2.6 Resonance and Formal Charge

- Formal Charge
- Resonance Structures
- Bond Order, Bond Length and Bond Energy

Formal Charge

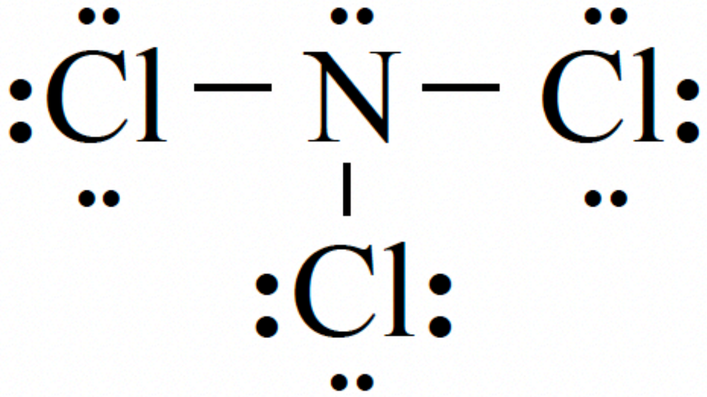
- In some cases, more than one Lewis diagram is possible for a given molecule.
- **Formal Charges** can be calculated to identify the most stable (likely) structure.
  - Neutral molecules: sum of charges will be zero
  - Polyatomic ion: sum will be equal to the overall charge

$$\text{Formal Charge} = \text{\# of valence electrons of the neutral atom} - \left(\text{number of lone e- around atom} + \frac{\text{number of bonding e-}}{2}\right)$$

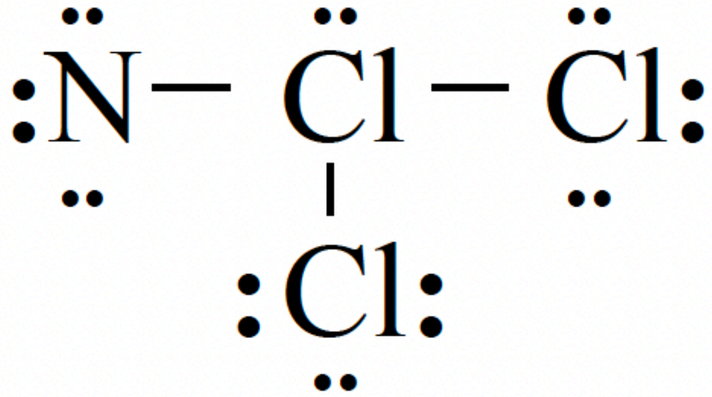
Example #1

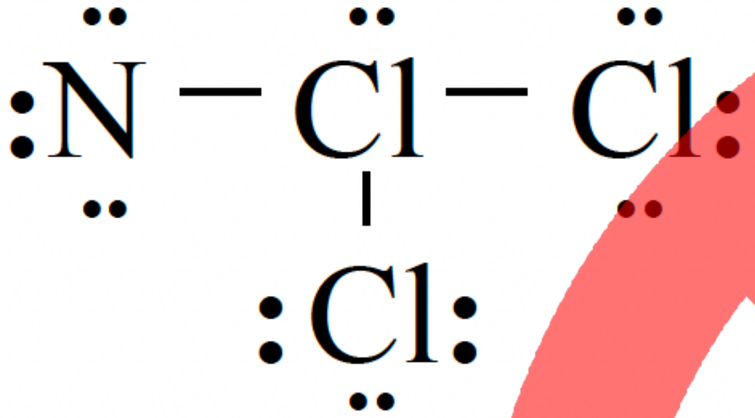
$$\text{Formal Charge} = \text{\# of valence electrons of the neutral atom} - \left(\text{number of lone e- around atom} + \frac{\text{number of bonding e-}}{2}\right)$$

- Which is the most likely structure?



