WRITING LEWIS DOT STRUCTURES

Lewis structure or formula shows electron-dot symbols for the atoms, the bonding pairs as lines, and the lone pairs that fill each atom's outer level (valence shell) as pairs of dots.

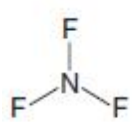
Step 1. Determine the total number of valence electrons.

- add up the valence electrons of the atoms. (Recall that the number of valence electrons equals = A-group number.)
- for ions, *add* one e^- for each negative charge, or *subtract* one e^- for each positive charge.

Step 2. Write the bond skeleton - Placement of atoms relative to each other

- place the atom with the *lower group number* in the center
- this is also the atom with the *lower electronegativity*
- If the atoms have the same group number, as in SO_3, place the atom with the *higher period number* (also lower EN) in the center. **H can form only one bond, so it is *never* a central atom.**

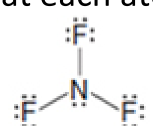
Step 3. Draw a single bond from each surrounding atom to the central atom, and subtract $2e^-$ for each bond from the total to find the number of e^- remaining:



$$3\ N{-}F \text{ bonds} \times 2e^- = 6e^- \quad \text{so} \quad 26e^- - 6e^- = 20e^- \text{ remaining}$$

Step 4. Distribute the remaining electrons in pairs so that each atom ends up with $8e^-$ (or $2e^-$ for H).

- First, place lone pairs on the *surrounding (more electronegative) atoms* to give each an octet. If any electrons remain, place them around the central atom—each F gets 3 pairs ($3 \times 6e^- = 18e^-$) and the N gets 1 ($2e^-$), for a total of $20e^-$.
- Check Always check that each atom has an octet or duet



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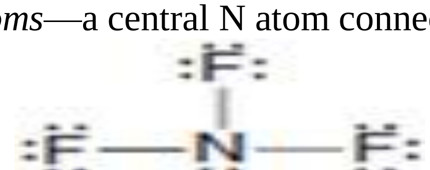
Since Lewis structures **do not indicate shape/geometry**, an equally correct depiction of NF_3 is any other that retains the *same connections among the atoms*—a central N atom connected by single bonds to each of three surrounding F atoms such as 

In nearly all their compounds,

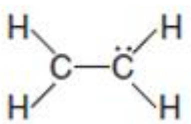
- Hydrogen atoms form one bond.
- Oxygen atoms form two bonds.
- Nitrogen atoms form three bonds.
- Carbon atoms form four bonds.
- Surrounding halogens form one bond; fluorine is *always* a surrounding atom

Writing Lewis Structures for Molecules with More Than One Central Atom:

CH_4O Here the 2 central atoms are C and O

Writing Lewis Structures for Molecules with Multiple Bonds:

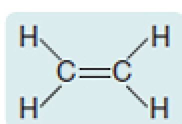
For C_2H_4. After steps 1 to 4, we have



The right C has an octet, but the left C has only $6e^-$ ☹ **!!!!!!!**

Step 5. Change a lone pair to a bonding pair if you run out of electrons before making all atoms HAPPY:

- ➢ Move the lone pair on C to a bonding pair between the 2 C atoms.



NOW ☺

Formal Charge in Lewis Structure: the charge it would have if the bonding electrons were shared equally.

$$\text{Formal charge of atom} = \text{no. of valence } e^- - (\text{no. of unshared valence } e^- + \tfrac{1}{2}\,\text{no. of shared valence } e^-)$$

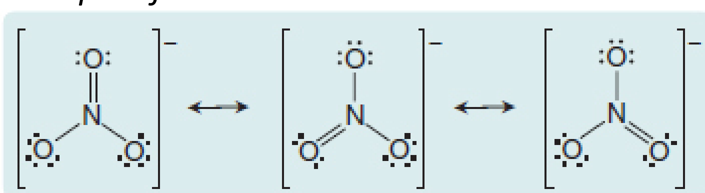
Formal charge for N, = 5 – (6+1) = - 2 ; for C = 4 - (0+4) = 0 ; for O = 6 – (2+3) = + 1

Sum of all the formal charges = - 2 + 0 +1 = - 1 = the charge of the polyatomic ion.

