1. Count valence electrons

2. Pick central atom and draw skeletal structure

   - central atom is usually the one that needs to gain the most 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.

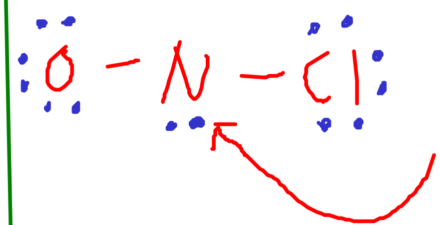
4. Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

NOCl

N : 1 × 5
O : 1 × 6
Cl : 1 × 7

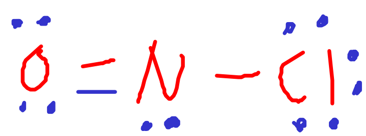
18 e^-

Choose N as central atom, since it needs to gain more electrons than O or Cl.



The last pair of electrons are put on the central atom since the outer atoms already have 8 ...

Central nitrogen has a share in only 6 valence electrons, so we need to make a double bond. Choose OXYGEN to make the bond, for the same reason as the last example!



With the double bond, all atoms have a share in eight valence electrons!

(1) Count valence electrons

(2) Pick central atom and draw skeletal structure

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

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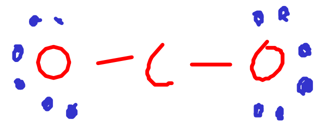
(4) Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

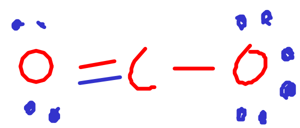
CO_2

C: 1 × 4
O: 2 × 6
16 e^-

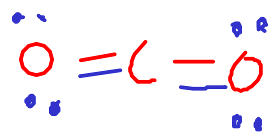
Pick C as central atom ...



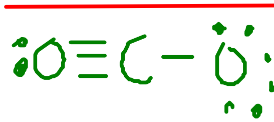
... distribute electrons, stop at 16 total. But C atom has a share in only four valence electrons!



... now six. Make another double bond.



... and now each atom has a share in 8 valence electrons!



What about this structure? This structure isn't correct. Why?

It shows two oxygen atoms in an identical environment behaving differently, and there's no reason here for that to happen. We expect them to bond the same way, as in the structure with the double bonds!

(1) Count valence electrons

(2) Pick central atom and draw skeletal structure

- central atom is usually the one that needs to gain the most 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.

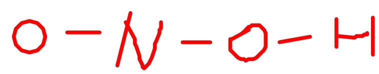
HNO_2 "nitrous acid"

In oxyacids, the acidic hydrogen atoms are attached to OXYGEN atoms in the structure!

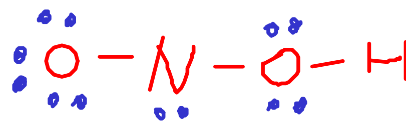
H: 1 x 1
N: 1 x 5
O: 2 x 6

18 e^-

Nitrogen is "central", but H must be attached to O for an oxyacid...



Distribute electrons, stop at 18 total!



... but nitrogen has a share in only six valence electrons!

... creating a double bond with the O on the left fixes this molecule. (Why the left? The other oxygen is already bonding twice ... with N and H!)

Notice that the bonding is a little different for the oxygen atoms here ... but that's because the environment is different (one bonds to N and H, the other to only N)

A DOT STRUCTURE FOR A LARGER MOLECULE

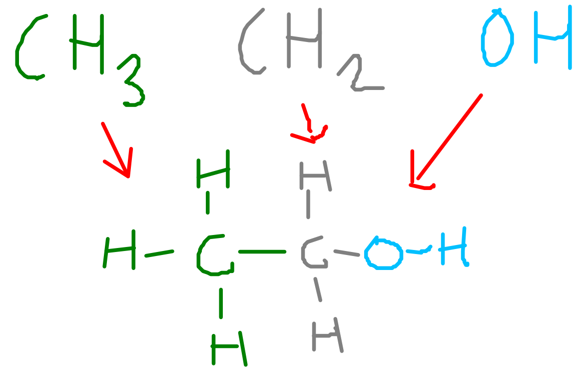
CH_3CH_2OH ETHANOL!

C : 4 x 2 = 8
H : 1 x 6 = 6
O : 6 x 1 = 6
| 20

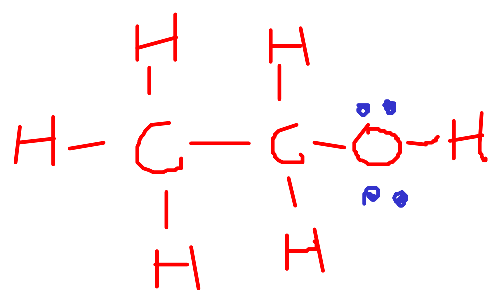
This formula gives us a hint to the structure of ethanol. Ethanol has THREE central atoms chained together.