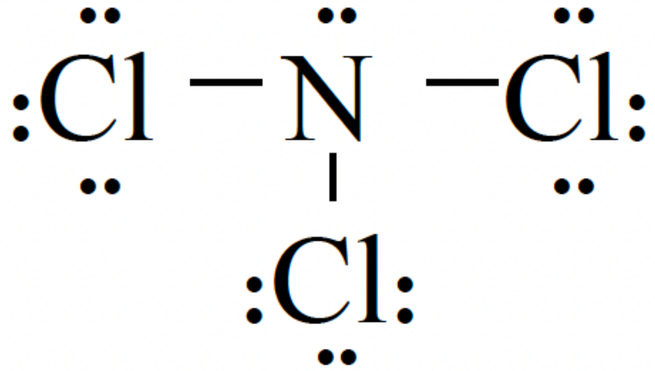
or





Example #1

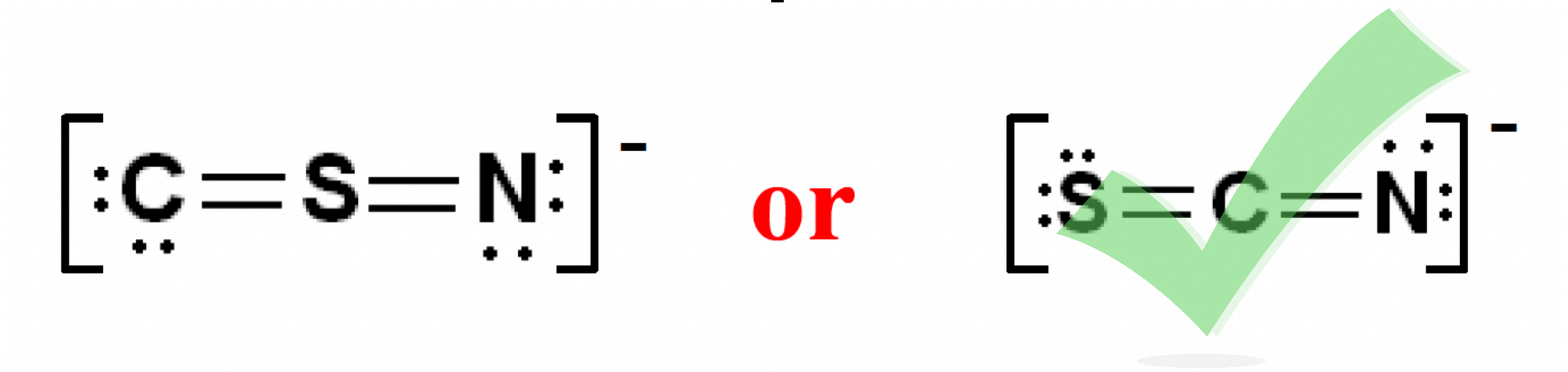
	N	Cl	Cl	Cl
Valence Electrons	5	7	7	7
Electrons Assigned	7	7	7	5
Formal Charge	-2	0	0	2