Resonance Structures:

- When you can write more than one possible Lewis dot structure for a molecule or ion, they are called resonance structures.
- You often find this in structures with *double bonds next to single bonds*
- Resonance structures *have the* *same bond skeleton* *but* *different locations of bonding and lone electron pairs*. You can convert one resonance form to another by moving lone pairs to bonding positions, and vice versa
- *Resonance structures are not real bonding depictions*
- The actual molecule is a **resonance hybrid,** an average of the resonance forms
- In a resonance hybrid, two of the electron pairs (one bonding and one lone pair) are *delocalized*- Delocalized Electron-Pair Bonding
- Partial bonding, as in resonance hybrids, often leads to fractional bond orders

Example of resonance structures in nitrate ion:

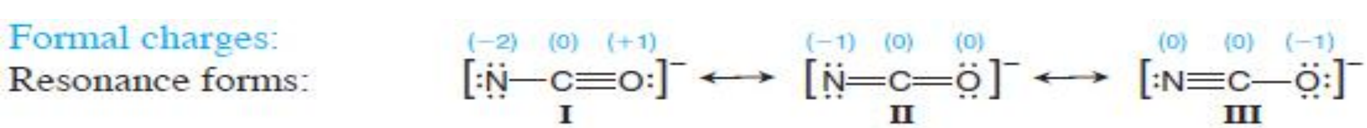


In fact, *t*he three nitrogen-oxygen bonds in NO_3^- ion are actually identical in length and energy. The bonds have properties between an N—O bond and an N═O bond, something like a “one-and-a-fraction” bond. The structure is shown more correctly with Lewis structures, called **resonance structures** (or **resonance forms),** and a two-headed resonance arrow ($(\longleftrightarrow)$) between them.

$$bond\ order = \frac{total\ electron\ pairs}{localized\ electron\ pairs}$$ = 4/3 = 1.33 in NO_3^- ion

Selecting the More Important Resonance Structure of the many resonance structures with varied formal charges for atoms:

- Smaller formal charges (positive *or* negative) are preferable to larger ones.
- A more negative formal charge should reside on a more electronegative atom.

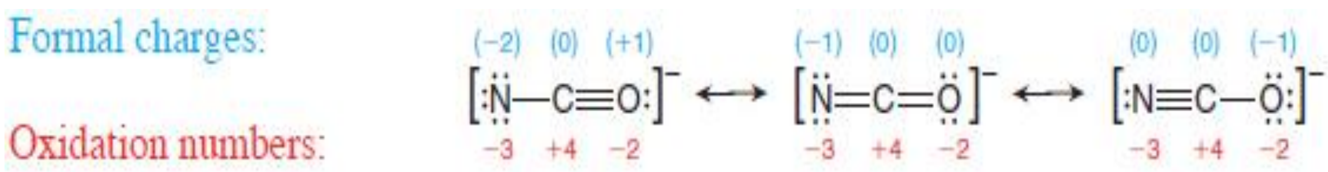


I is has a larger charge on N and a positive charge on the more electronegative O, so not preferred.
II and III have the same magnitude of charges, but III has a −1 charge on the more electronegative O, so III is more important than II.

Formal Charge Versus Oxidation Number :

For an *oxidation number*, bonding electrons are given *completely* to the more electronegative atom (as if the bonding were *pure ionic*):

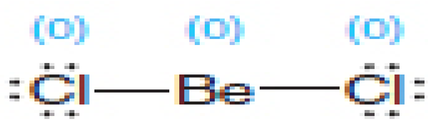
$$\text{Oxidation number} = \text{valence } e^- - (\text{lone pair } e^- + \text{bonding } e^-)$$

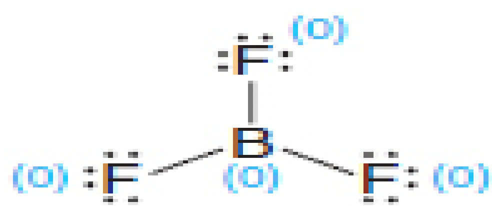


Notice that the oxidation numbers *do not* change from one resonance form to another (because the electronegativities *do not* change), but the formal charges *do* change (because the numbers of bonding and lone pairs *do* change).

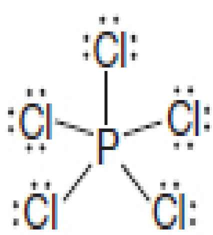
Lewis Structures for Exceptions to the Octet Rule:

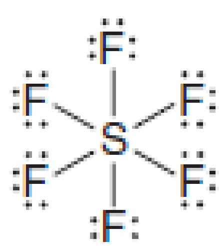
a) Molecules with Electron-Deficient Atoms- **LESS THAN OCTET**: There are only four electrons around Be and six around B

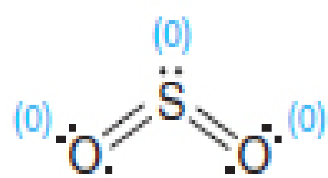




b) Molecules with **expanded valence shells** - MORE THAN OCTET –more than s^2, p^6
These occur only with *nonmetals from Period 3 or higher because they have empty d orbitals available.*







For SO_2 , the above structure is preferred based on formal charges whereas the one below obeys octect rule: