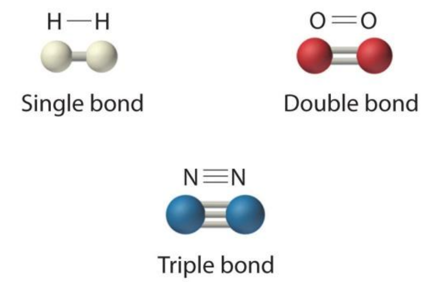
SCH 4U

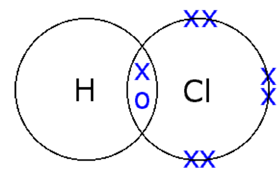
POLARITY OF BONDS & FORMAL CHARGES

When 2 identical atoms form a covalent bond, each atom has an equal share of the electron pair in the bond.

- Electron density is the same at both ends.
- Electrons are equally attracted to both nucleii.

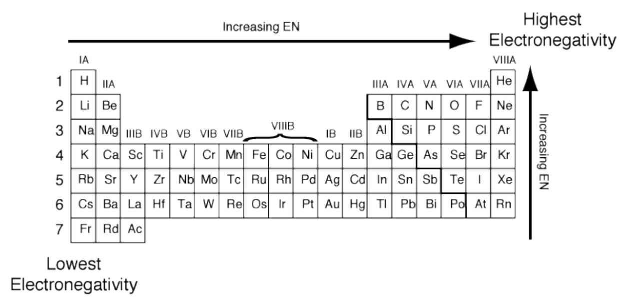


However, when bonding atoms are not alike, as in the H – Cl molecule, one nucleus usually attracts the electrons in the bond more than the other. The bonding pair of electrons are located closer to the stronger nucleus.



ELECTRONEGATIVITY = the relative attraction of an atom for the electrons in a bond. The larger the electronegativity of an atom, the greater the attraction for the bonding pair of electrons.

The general trend of the Electronegativity in the periodic table follows the trend of ionization energy.

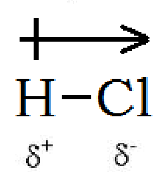


The nature of the bond between 2 atoms is often characterized by the difference in the electronegativities (ΔEN) of the atoms. If...

- **ΔEN = 0**: purely covalent (equal sharing of e^-)
  → as in diatomic molecules
- **ΔEN is between 0 and 1.7**: polar covalent → shared electrons are pulled towards the more electronegative atom.
- **ΔEN > 1.7:** bond is ionic.

When unequal sharing of electrons occurs between 2 atoms, a **POLAR covalent bond** is formed and each atom generates (or carries) a **partial charge**. Partial charges (represented with a lowercase Greek letter delta) and a vector pointing in the direction of the atom with the greater EN illustrate the polarity in the Lewis structure.

For instance, the H – Cl molecule has an unequal sharing of electrons:



EN of H = 2.1

EN of Cl = 2.9

ΔEN = 2.9 – 2.1 = 0.8

Since 0.8 falls in the range of 0 to 1.7, the bond is characterized as a **polar bond**.

HCl is a **polar molecule** due to the **dipole** created by the unequal sharing of electrons.

<u>EXERCISE:</u> For each compound/molecule,

- Draw the Lewis & structural diagrams of the following molecules/ions.
- Determine the difference in electronegativity of the bonded atoms and describe the <u>polarity of the bond</u> and <u>polarity of the molecule</u> formed.

1. OF_2

2. NH_4^+

3. $CaCl_2$

4. NO_3^-

5. ClF_3

6. $HClO_4$

7. Br_2

8. H_2CO_3

9. bromous acid

10. sulfite ion

11. sulfuric acid

12. phosphoric acid

FORMAL CHARGES & THE SELECTION OF LEWIS STRUCTURES

BOND ORDER = number of pairs of electrons shared between 2 atoms.

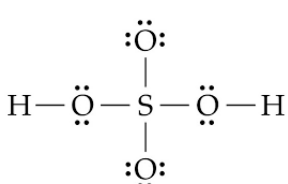
- As the bond order increases, the bond length decreases and the bond energy increases, when comparing bond orders between the same elements.

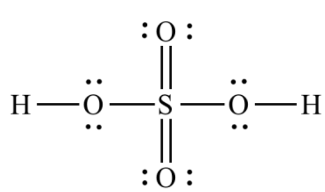
The Relation of Bond Order, Bond Length and Bond Energy

Bond	Bond Order	Average Bond Length (pm)	Average Bond Energy (kJ/mol)
C — O	1	143	358
C = O	2	123	745
C ≡ O	3	113	1070
C — C	1	154	347
C = C	2	134	614
C ≡ C	3	121	839
N — N	1	146	160
N = N	2	122	418
N ≡ N	3	110	945

Consider the structure drawn in #11 of sulfuric acid. We would predict that the bond lengths of the S – O bonds should all be equal since their bond order is 1. Experimentally, however, they do not all have equal bond length. The S – O bond lengths are shorter than the S – O – H bond lengths, which means they must have a larger bond order. In fact, the S – O bond lengths correspond with bond order 2, meaning that a double bond exists between the S and O atoms in the S – O bond, but a single bond exists in the S – OH bond.

The Lewis structure of sulfuric acid must be modified.



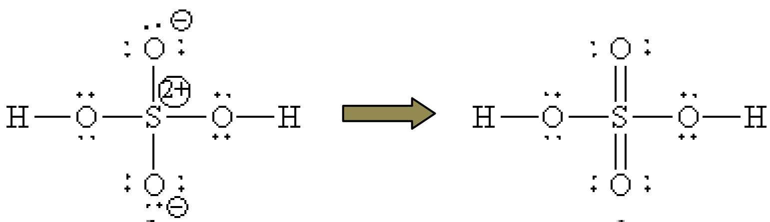


Note that the valence shell of sulfur has an expanded valence, which is permitted for elements below period 2.

Calculating **__FORMAL CHARGE__** on each atom in a given molecule, rather than depending on experimental data, is a convenient way of determining the best illustration of its structure.

$$[\mathit{formal\ charge}] = \begin{bmatrix} \#\ of\ valence\ e^- \\ in\ isolated\ atom \end{bmatrix} - [\#\ of\ \boldsymbol{bonds}] - [\#\ of\ \boldsymbol{unshared\ e^-}]$$

The **BEST structure** is the one with **fewest formal charges** and closest to zero.
The net charge of the formal charges of all atoms in a particle must sum to the charge of the particle. For instance, the sum of all formal charges within the nitrate (NO_3^-) ion must be -1, and the sum of all formal charges within the $HClO_2$ molecule must be 0.



1 2

Structure #2 wins the prize!

__EXAMPLES__:

Draw the structure of each molecule/ion. Use formal charges to check for a better structure.

1. HNO_3
2. $HClO_2$
3. $POCl_3$
4. BCl_3
5. SO_2
6. NOF_3
7. chromate ion
8. dichromate ion