1. Count valence electrons

2. Pick central atom and draw skeletal structure
   - central atom is usually the one that needs to gain the most 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.

A DOT STRUCTURE FOR A MOLECULE WITH DELOCALIZED BONDS

O: 3 x 6 = 18

See text, 9,7
p 356-357

O_3 (OZONE)

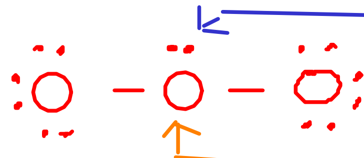
(1) Count valence electrons

(2) Pick central atom and draw skeletal structure

- central atom is usually the one that needs to gain the most electrons!
- skeletal structure has all atoms connected to center with single bonds

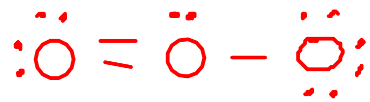
(3) Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

(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

Central oxygen has only six electrons

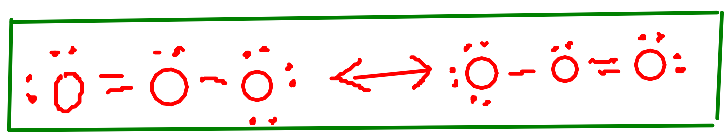


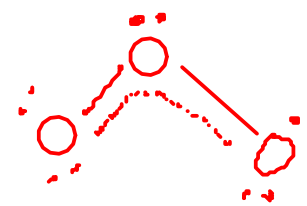
All atoms have a share in eight electrons!

The structure we drew implies that one of the outer oxygen atoms is closer to the central oxygen atom than the other one.

Experimentally, though, we find the two oxygen atoms to be the SAME distance from the center.

In the ozone molecule, electrons are actually being shared between ALL THREE oxygen atoms at the same time. This is called a DELOCALIZED BOND.





The structures in the green box are called RESONANCE STRUCTURES. The "real" structure of ozone is an "average" of the two resonsnce structures. The "double bond" electrons in these structures are actually 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 most electrons!
   - skeletal structure has all atoms connected to center with single bonds

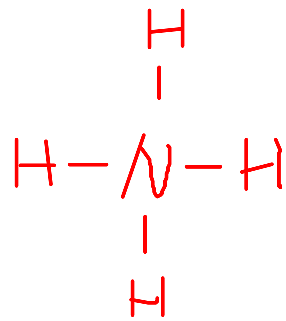
3. Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

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

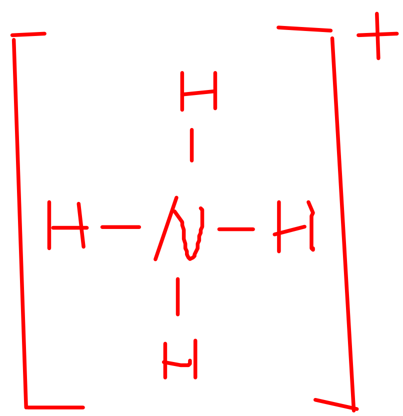
NH_4^+

N - 5
H - 1x4 = 4
9 e^-
-1 e^- (+1 charge)
8 e^-

For a polyatomic ion, the electron count must be adjusted to reflect the charge!



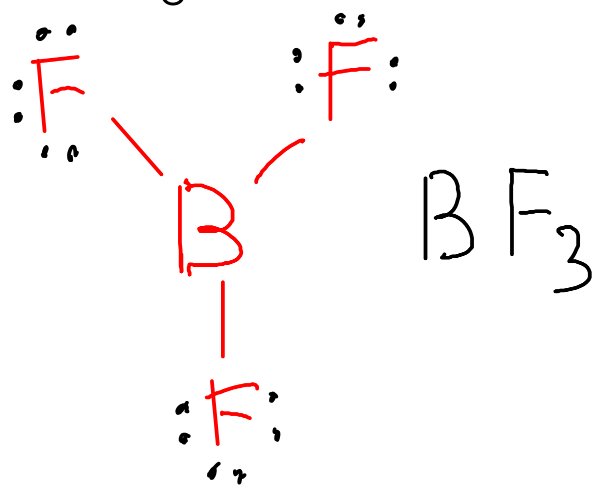
Skeletal structure with N central...



To indicate the charge, put brackets around the entire molecule and indicate the charge in the upper right corner...

