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 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.

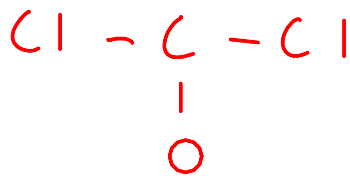
(4) Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

$COCl_2$

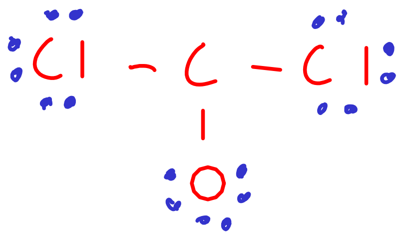
C: 1 x 4
O: 1 x 6
Cl: 2 x 7 = 14

24 valence electrons

Pick C as central atom because it needs to form more bonds (to get more electrons) than the other two elements in the molecule.

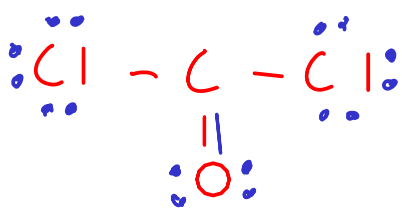


Skeletal structure. Now distribute remaining electrons



Stop when we reach the total number of valence electrons (24, here). But CARBON has a share in only 6 electrons. How to fix? Try a double bond.

... but with which atom? Pick OXYGEN, since it needed more electrons than chlorine to begin with (and thus is likely to form more bonds!)



The double bond gives carbon a share in eight valence electrons!

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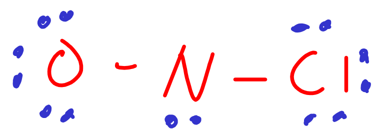
NOCl

N : 1 x 5
O : 1 x 6
Cl : 1 x 7

18 e^-

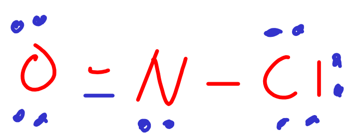
Pick N for central atom (it needs to gain more electrons than the other elements, and will likely form more bonds.)

Skeletal structure.



Distribute electrons. We ran out of space on the outer atoms, so the last pair goes on the central N.

... but N has a share in only SIX valence electrons. Let's try to fix this with a double bond. As before, choose O to contribute the electrons for the bond.



Now each atom has a share in eight outer shell electrons.

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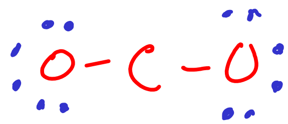
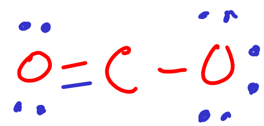
CO_2

C: 1 × 4
O: 2 × 6
16 e^-

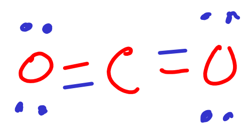
Pick C for central atom.



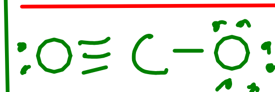
Distribute electrons. C doesn't have enough valence electrons (has 4, needs 8)



Now 6 ...



Now all atoms have a share in eight valence electrons.



Why not this? This structure suggests that two oxygen atoms put in exactly the same chemical situation would bond in different ways. This goes against the idea that all atoms of the same element are chemically identical!

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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.

HNO_2 "nitrous acid"

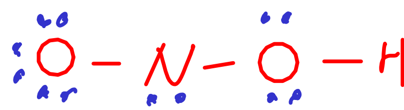
In oxyacids, the acidic hydrogen atoms are attached to OXYGEN atoms in the structure!

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

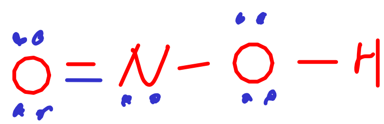
18 e^-

Since this is an oxyacid, we MUST have at least one H attached to an O.

(This molecule effectively has TWO central atoms, the N and the O on the right. Large molecule are made of smaller molecules joined to each other!)



Distribute. After showing all 18 electrons, N has only six.



Pick the O on the left for a double bond, since the O on the right already has two bonds!

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 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.

