DRAWING DOT STRUCTURES FOR SIMPLE MOLECULES

① Count valence electrons

② Pick central atom and draw skeletal structure

- central atom is usually the one that needs to gain the ost electrons!

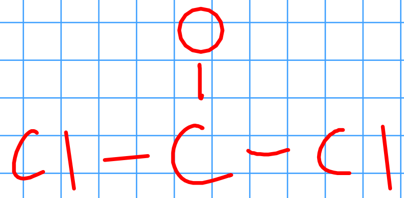
- skeletal structure has all atoms connected to center with single bonds

③ Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

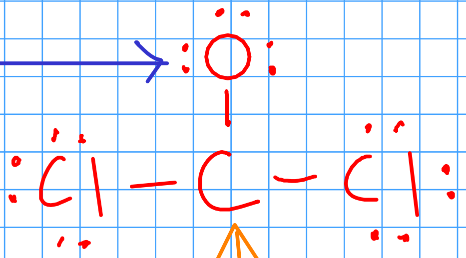
④ Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

$COCl_2$

C : 4
O : 6
Cl: 7 x 2
24



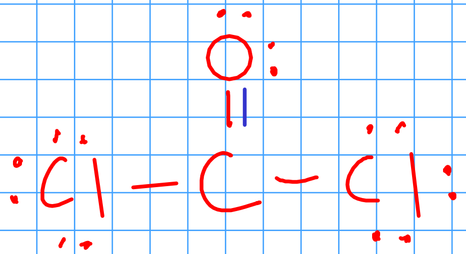
Choose carbon as the central atom, and draw skeleton



Distribute electrons - have to stop here because we've used all 24!

Carbon only has six electrons!

We'll pick OXYGEN to share two pairs of electrons. It's likely to be able to share two pairs since it needs to gain two electrons anyway!



This structure looks better - all atoms have a share in the correct number of electrons!

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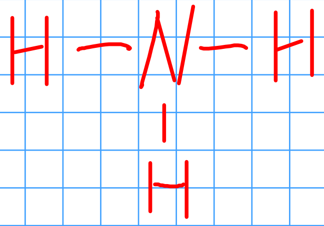
④ Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

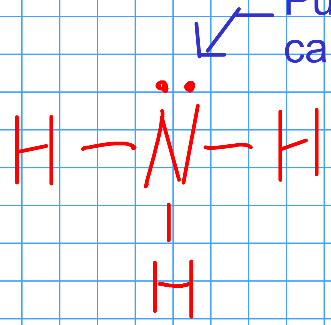
NH_3

$N: 5$

$H: \underline{1 \times 3}$

8





Put the electrons here, since hydrogen atoms can only hold two electrons in a 1s orbital!

A DOT STRUCTURE FOR A LARGER MOLECULE

① Count valence electrons

② Pick central atom and draw skeletal structure

- central atom is usually the one that needs to gain the ost electrons!

- skeletal structure has all atoms connected to center with single bonds

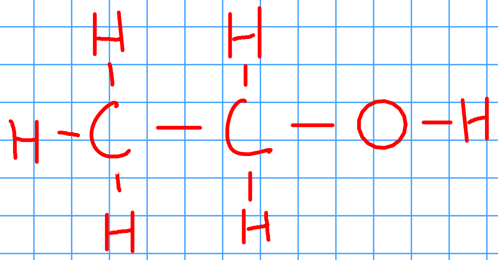
③ Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

④ Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

CH_3CH_2OH ETHANOL!

This formula gives us a hint to the structure of the molecule. Ethanol has THREE centers: the two carbon atoms and the oxygen atom.

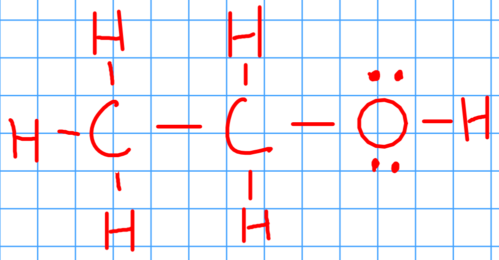
Draw the skeleton by connecting the centers, then distributing the atoms around each center.



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

$\overline{\quad 20 \quad}$

Now, distribute electrons!