Example #1

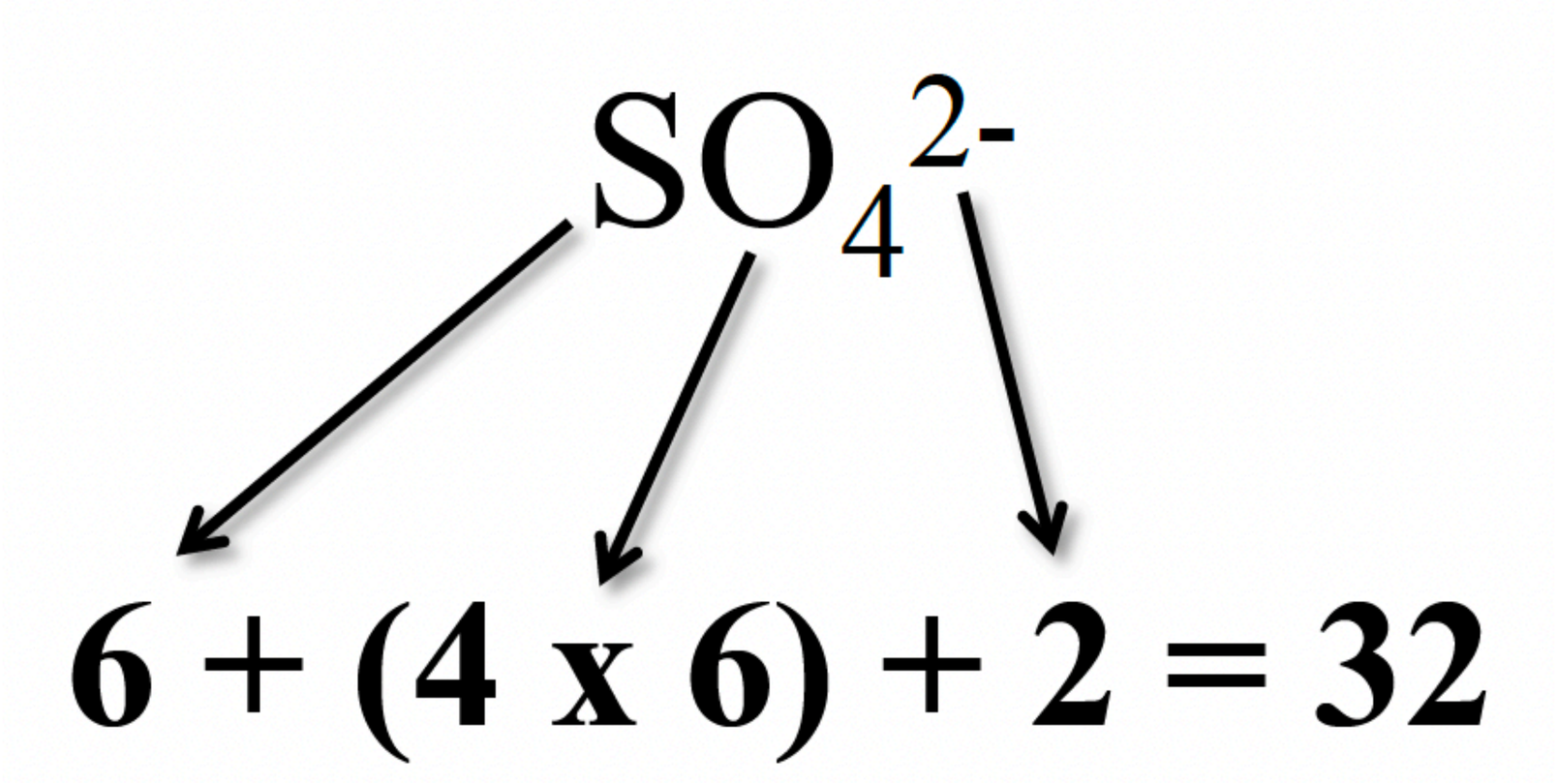
	N	Cl	Cl	Cl
Valence Electrons	7	7	7	5
Electrons Assigned	7	7	7	5
Formal Charge	0	0	0	0

Example #2



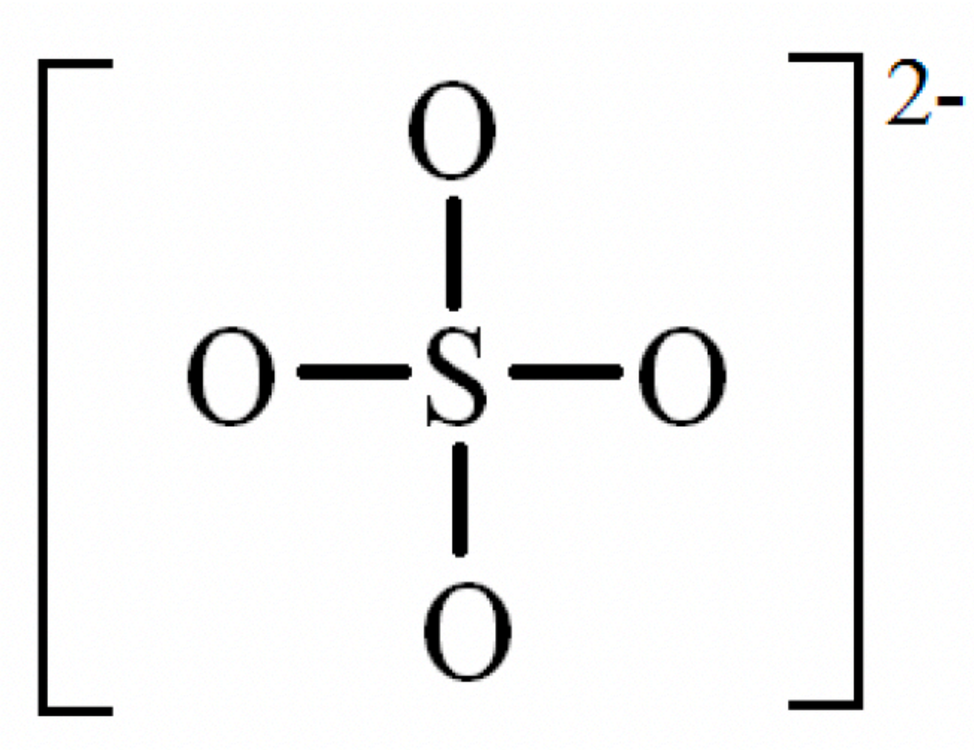
Example #3

- Draw the Lewis structure for SO_4^{2-} and check it using formal charges.
  - Count the total number of valence electrons in the polyatomic ion.