EXPANDED VALENCE and other exceptions to the "octet rule"

- 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.



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

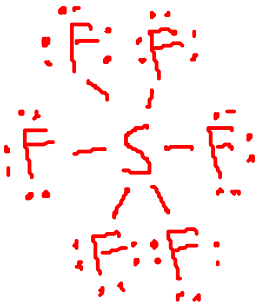
- Any atom in period three or greater can do this. SULFUR and PHOSPHORUS compounds commonly do this!

... 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: 7x6
48

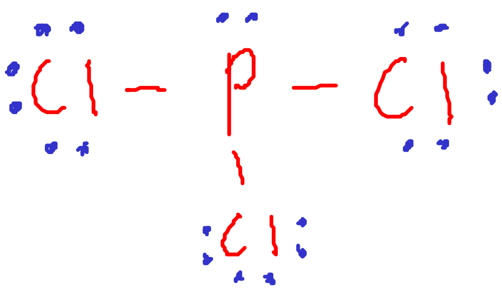
- The central SULFUR atom has a share in TWELVE total electrons, not eight!

- The SHAPE of the sulfur hexafluoride molecule in three dimensions agrees with the picture of six fluorine atoms each sharing a pair of electrons with a sulfur center.

PCl_3 vs PCl_5

PCl_3

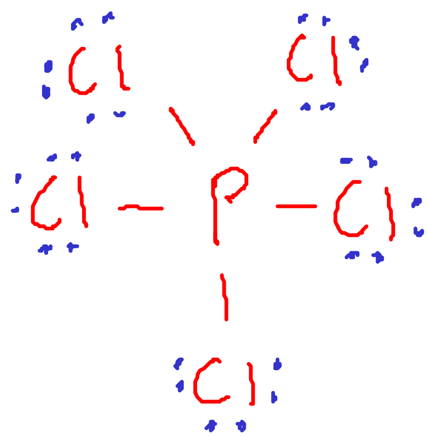
P : 5
Cl : 7x3 = 21
26



This structure obeys the octet rule.

PCl_5

P : 5
Cl : 7x5 = 35
40



This molecule does NOT obey the octet rule. Phosphorus ends up with ten electrons instead of eight.

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.

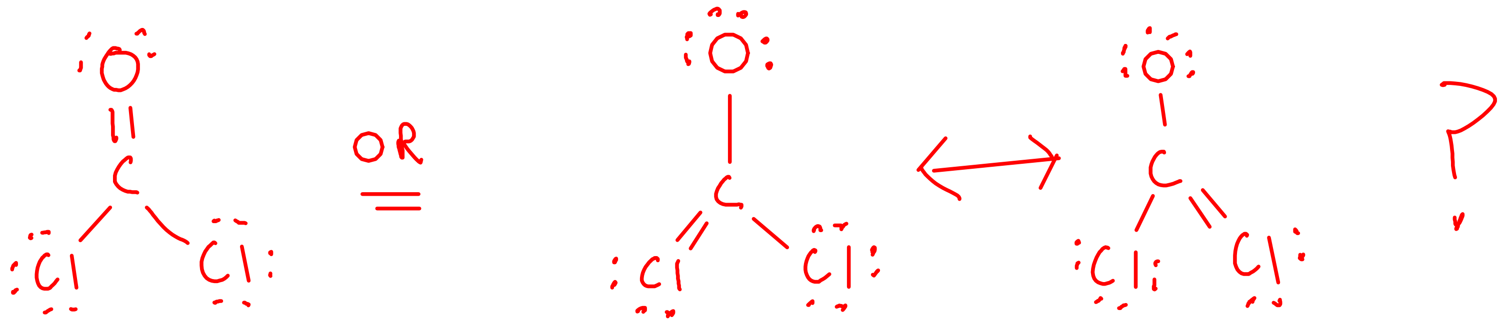
FORMAL CHARGE	=	ORIGINAL # OF VALENCE ELECTRONS	—	NUMBER OF BONDS	—	NUMBER OF UNSHARED ELECTRONS

* 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, or positive formal charges on atoms that are less electronegative.

EXAMPLE: $COCl_2$



... 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

O: 6 − 1 − 6 = −1
C: 4 − 4 − 0 = 0
=Cl: 7 − 2 − 4 = +1
−Cl: 7 − 1 − 6 = 0

In this case, the structure on the left is preferable, as it has lower formal charges (0,0,0,0) than the resonance structures...

$H-N\equiv C:$ vs $H-C\equiv N:$?

