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.

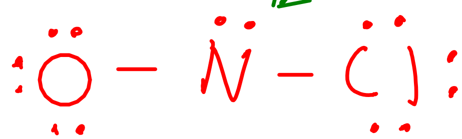
4. Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

NOCl

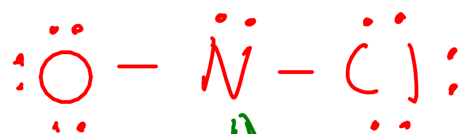
N : 5 x 1
O : 6 x 1
Cl : 7 x 1

18e⁻

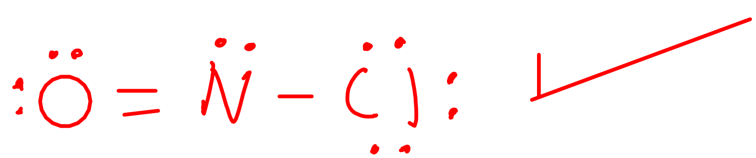
We will use nitrogen as the central atom, since it needs to gain 3 more electrons (and thus is likely to share more than oxygen or chlorine)



We ran out of "space" on the outer atoms, so we put the remaining electrons on the nitrogen atom in the center.



Only six electrons on nitrogen!



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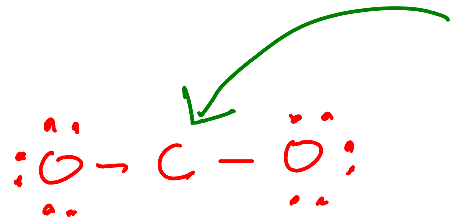
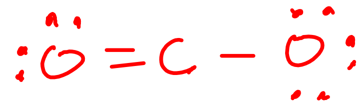
CO_2

C: 4
O: 6 x 2
16 e^-

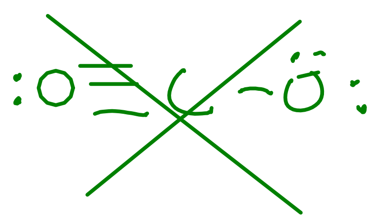


Carbon only has a share in four electrons!



One double bond give the carbon a share in SIX electrons.

Two double bonds are needed to get carbon a share in EIGHT electrons.



There's nothing different about the oxygen on the left than the oxygen on the right, so we expect them to bond the same way to the central carbon!

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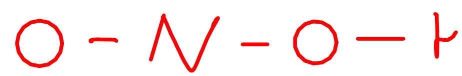
4. Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

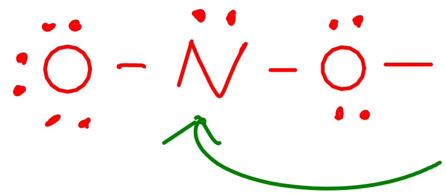
HNO_2 "nitrous acid"

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

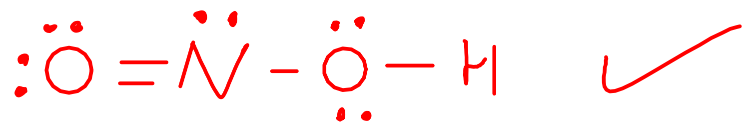
H: 1 x 1
N: 5 x 1
O: 6 x 2

18 e^-





Nitrogen has a share in only six!