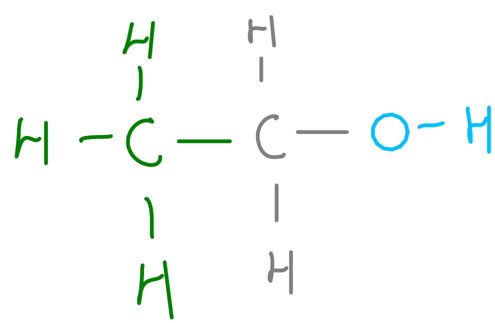
(4) Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

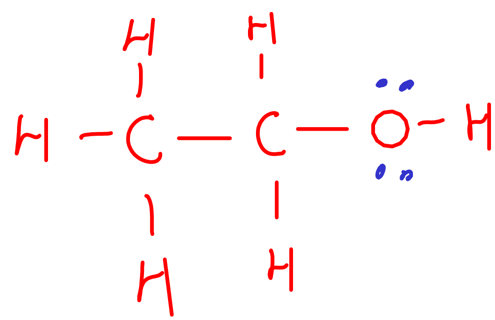
CH_3CH_2OH ETHANOL!

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.

CH_3 CH_2 OH





Distribute electrons

O: 3 x 6 = 18

A DOT STRUCTURE FOR A MOLECULE WITH DELOCALIZED BONDS

See text, 9,7
p 356 - 357

(1) Count valence electrons

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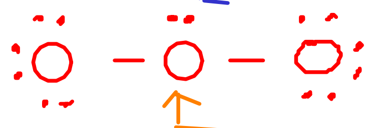
- skeletal structure has all atoms connected to center with single bonds

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

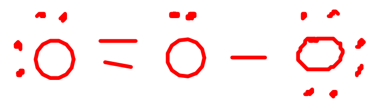
(4) Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

O_3 (OZONE)



OUT OF ELECTRONS

Central oxygen has only six electrons

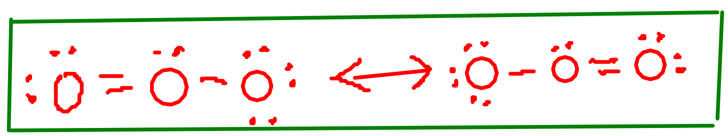


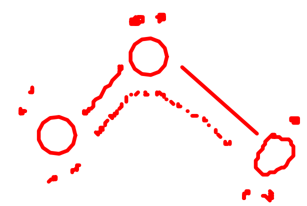
All atoms have a share in eight electrons!

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

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- 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: 1 x 5

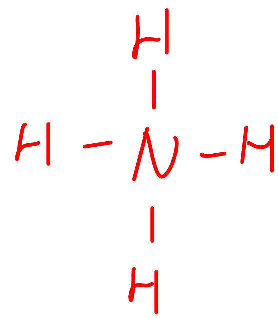
H: 4 x 1 = 4

9 e^-

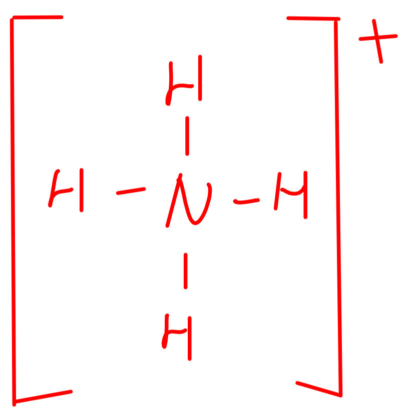
−1 (+1 charge)

8 e^-

For a polyatomic ion, adjust the electron count to give the correct charge (add electrons for anions, subtract them for cations)



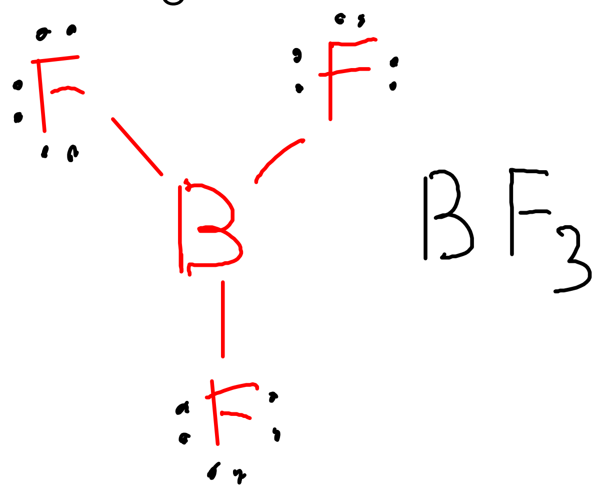
All atoms (except H) have eight valence electrons.