A DOT STRUCTURE FOR A MOLECULE WITH DELOCALIZED BONDS

O: 3 x 6 = 18

O_3 (OZONE)

① Count valence electrons

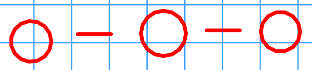
② Pick central atom and draw skeletal structure

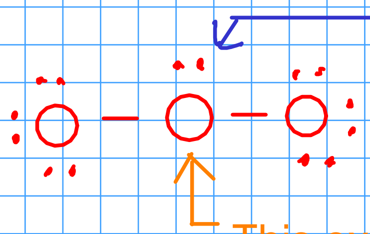
- central atom is usually the one that needs to gain the ost electrons!

- skeletal structure has all atoms connected to center with single bonds

③ Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

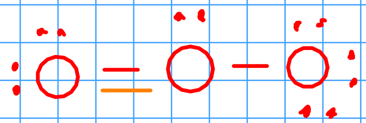
④ Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.





Out of electrons!

This oxygen atom only has six electrons!

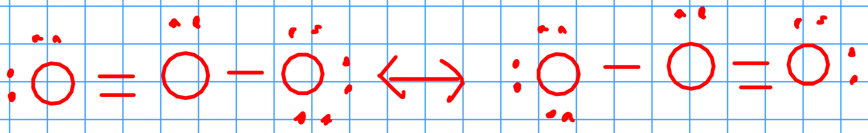


All atoms have a share in eight electrons here.

This structure suggests that one of the outer oxygen atoms is closer to the central oxygen atom than the other one!

Experimentally, we observe that both outer oxygen atoms are the SAME distance from the center.

In the molecule, electrons are actually being shared between ALL THREE oxygen atoms. This is a DELOCALIZED bond!



These are RESONANCE structures. The real structure is an "average" of these two. The "double bond"'s electrons are shared between all three oxygen atoms!

A DOT STRUCTURE FOR A POLYATOMIC ION

① Count valence electrons

② Pick central atom and draw skeletal structure

- central atom is usually the one that needs to gain the ost electrons!

- skeletal structure has all atoms connected to center with single bonds

③ Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

④ Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

NH_4^+

N: 5

H: 1 x 4

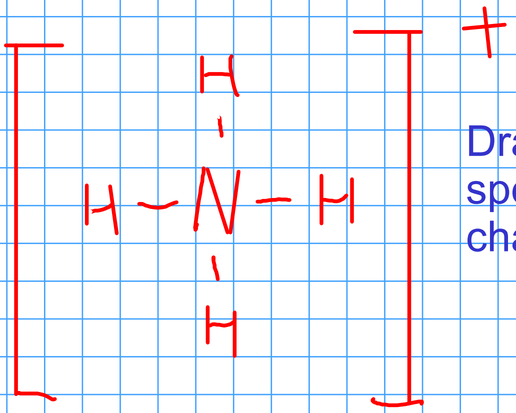
9

An odd number of electrons? But Lewis structures deal in PAIRS of electrons!

-1

8

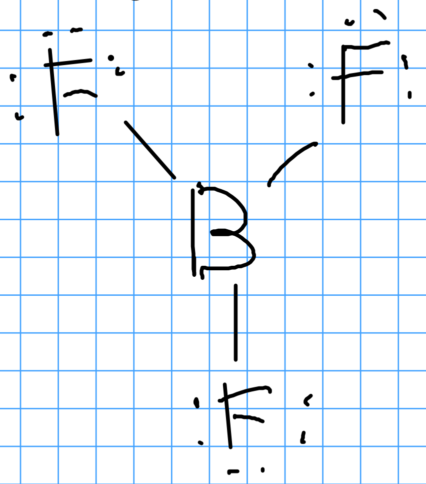
Subtract one electron from the total to get the correct charge (+1) on the ion.



Draw brackets around charged species and indicate the overall charge!

EXPANDED VALENCE

- Some atoms do not always obey the octet rule. A few, like BORON, will bond in such a way that they end up with less than eight electrons.



BF_3

... but many more bond in such a way that they end up with a share in MORE THAN EIGHT electrons!

- Any atom in period three or greater can do this. SULFUR and PHOSPHORUS compounds commonly do this!

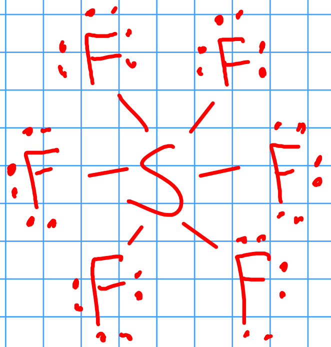
... these atoms have unfilled "d" orbitals that may participate in bonding!