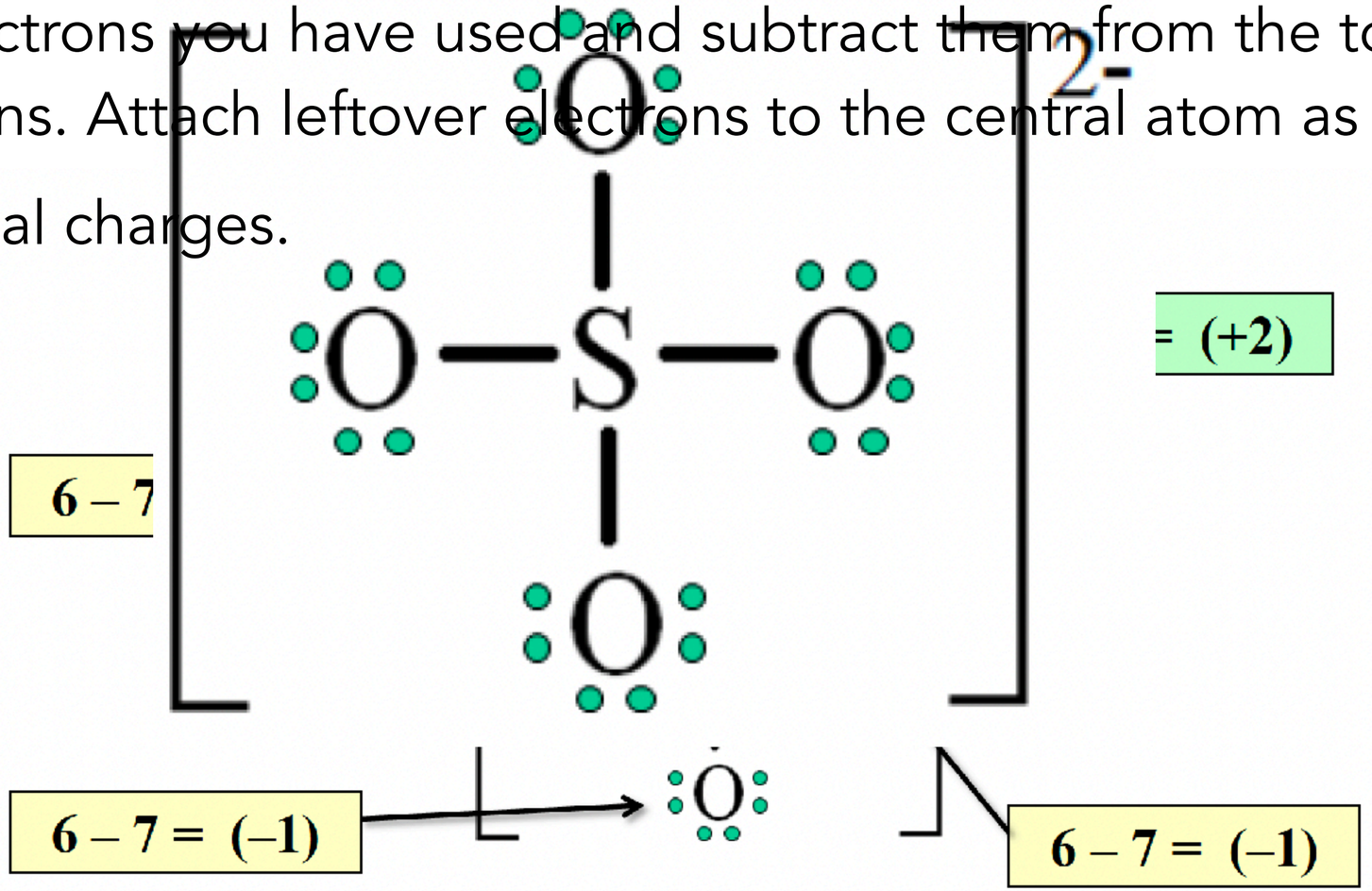
Example #3

- Put the **<u>least</u>** electronegative atom in the center and connect terminal atoms to it with single bonds.