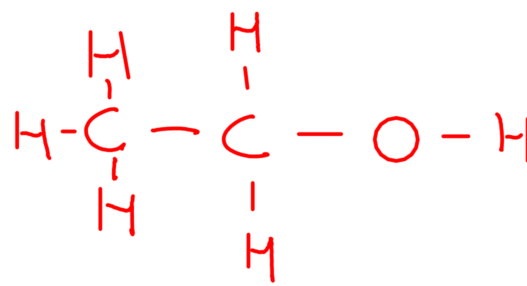
A DOT STRUCTURE FOR A LARGER MOLECULE

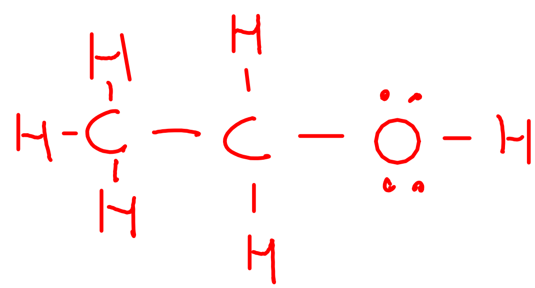
1. Count valence electrons
2. Pick central atom and draw skeletal structure
   - central atom is usually the one that needs to gain the most electrons!
   - skeletal structure has all atoms connected to center with single bonds
3. Distribute remaining valence electrons around structure, outer atoms first. 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
Total: 20

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





A DOT STRUCTURE FOR A MOLECULE WITH DELOCALIZED 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

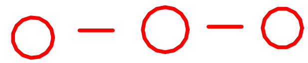
(3) Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

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

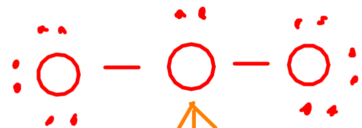
O_3 (OZONE)

O: 3 x 6 = 18

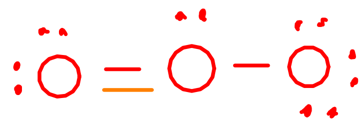
See text, 9,7 p 350-352



Out of electrons!



This oxygen atom only has six electrons!

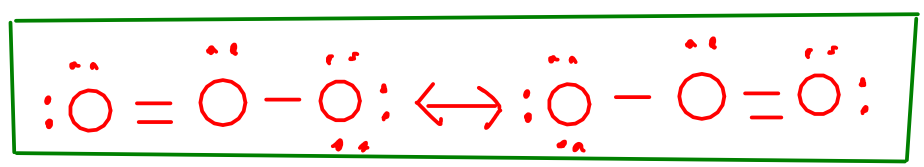


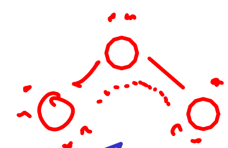
All atoms have a share in eight electrons here.

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 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^+

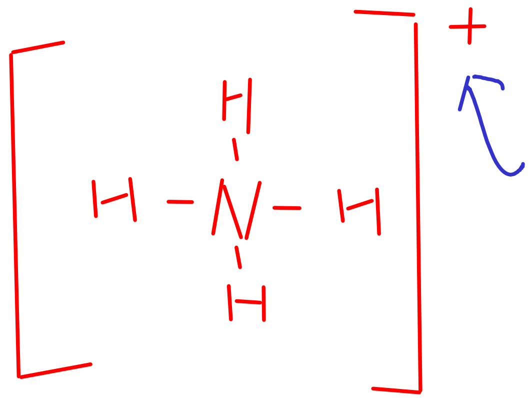
N : 5

H : 1 x 4

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

− 1 ← Subtract an electron to account for ammonium's +1 charge

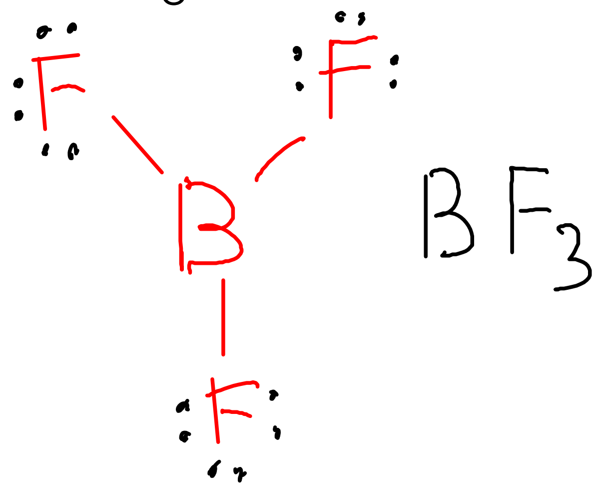
8



Draw brackets around the structure so that we can see the entire molecule is CHARGED.

