(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

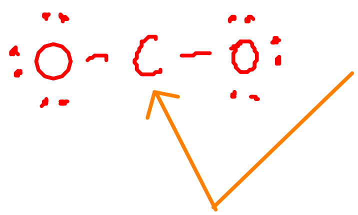
(3) Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

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

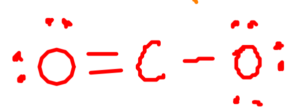
CO_2

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

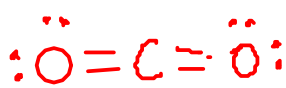
Use CARBON as the central atom.



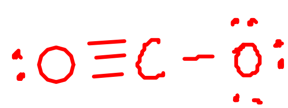
Carbon has a share in only four electrons (same as before bonding)



Adding one double bond gives carbon a share in SIX electrons



Giving the other oxygen arom a double bond like the first gives carbon a share in eight electrons.



These two oxygen atoms SHOULD bond the same way to the carbon center. They are identical atoms in an identical environment.

EXPERIMENTALLY, we find that the two oxygen atoms are the same distance from the carbon center, so they should both have the same kind of bond with the carbon.

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(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

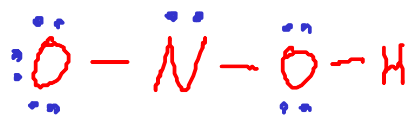
(3) Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

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: 5 x 1
O: 6 x 2
] 18 e^-



... but NITROGEN has a share in only SIX electrons.

These two oxygens are in DIFFERENT environments, so we're not surprised that one oxygen is bonded differently from the other.

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

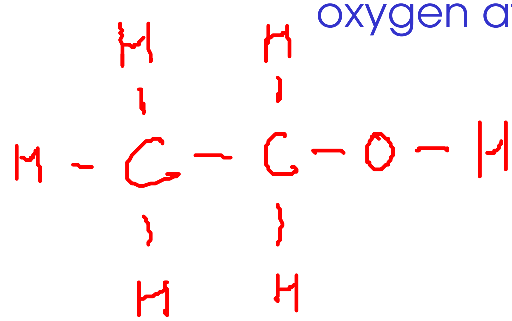
(3) Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

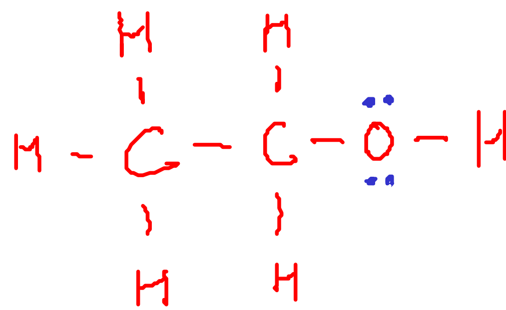
(4) Check octet rule - each atom should have a share in 8 electrons (H gets 2). if not, make double or triple bonds.

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 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

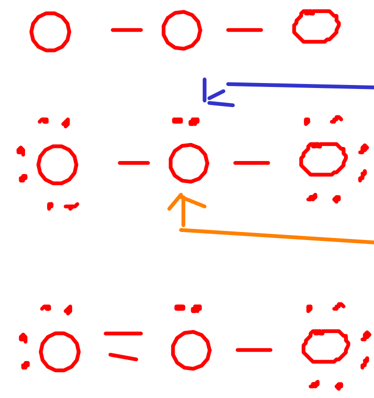
3. Distribute remaining valence electrons around structure, outer atoms first. Follow octet rule until you run out of electrons.

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

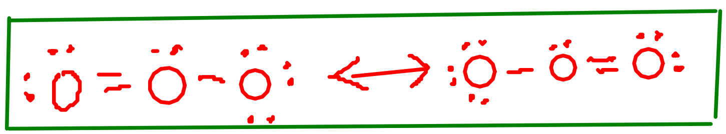
Central oxygen has only six electrons

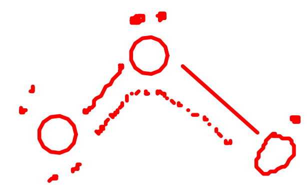
All atoms have a share in eight electrons!