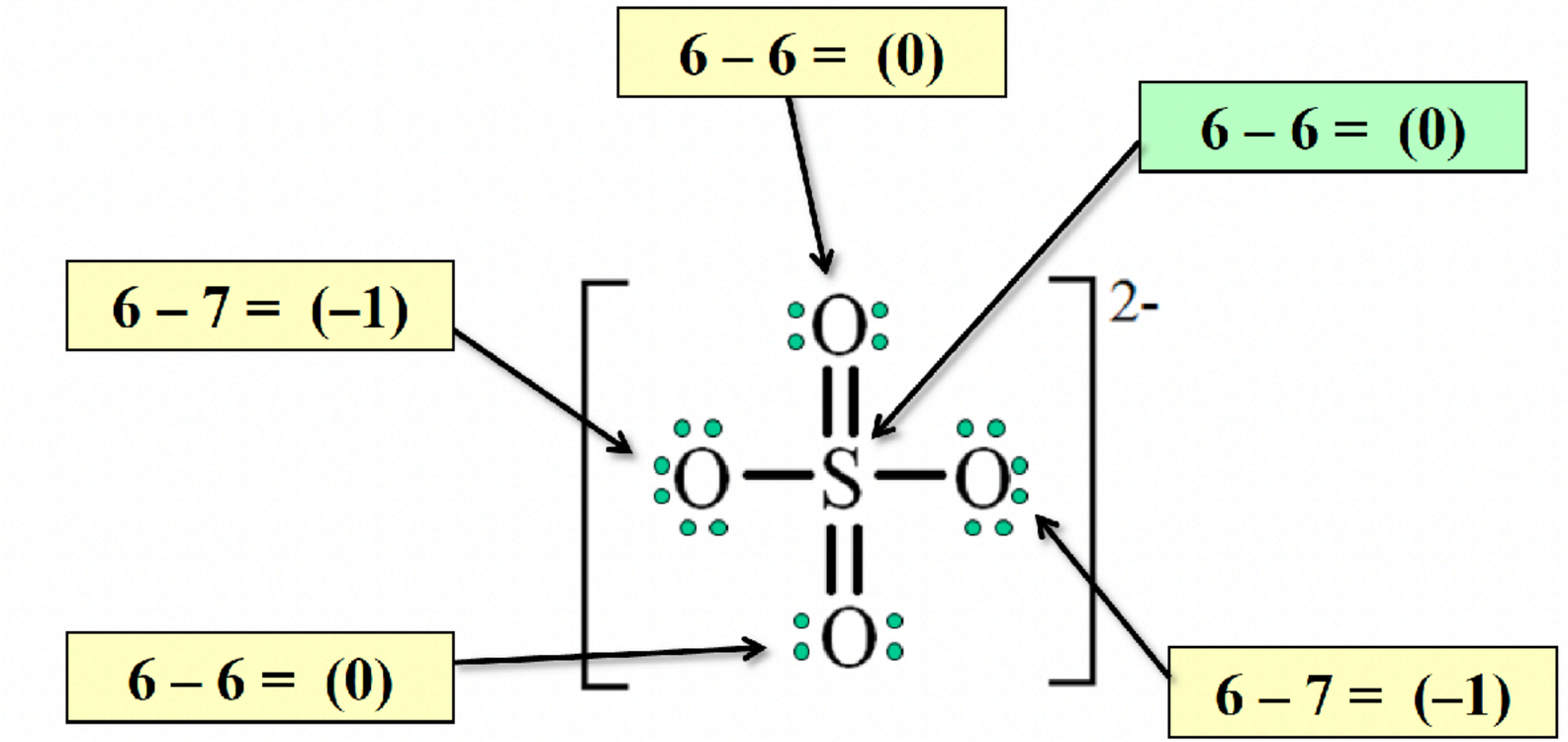
Example #3

- Complete the octets for all terminal atoms.
- Add up the electrons you have used and subtract them from the total number of valence electrons. Attach leftover electrons to the central atom as lone pairs.
- Check the formal charges.