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

$H-N\equiv C:$	$H-C\equiv N:$
H: 1 − 1 − 0 = 0	H: 1 − 1 − 0 = 0
C: 4 − 3 − 2 = −1	C: 4 − 4 − 0 = 0
N: 5 − 4 − 0 = +1	N: 5 − 3 − 2 = 0

Which structure is more likely?

The one on the right with the central C atom, as the formal charges are lower.

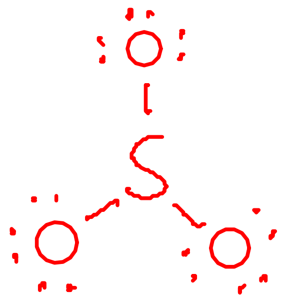
Let's look at sulfur trioxide. SO_3

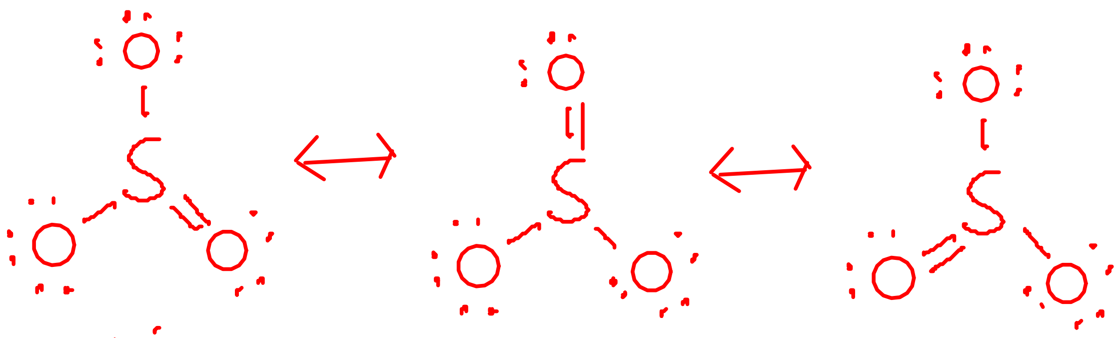
S: 6

O: 6 x 3 = 18

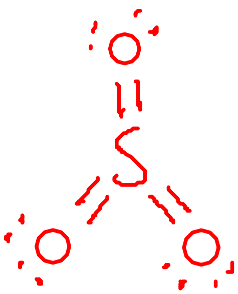
24 e^-

Skeletal structure:



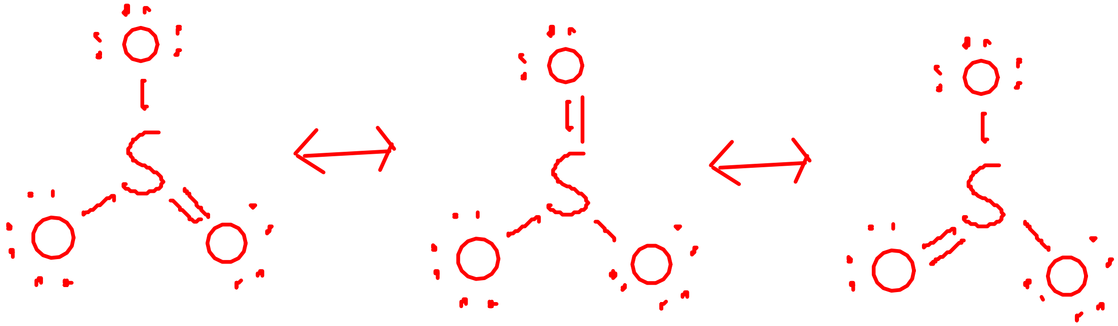


Resonance structures.



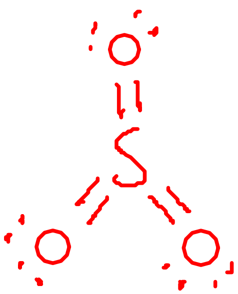
Expanded valence
(Sulfur is period 3)

To decide which structure is preferred, let's look at formal charges.



Resonance structures.

S: 6 − 4 − 0 = +2
O−: 6 − 1 − 6 = −1
O−: 6 − 1 − 6 = −1
O=: 6 − 2 − 4 = 0



Expanded valence
(Sulfur is period 3)

S: 6 − 6 − 0 = 0
O=: 6 − 2 − 4 = 0
O=: 6 − 2 − 4 = 0
O=: 6 − 2 − 4 = 0

Based on formal charge, we should prefer the sulfur trioxide structure with expanded valence, as it has lower formal charges.

In general, choose the stucture with lower formal charges even if it violates the octet rule ... provided the atoms actually CAN violate the octet rule (period 3 or higher).

Elements like C, N, O, F will never have more than eight valence electrons! (they can't do expanded valence)