which makes it happy, since it will look like He (a noble gas). C is happy, since it has 4 bonds of 2 electrons each around it for a total of 8 electrons. The electrons in the H's hate each other, so the H's will try to get away from each other as much

as possible. If the H's were in a cross (+), the bond angle would be 90^o. **If we draw it 3-dimensionally, where the wedged H is sticking out towards you and the dashed H is sticking behind the paper,** the H's will form an angle of 109.5^o, which puts the H's farther away from each other, than in the 90^o case. This will form a pyramid with 1 face on the bottom and 3 faces around the top, for a total of 4 faces, so tetrahedral (4 faces).

Ex. 5) PCl_3

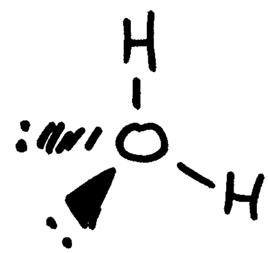




trigonal pyramidal, 107^o

P has 5 electrons and Cl has 7 electrons. The 3 Cl's will each grab 1 electron from P to make a bond. That will leave 2 extra electrons on the P, which will form a lone pair of electrons. If there are 3 bonds and 1 pair of electrons, there are 4 groups that will repel and hate each other. These 4 groups will arrange the same way as the last example. ****Notice the sticks will always be the same, if there are 4 groups.**** The lone pair of electrons on the P could go in any position, but if it is placed on top, it is easier to figure out its' name. ****When we name the structure, we only look at where the atoms are located and not at the lone pair of electrons.**** Look at the 3 Cl's and the 1 P. They form a pyramid that has 3 sides, so trigonal pyramidal. **The lone pair of electrons is very negative and the Cl's are very repelled by them,** so the Cl's will come closer together, making the bond angle smaller than 109.5^o; it will now be 107^o.

Ex. 6) H_2O

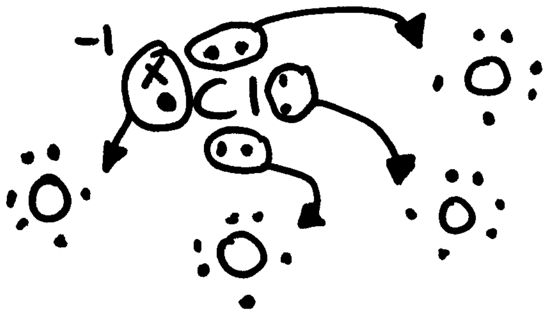


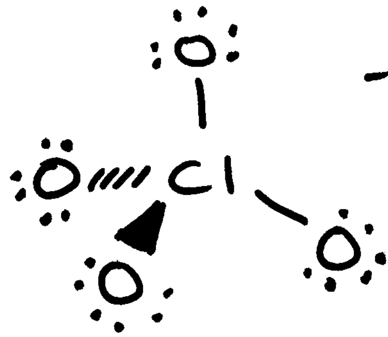
bent, 104.5^o

Each H has 1 electron and O has 6 electrons. Each H grabs 1 electron from the O to make a total of 2 bonds. There will be 4 electrons left on the O, forming 2 lone pairs of electrons. Again there are 4 groups around the O, so the sticks will be drawn just as before. The lone pairs can go anywhere. ****Again to name it, we only look at the atoms.**** The H-O-H bonds are linked in a line, but it is not straight; it is bent, so bent. (Ignore the lone pairs when naming!) **The lone pairs of electrons are very negative and the H's are very repelled by**

them, so the H's will come closer together, making the bond angle smaller than 107°; it will now be 104.5°.

Ex. 7) ClO_4^-

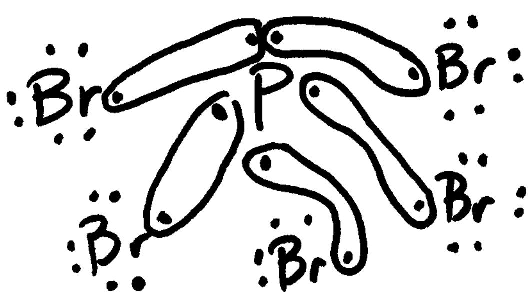


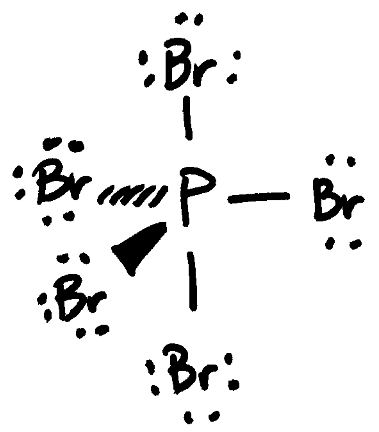


tetrahedral, 109.5°

Cl has 7 electrons. Each O has 6 electrons. **Oxygen is weird**! Look at where it is on the periodic table. Each O wants 2 electrons to look like noble gas Ne, so **each O will take 2 electrons from Cl to use for its' bonds**. **<u>Oxygen is greedy!</u>** Since each O needs 2 electrons and Cl only has 7 electrons, we are short. That is why perchlorate is charged -1. **<u>Since it is negative one (-1), we can add an extra electron wherever we need one.</u>** If we add the extra electron to Cl, then there will be enough electrons for each O to grab 2 electrons. (**<u>The extra electron on Cl is the "x".</u>**) If each O grabs 2 electrons from Cl, Cl will have no extra electrons. We will have a total of 4 bonds. Note the sticks are drawn the same as the last 3 examples. We again have the atoms in a pyramid with 1 face on the bottom and 3 faces around the top, for a total of 4 faces, tetrahedral. The bond angle will be back to 109.5°.

Ex. 8) PBr_5

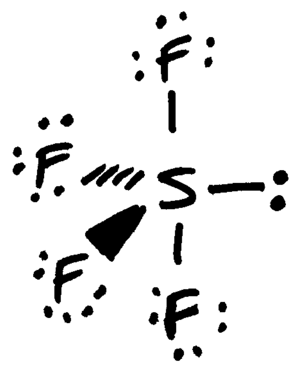




trigonal bipyramidal, 90° & 120°

P has 5 electrons and Br has 7 electrons. Each Br grabs 1 electron from P to make a total of 5 bonds. This will give the P more than 8 electrons around it (it will not follow the octet rule), but we can't do anything about it. We will find out that this is OK, since it can use empty "d" orbitals for the bonds. Again the Br's hate each other. We can take the tetrahedral shape and add a Br to the bottom of it. Shifting the 3 (bottom/tripod) Br's into a plane around the middle of the P. Around the middle, one stick is in the plane of the top and bottom sticks. The other two sticks are out of the plane. One coming out towards you (the wedge) and one going back behind the structure (the dashed line). From the middle up we form a 3 faced pyramid and from the middle down we form a 3 faced pyramid, trigonal **bi**pyramidal (**2** trigonal pyramids). The bond angle from the middle to the top and from the middle to the bottom is 90^o. The bond angle between the middle 3 Br's is $360^o / 3 = 120^o$.