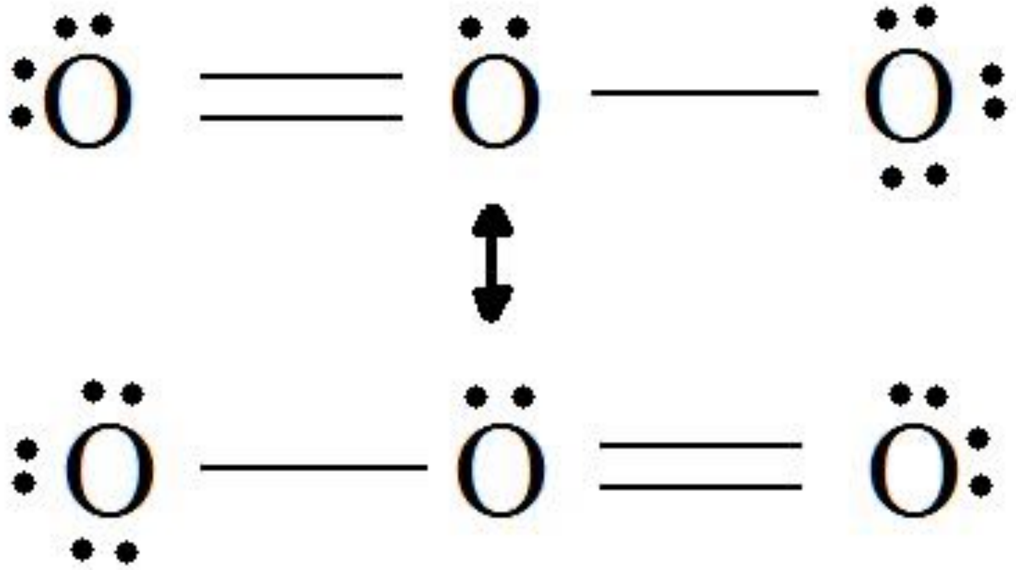
Example #3

- Add multiple bonds or change the arrangement of atoms to eliminate formal charges if necessary.



Resonance Structures

- For many molecules, double or triple bonds are located between different atoms.
- The result is more than one Lewis structure is possible.
  - Be prepared to draw all possible structures with ↔ arrows.
  - Ex: O_3

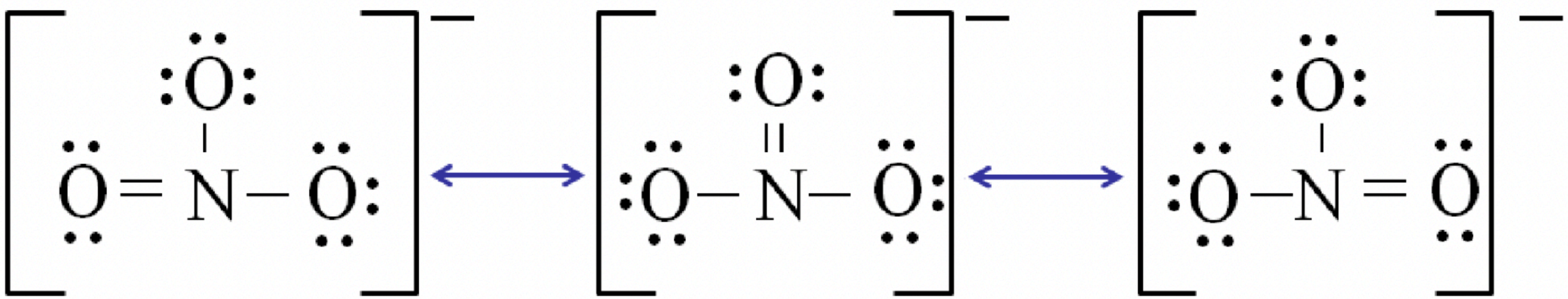


Bond Order = 1.5

Resonance Structures

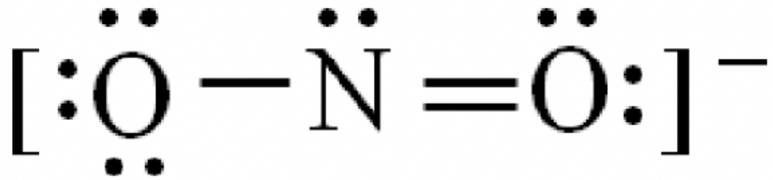
Effective number of bonds between atoms
= # of bonds / # of atoms

- Example: NO_3^-

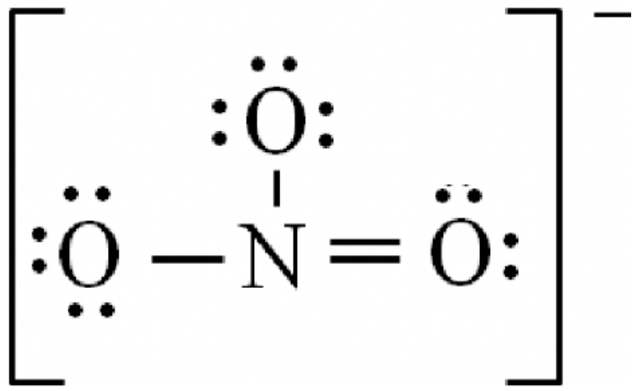


Resonance, Bond Length & Bond Energy

- Which structure has the shortest bonds?