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: 1 x 5

H: 4 x 1

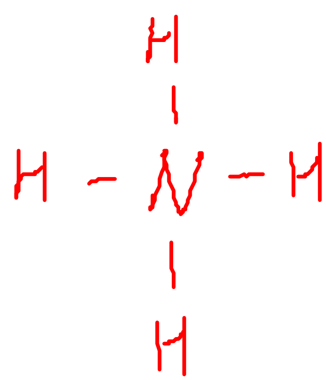
9

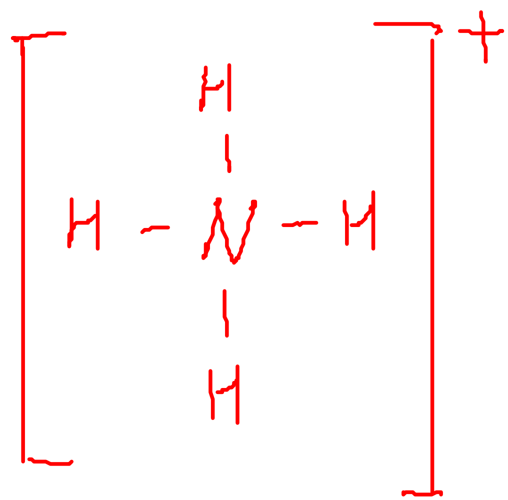
An odd number of electrons? But Lewis structures for molecules generally involve PAIRS of electrons.

− 1

Subtract an electron to account for the +1 charge.

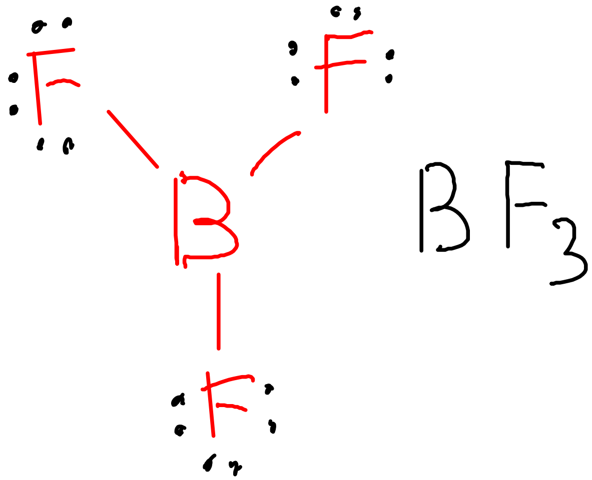
8





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!

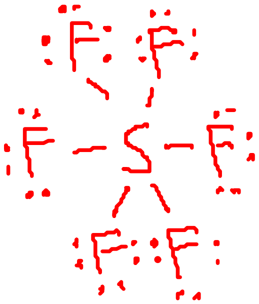
... these atoms have unfilled "d" orbitals that may participate in bonding!

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

EXAMPLES:

SF_6

S: 6
F: 7 x 6
48



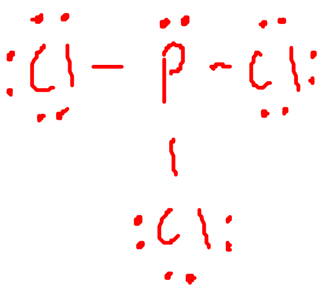
- The central SULFUR atom has a share in TWELVE total electrons, not eight!

- 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

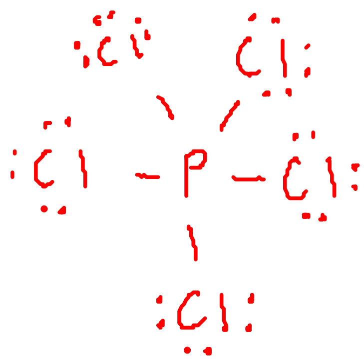
P : 5
Cl : 7 x 3 = 21
26



This structure obeys the octet rule.

PCl_5

P : 5
Cl : 7 x 5 = 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.

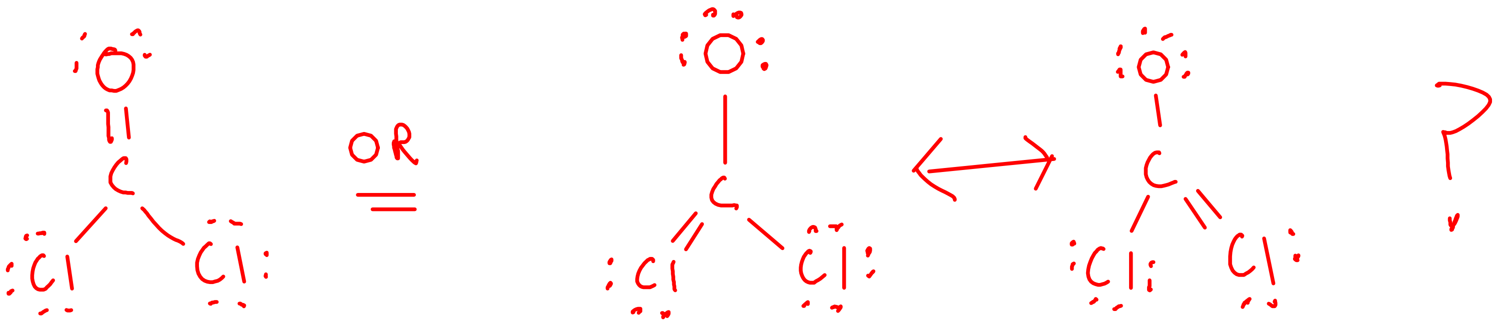
FORMAL CHARGE = ORIGINAL # OF VALENCE ELECTRONS − NUMBER OF BONDS − NUMBER OF UNSHARED ELECTRONS

* 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, choose the structure on the left. It has lower formal charges than the other.