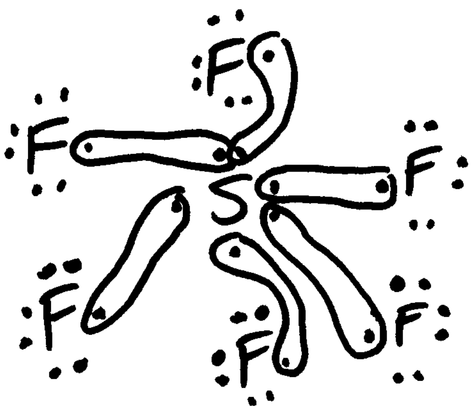
Ex. 9) SF_4

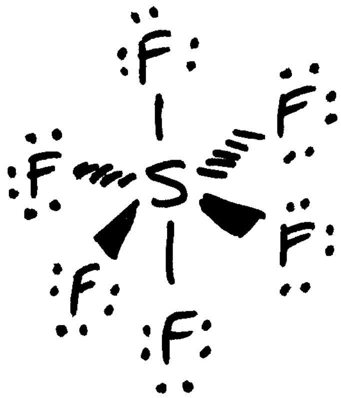


****e⁻ must be around the middle** seesaw, $<90^o$ & $< 120^o$
(irregular tetrahedran, bisphenoid)

S has 6 electrons and F has 7 electrons. Each F grabs 1 electron for a total of 4 bonds. That leaves 2 extra electrons on S, for a lone pair. We have 4 bonds and 1 lone pair, for a total of 5 groups. <u>****Notice if we have 5 groups, the sticks are always drawn the same.****</u> The lone pair electrons must go around the middle. If we put the lone pair on top (or bottom), it will be 90^o to 3 atoms around the middle. But if we put the lone pair around the middle, it will be 90^o to only 2 atoms (the top and bottom). <u>**The electrons will have more room around the middle, so they must be around the middle (not the top or bottom). They can be anywhere around the middle.**</u> The lone pair will again repel the F's, pushing the F's closer together, so the bond angles will be less than 90^o and less than 120^o. The name can be different for this one. Remember we look at only the atoms, not the lone pair of electrons. The 4 Fluorines around the Sulfur form an **irregular tetrahedran**, a **bisphenoid** and a **seesaw**.

Ex. 10) SF_6

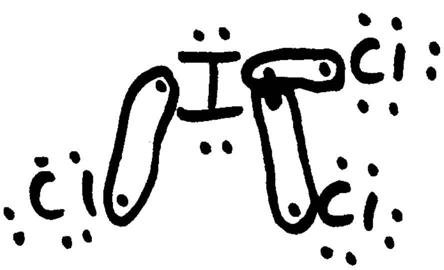


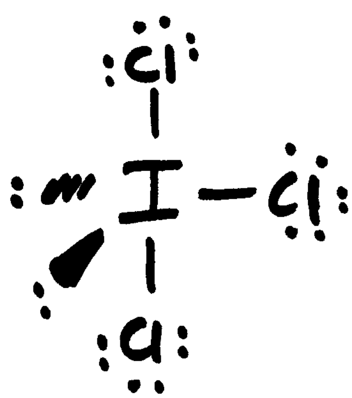


octahedral, 90°

S has 6 electrons and each fluorine has 7. The 6 fluorines will each grab an electron from sulfur, making 6 bonds. If we take the 5 stick picture and add another stick around the middle we will get the 6 stick picture. The top and bottom sticks are in the plane of the paper. Around the middle two sticks are coming out towards you (wedges) and two sticks are going back behind the structure (dashed lines). From the middle up to the top, there is a four faced pyramid and from the middle down to the bottom, there is a four faced pyramid. There are 4 + 4 = 8 faces total, so octahedral. The bond angle from the middle to the top and from the middle to the bottom is 90°. The bond angle between the middle 4 F's is 360° / 4 = 90°. So, all of the angles are 90°.

Ex. 11) ICl_3



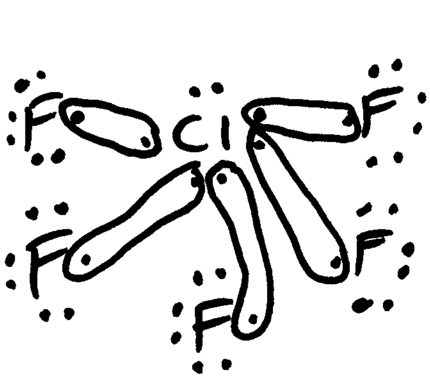


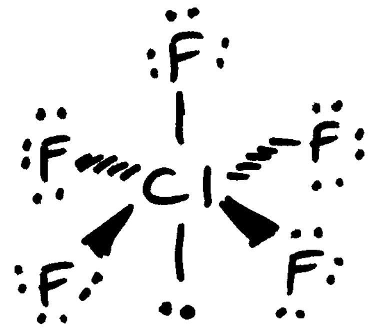
T-shaped, <90°

(e^- must be around middle)

