Chemical Bonding and Molecular Structure

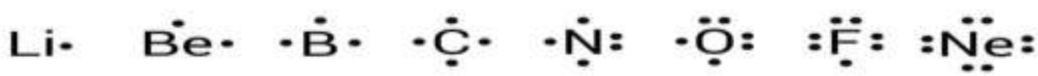
Matter is made up of one or different type of elements. Under normal conditions no other element exists as an independent atom in nature, except noble gases. However, a group of atoms is found to exist together as one species having characteristic properties. Such a group of atoms is called a molecule.

The attractive force which holds various constituents (atoms, ions, etc.) together in different chemical species is called a chemical bond.

Every system tends to be more stable and bonding is nature's way of lowering the energy of the system to attain stability.

Lewis Symbols: In the formation of a molecule, only the outer shell electrons take part in chemical combination and they are known as **valence electrons.**

G.N. Lewis, an American chemist introduced simple notations to represent valence electrons in an atom. These notations are called **Lewis Symbols.**



Kossel, in relation to chemical bonding, drew attention to the following facts.

- In the periodic table, the highly electronegative halogens and the highly electropositive alkali metals are separated by the noble gases;
- The formation of a negative ion from a halogen atom and a positive ion from an alkali metal atom is associated with the gain and loss of an electron by the respective atoms;
- The negative and positive ions thus formed attain stable noble gas electronic configurations. The noble gases (with the exception of helium which has a duplet of electrons) have a particularly stable outer shell configuration of eight (octet) electrons, ns^2np^6.
- The negative and positive ions are stabilized by electrostatic attraction.

Na	$\rightarrow$	$Na^+ + e^-$
$[Ne]\ 3s^1$	$\rightarrow$	$[Ne]$
$Cl + e^-$	$\rightarrow$	Cl^-
$[Ne]\ 3s^2\ 3p^5$		$[Ne]\ 3s^2\ 3p^6$ or $[Ar]$
$Na^+ + Cl^-$	$\rightarrow$	$NaCl$ or Na^+Cl^-

Similarly the formation of CaF_2 may be shown as:

Ca	$\rightarrow$	$Ca^{2+} + 2e^-$
$[Ar]\ 4s^2$		$[Ar]$
$F + e^-$	$\rightarrow$	F^-
$[He]\ 2s^2\ 2p^5$		$[He]\ 2s^2\ 2p^6$ or $[Ne]$
$Ca^{2+} + 2F^-$	$\rightarrow$	CaF_2 or $Ca^{2+}(F^-)_2$

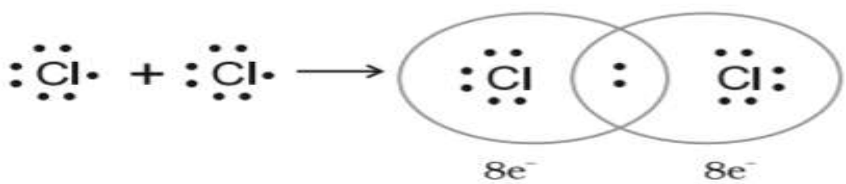
The bond formed, as a result of the electrostatic attraction between the positive and negative ions was termed as the ionic bond. The electrovalence is thus equal to the number of unit charge(s) on the ion.

Octet Rule

Kossel and Lewis in 1916 developed an important theory of chemical combination between atoms known as **electronic theory** of **chemical bonding.** According to this, atoms can combine either by transfer of valence electrons from one atom to another (gaining or losing) or by sharing of valence electrons in order to have an octet in their valence shells. This is known as **octet rule.**

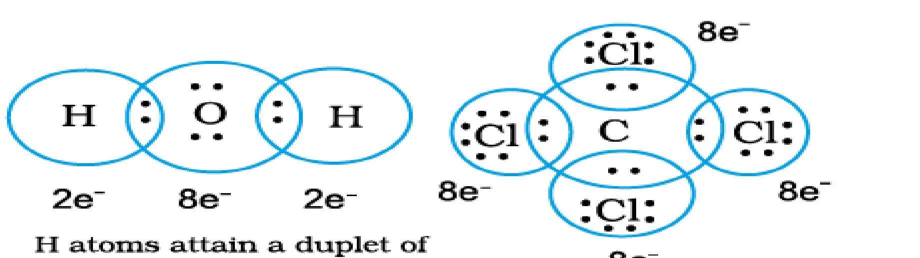
Covalent Bond

The formation of the Cl_2 molecule can be understood in terms of the sharing of a pair of electrons between the two chlorine atoms, each chlorine atom contributing one electron to the shared pair.