To indicate the charge, draw square brackets around the structure and put the charge in the upper left.

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!

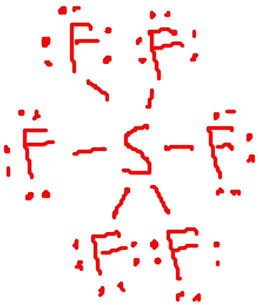
... these atoms have unfilled "d" orbitals that may participate in bonding!

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

EXAMPLES:

SF_6

S: 6
F: 7x6
48



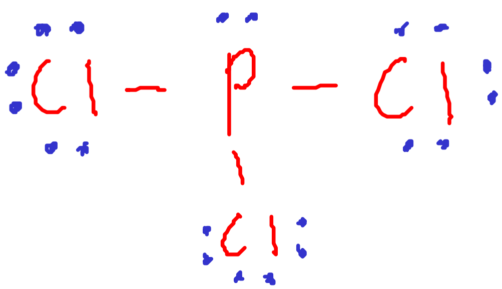
- The central SULFUR atom has a share in TWELVE total electrons, not eight!

- 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

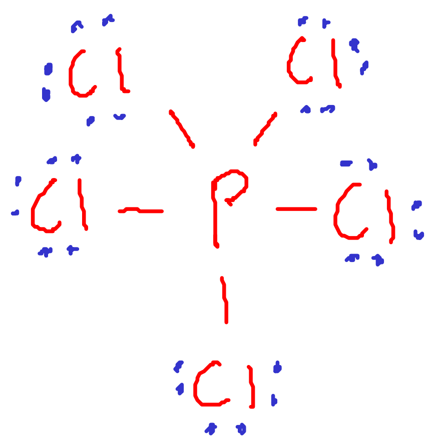
P : 5
Cl : 7x3 = 21
26



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.

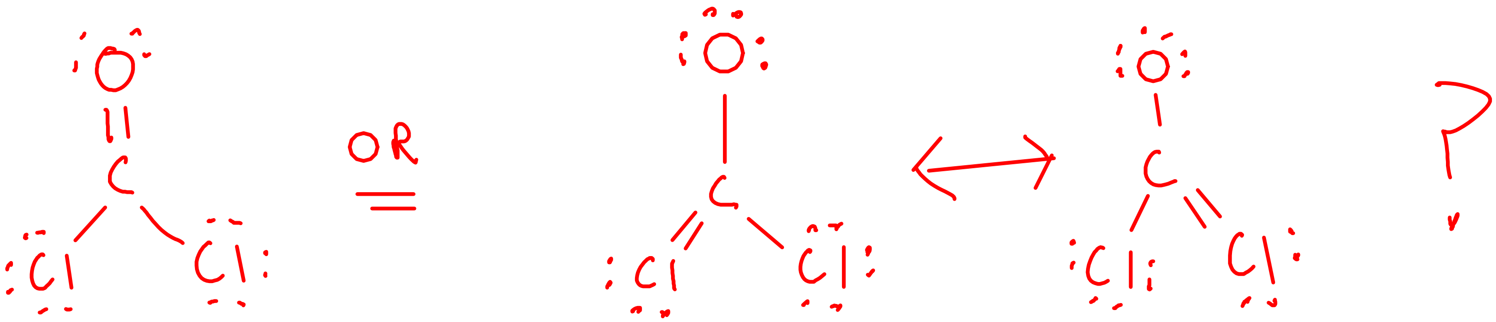
FORMAL CHARGE = ORIGINAL # OF VALENCE ELECTRONS — NUMBER OF BONDS — NUMBER OF UNSHARED ELECTRONS

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

Based on formal charge, the structure on the left is "better". It has a lower magnitude of formal charge than the one on the right.