I has 7 electrons and each Cl has 7 electrons. Each Cl will grab one electron from I, leaving 4 electrons on I (2 lone pairs). We have 3 bonds and 2 lone pairs, so 5 sticks are needed. Look at the 5 stick drawing, the sticks are always the same for 5 groups. Again the electron pairs must be around the middle, since they will have more room around the middle, than at the top or bottom. The Cl around the middle can go anywhere around the middle. Again the electrons around the middle will repel/push the chlorines closer together, reducing the bond angle, so less than 90°. Name wise we look only at the 3 chlorines. If you rotate the structure 90° to the right, you get a letter "T", so T-shaped.

Ex. 12) ClF_5

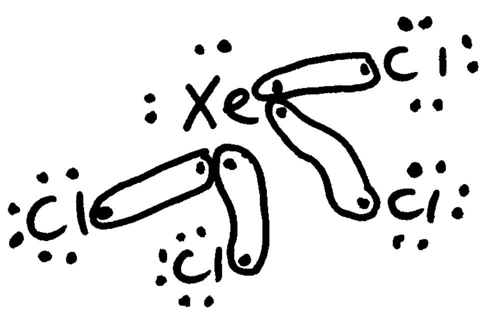


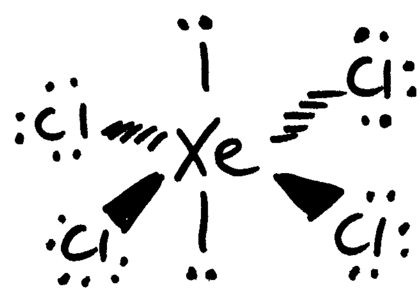


square pyramidal, $<90^o$

Cl has 7 electrons and each F has 7 electrons. Each F will grab one electron from the Cl, leaving 2 electrons (1 lone pair). We have 5 bonds and 1 lone pair, so 6 sticks will be needed for the 6 groups. The 6 sticks are always drawn the same. This time the electrons can go anywhere, since the angles are all 90^o on an octahedral type shape. But if we put the electrons on the bottom, the name makes more sense. From the middle up to the top there is a 4 sided pyramid, with a base that is a square, so square pyramidal. The electrons added to the bottom, will repel/push the fluorines closer together, making the angle decrease to less than 90^o.

Ex. 13) $XeCl_4$

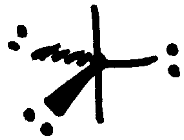




square planar, 90^o

**** e- must be across from each other**

Xe has 8 electrons and each Cl has 7 electrons. Each Cl will grab one electron, leaving 4 electrons (2 lone pairs). We have 4 bonds and 2 lone pairs, so 6 sticks are needed for the 6 groups. This time the electrons must go opposite each other. If we put them on the top and bottom, the name will make more sense. Around the middle there are 4 atoms forming a square in a flat plane, so square planar. The electrons on top and bottom both repel/push the chlorines, but since both are pushing from opposite directions the chlorines will not move, the bond angle remains 90^o.