- All noble gas compounds (example: XENON compounds with oxygen and fluorine) exhibit this behavior!

EXAMPLES:

SF_6

S: 6
F: 7 x 6
48

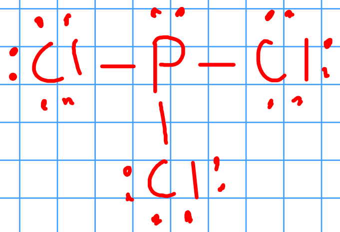


The sulfur atom ends up with a share in twelve electrons, not eight!

The shape of the sulfur hexafluoride molecule suggested by this structure checks with experimental data.

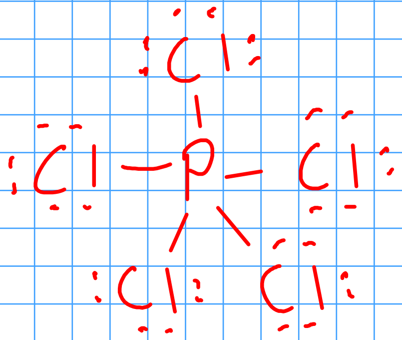
PCl_3 vs PCl_5

P: 5
Cl: 7 x 3
26



This structure obeys the octet rule!

P: 5
Cl: 7 x 5
40



This structure does NOT obey the octet rule - the phosphorus atom has a share in TEN electrons!

FORMAL CHARGE

- You can often draw more than one structure for a molecule that appears correct. How can you determine which one is more likely?

- USE FORMAL CHARGE!

  - Formal charge is a hypothetical charge on each atom in a structure. It assumes:

    ① All bonding electrons are shared EQUALLY between atoms

    ② Lone pairs are NOT shared.

$$\text{FORMAL CHARGE} = \text{ORIGINAL \# OF VALENCE ELECTRONS} - \text{NUMBER OF BONDS} - \text{NUMBER OF UNSHARED ELECTRONS}$$

* The sum of the formal charges of all atoms in a structure should equal to the charge of the molecule (0 for neutral molecules)

The "better" Lewis structure will have:

- Lower magnitudes of formal charge (0 0 is better than +2 -2)
- Negative formal charges on ELECTRONEGATIVE atoms

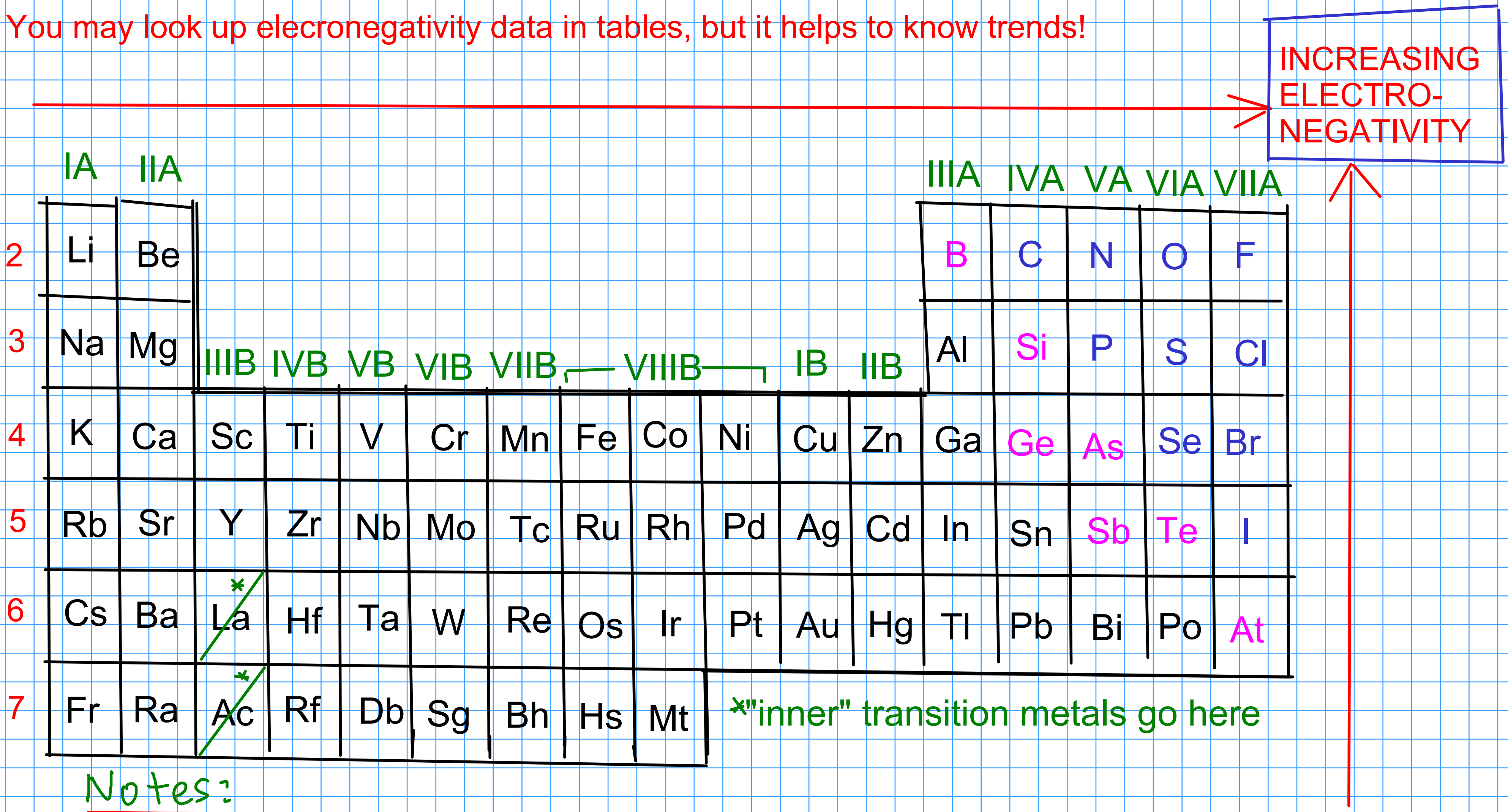
... but what is ELECTRONEGATIVITY?