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!

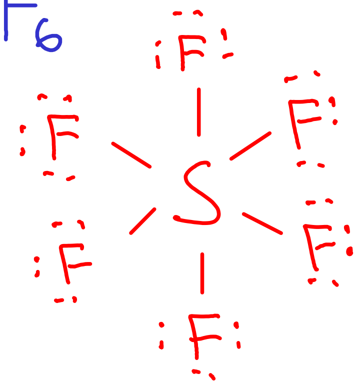
  - Any atom in period three or greater can do this. SULFUR and PHOSPHORUS compounds commonly do this!

    ... 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

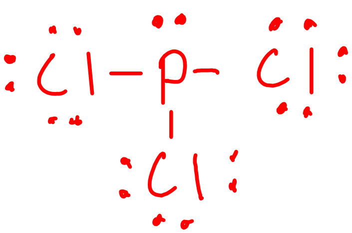
- The central SULFUR atom has a share in TWELVE total electrons, not eight!

- 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

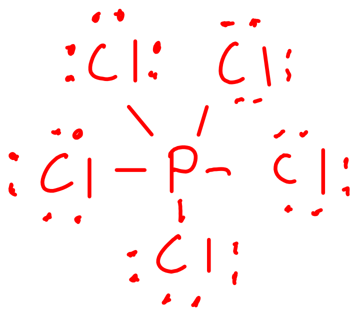
P : 5
Cl : 7x3 = 21
= 26



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.

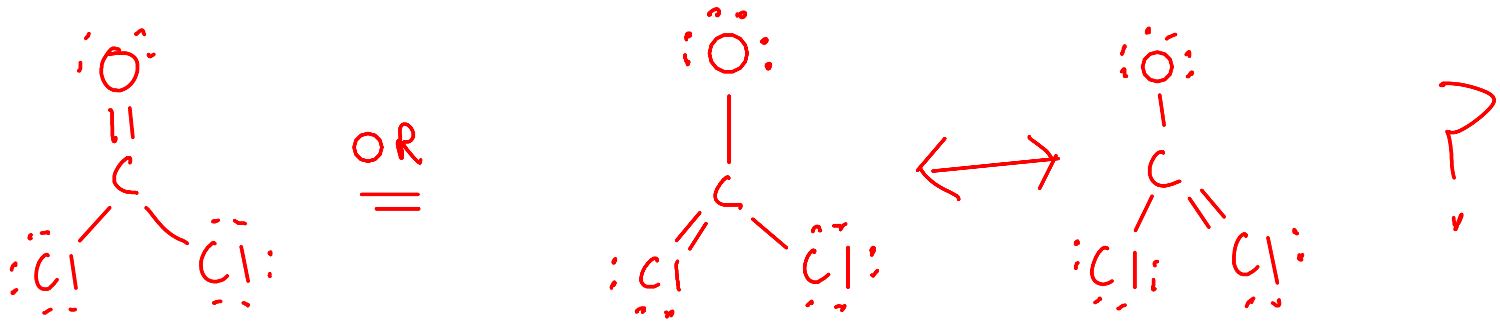
FORMAL CHARGE	=	ORIGINAL # OF VALENCE ELECTRONS	—	NUMBER OF BONDS	—	NUMBER OF UNSHARED ELECTRONS

* 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

* The sum of the formal charges of a correct Lewis structure will sum to the overall CHARGE of the molecule.

* The structure on the left is preferred. It has LOWER formal charges than the one on the right, plus it does not have positive formal charge on electronegative elements like CHLORINE.

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?

* HCN structure (on the right) is more likely.
- Lower magnitude of formal charges (all zeros)
- The HNC structure has a positive formal charge on nitrogen and a negative formal charge on carbon, when nitrogen is more electronegative.