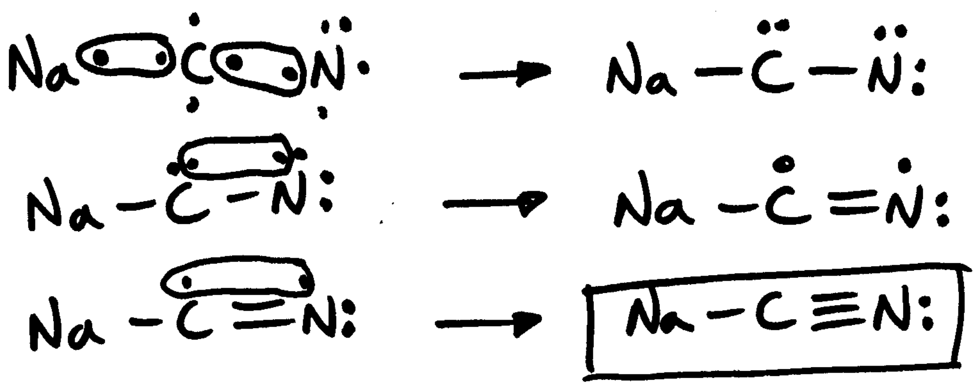


linear, 180°

If you have 2 bonds and 3 pairs of electrons, you will need 5 sticks for the 5 groups. Remember for this structure the electrons must go around the middle, where they have more room (not the top or bottom). Looking at the middle atom and the top and the bottom atoms, you can see that they all fall in a line (top to bottom), so linear. (Ignore the electron pairs.) The angle top to bottom is half a circle, so 360 /2 = 180°.

Remember the atoms would like to have an octet of 8 electrons around them, so that they resemble the noble gases. Sometimes it is necessary to make multiple bonds to make the atoms happy and stable!

Ex.14) NaCN



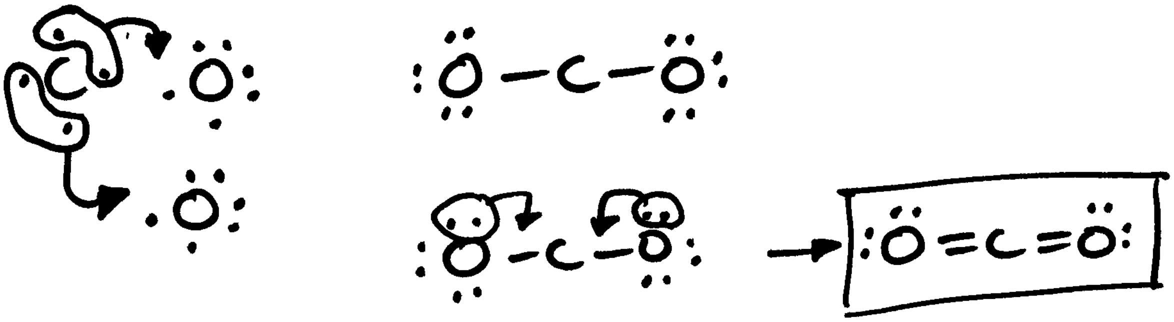
linear, 180°

In the 1st line,we just make bonds to connect the atoms, by sharing atoms. Notice we have single bonds between the Na—C—N. The Na appears unhappy, but remember it loses its' one electron ionically. Its' 2nd layer will be full with 8 electrons, so it is happy. C is unhappy; it only has 6 electrons (2 in the lone pair and 2 electrons in each of the 2 bonds). N is also unhappy, since it only has 6 electrons (4 in the 2 lone pairs and 2 electrons in the bond).

In the 2nd line, we make a double bond between the C and the N. Now C has 7 electrons around it (1 electron dot and 2 electrons in each of the 3 bonds). N has 7 electrons around it (3 electron dots and 2 electrons in each of the 2 bonds). Both still do not have 8, so make a triple bond.

In the 3rd line, we make a triple bond. Now C has 8 electrons (2 electrons in each of the 4 bonds) and N has 8 electrons (2 in each of the 3 bonds and the 2 electron dots).

Ex. 15) CO_2



linear, 180°

Remember **Oxygen is weird and greedy**; it wants two more electrons to look like the noble gas, Ne. **So **each oxygen will grab 2 electrons to make its' bonds**.**
At this point there will be single bonds between the C and the O's. Oxygen is happy/stable, since it has 8 electrons (an octet) around it. (6 electron dots and 2 electrons in the one bond) Carbon is unhappy, since it has only 4 electrons (2 in each of the 2 bonds). We will need to make double bonds on both sides of the C to make it happy. In the final picture, C has 8 electrons (2 in each of the 4 bonds) and O is happy, since it has 8 electrons (4 electron dots and 2 electrons in each of the 2 bonds).

End of Notes