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

H: 1 − 1 − 0 = 0

C: 4 − 4 − 0 = 0

N: 5 − 3 − 2 = 0

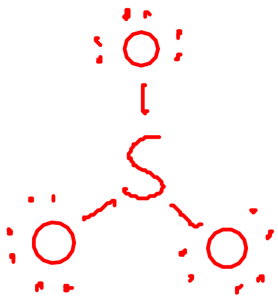
Which structure is more likely?

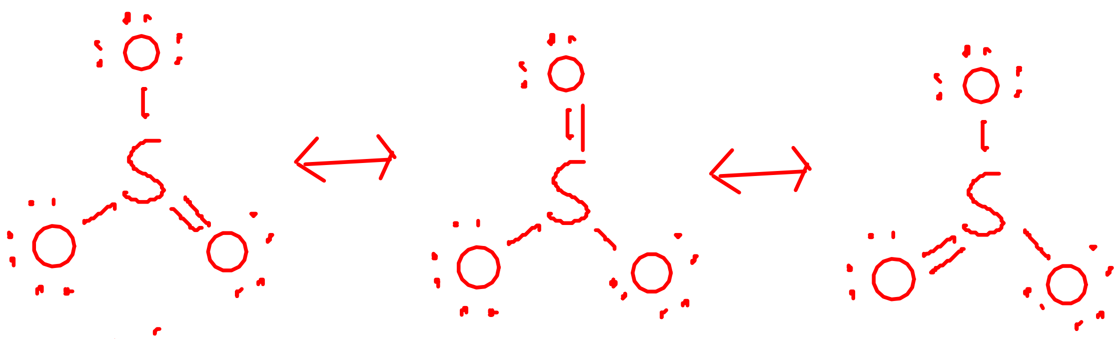
* The HCN structure is more likely. it has lower overall formal charges. Also, the HNC structure has a positive formal charge on nitrogen and a negative on carbon. Since nitrogen is more elecronegative than carbon, this seems backwards.

Let's look at sulfur trioxide. SO_3

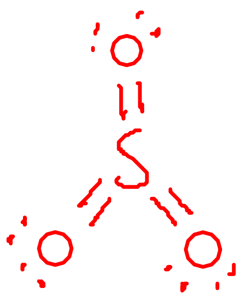
S: 6
O: 6 x 3 = 18
24 e^-

Skeletal structure:



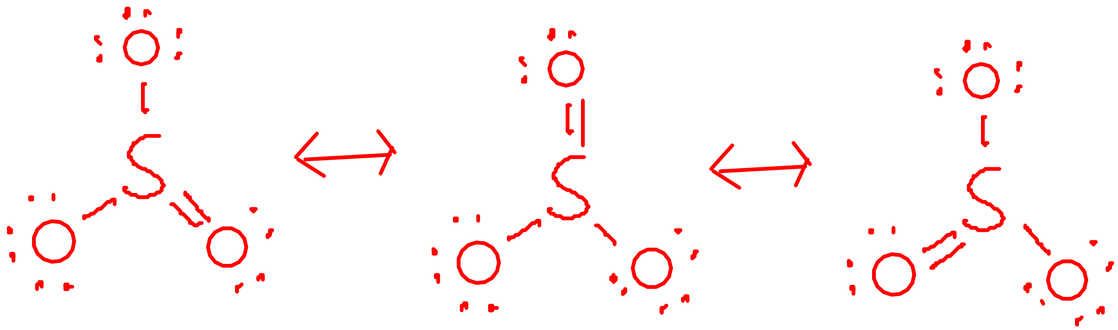


Resonance structures.



Expanded valence
(Sulfur is period 3)

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



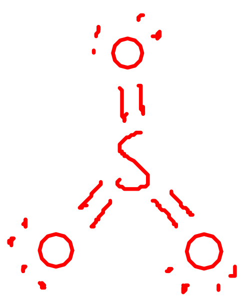
Resonance structures.

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 CHARGES, the expanded valence structure is preferred.

The correct structure is usually the one with minimized formal charge, EVEN IF the structure violates the octet rule!

NOTE: PERIOD 2 never violates the octet rule (except boron, which doesn't have expanded valence anyway)