H–N≡C: vs   H–C≡N: ?

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

H–N≡C:	H–C≡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: $5 - 3 - 2 = 0$

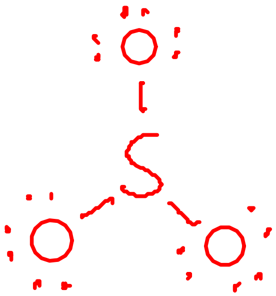
Which structure is more likely?

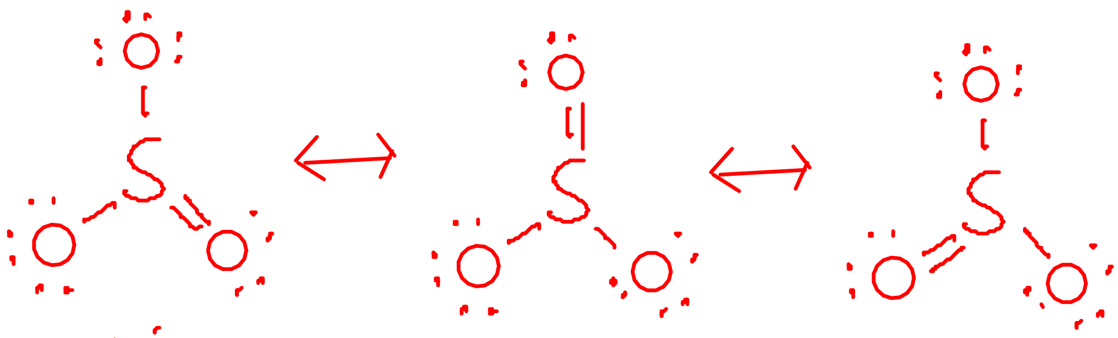
Based on formal charge, the structure on the right is more likely. (Lower mangnitude of formal charge.)

Let's look at sulfur trioxide. SO_3

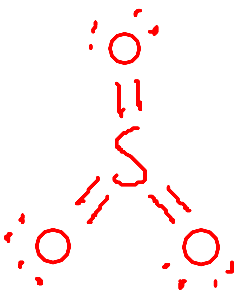
S: 6
O: 6 x3 = 18
24 e^-

Skeletal structure:



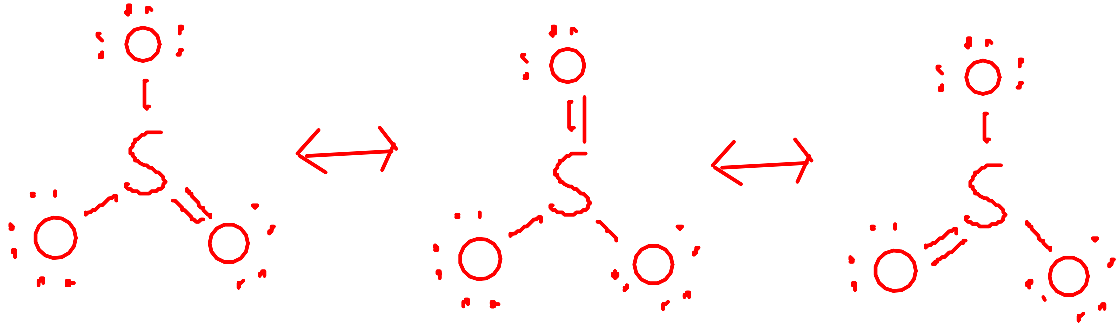


Resonance structures.



Expanded valence
(Sulfur is period 3)

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



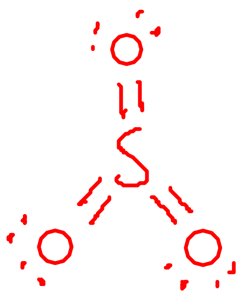
Resonance structures.

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, the sufur trioxide molecule should have the expanded valence structure, and NOT the resonance structures that obey the octet rule.