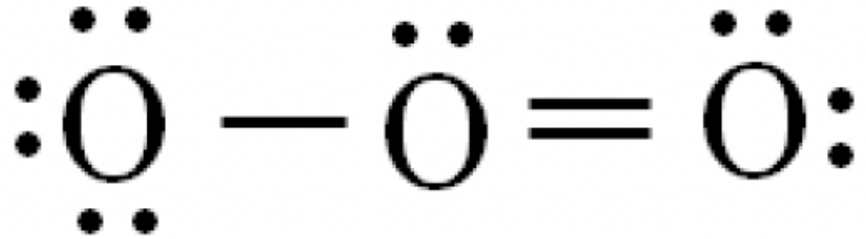
Bond order = 1.5



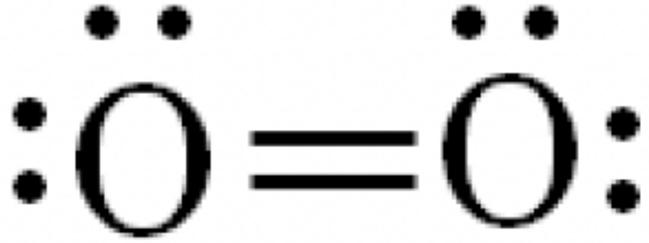
Bond order = 1.33

Resonance, Bond Length & Bond Energy

- Which structure has the greatest bond energy?



Bond order = 1.5

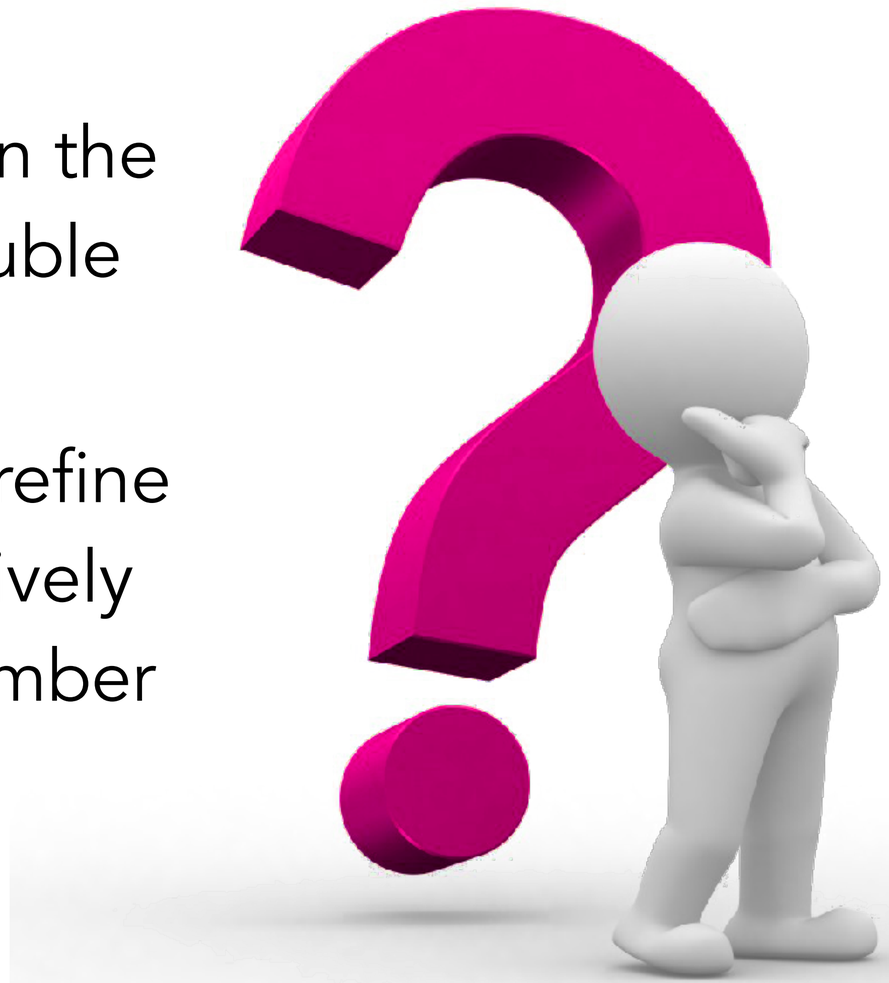


Bond order = 2.0

Limitations of the Lewis Structure Model

Part 1

- Many of the double bonds that are shown in the accepted Lewis structures are not really double bonds - they are 1.5, 1.33, or 1.25 bonds.
- In some cases, resonance must be used to refine a Lewis structure in order to obtain qualitatively accurate predictions about the effective number of bonds, bond energy and bond length.