ELECTRONEGATIVITY:
-A measure of how closely to itself an atom will hold shared electrons

... in other words, how ELECTRON-GREEDY an atom is!

ELECTRONEGATIVITY TRENDS

- You may look up elecronegativity data in tables, but it helps to know trends!



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

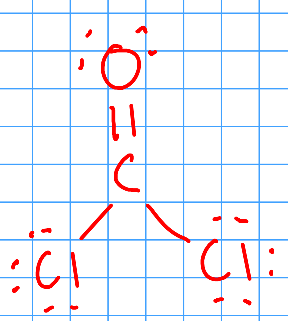
Notes:

① - FLUORINE is the most elecronegative element, while FRANCIUM is the least!

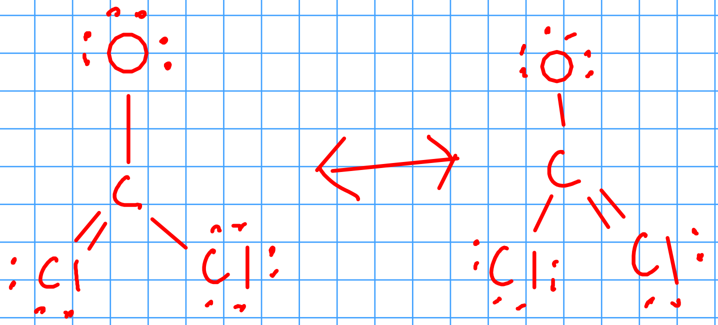
② - All the METALS have low electronegativity

③ - HYDROGEN is similar in electronegativity to CARBON

EXAMPLE: $COCl_2$



OR



?

... calculate formal charges to tell which structure is more likely!

O $6 - 2 - 4 = 0$

C $4 - 4 - 0 = 0$

Cl $7 - 1 - 6 = 0$

Cl $7 - 1 - 6 = 0$

0

✓

O $6 - 1 - 6 = -1$

C $4 - 4 - 0 = 0$

=Cl $7 - 2 - 4 = +1$

−Cl $7 - 1 - 6 = 0$

0

The structure on the left has lower magnitude formal charges!

H—N≡C: vs H—C≡N: ?

... we can determine which of these structures is more likely by calculating formal charges!

H $1-1-0=0$

C $4-3-2=-1$

N $5-4-0=+1$

$\overline{}$
0

H $1-1-0=0$

C $4-4-0=0$

N $5-3-2=0$

$\overline{}$
0

✓

The structure on the left has higher formal charges than the structure on the right. ALSO, the structure on the left assigns a negative formal charge to CARBON, while the MORE electronegative NITROGEN atom has a positive formal charge.