Limitations of the Lewis Structure Model

Part 2

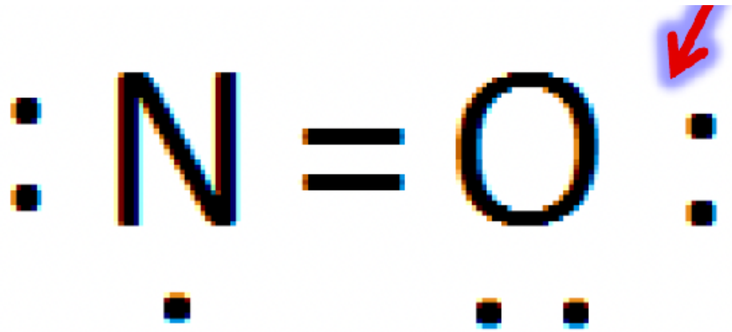
- The octet rule fails when there are numbers of valence electrons. (Wait, what??)
- Nitrogen monoxide, NO

N has 5 valence e^-

O has 6 valence e^-

11 valence e^-

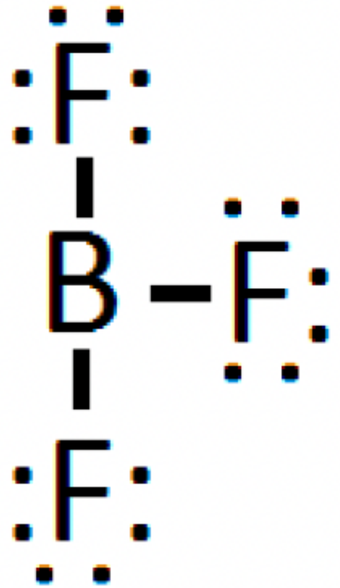
O gets 8, as it is more electronegative

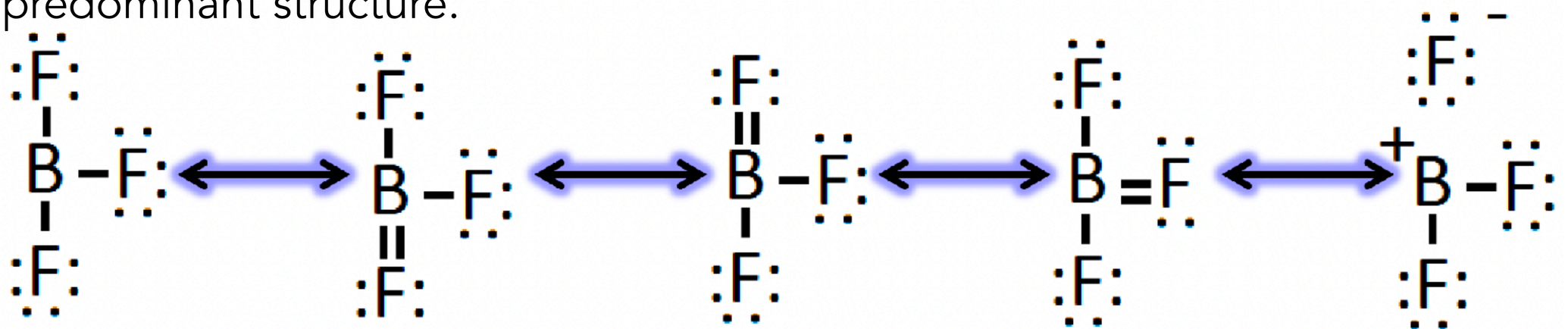


Limitations of the Lewis Structure Model

Part 3

- Incomplete octets and other issues
- **This is the accepted Lewis structure for BF_3,** and other compounds off boron for 2 reasons.
  - Boron has less ability to attract electrons to fill its octet, as it only has 5 protons in its nucleus.
  - The formal charges work out.
  - Several resonance forms exist, but experiments suggest this is the predominant structure.





Limitations of the Lewis Structure Model

Part 4

- Expanded octets also fail the octet rule.