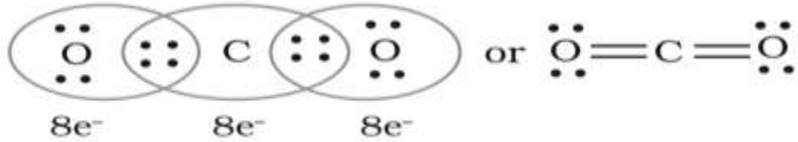
Covalent bond between two Cl atoms

- Each bond is formed as a result of sharing of an electron pair between the atoms.
- Each combining atom contributes at least one electron to the shared pair.
- The combining atoms attain the outer-shell noble gas configurations as a result of the sharing of electrons.
- Thus in water and carbon tetrachloride molecules, formation of covalent bonds can be represented as:

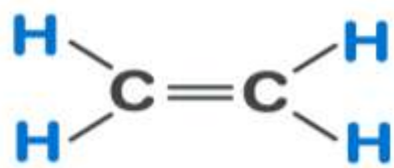


Thus, when two atoms share one electron pair they are said to be joined by a single covalent bond.

If two atoms share two pairs of electrons, the covalent bond between them is called a double bond. For example, in the carbon dioxide molecule, we have two double bonds between the carbon and oxygen atoms.

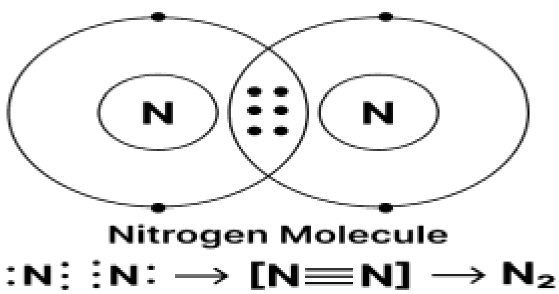


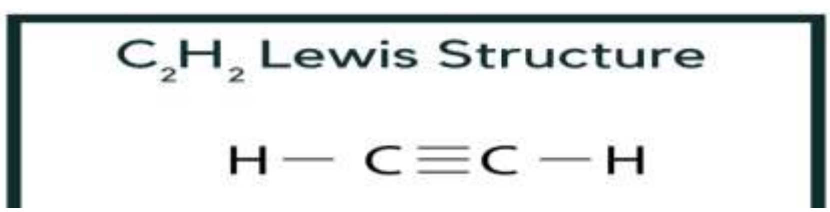
Double bonds in CO_2 molecule



C_2H_4 molecule

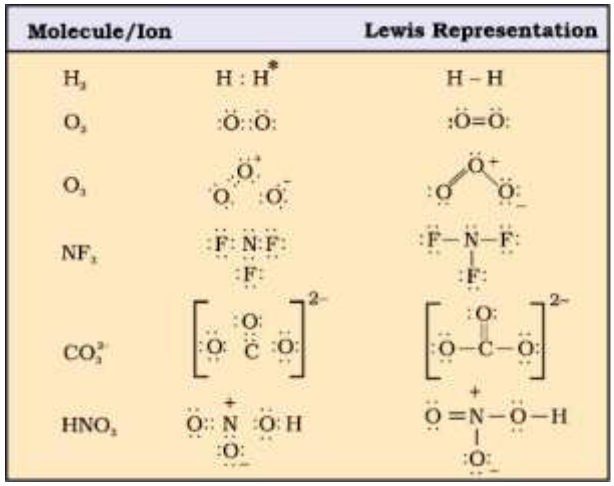
When combining atoms share three electron pairs as in the case of two nitrogen atoms in the N_2 molecule and the two carbon atoms is the ethyne molecule, a triple bond is formed.





Lewis representation of simple molecules (the Lewis structures)

The Lewis representation of Some Molecules



Each H atom attains the configuration of helium (a duplet of electrons)

Hydrogen Bonding

Nitrogen, oxygen and fluorine are the highly electronegative elements. When they are attached to a hydrogen atom to form covalent bond, the electrons of the covalent bond are shifted towards the more electronegative atom. This partially positively charged hydrogen atom forms a bond with the other more electronegative atom. This bond is known as hydrogen bond and is weaker than the covalent bond. For example, in HF molecule, the hydrogen bond exists between hydrogen atom of one molecule and fluorine atom of another molecule as depicted below:

$$---H^{\delta+} - F^{\delta-} --- H^{\delta-}\ F^{\delta-} --- H^{\delta-} - F^{\delta-}$$

Here, hydrogen bond acts as a bridge between two atoms which holds one atom by covalent bond and the other by hydrogen bond. Hydrogen bond is represented by a dotted line (– – –) while a solid line represents the covalent bond. Thus, hydrogen bond can be defined as the attractive force which binds hydrogen atom of one molecule with the electronegative atom (F, O or N) of another molecule.

Cause of Formation of Hydrogen Bond

When hydrogen is bonded to strongly electronegative element 'X', the electron pair shared between the two atoms moves far away from hydrogen atom. As a result the hydrogen atom becomes highly electropositive with respect to the other atom 'X'. Since there is displacement of electrons towards X, the hydrogen acquires fractional positive charge (δ^+) while 'X' attain fractional negative charge (δ). This results in the formation of a polar molecule having electrostatic force of attraction which can be represented as:

$$H^{\delta+} - X^{\delta-} --- H^{\delta+} - X^{\delta-} --- H^{\delta+} - X^{\delta-}$$

The magnitude of H-bonding depends on the physical state of the compound. It is maximum in the solid state and minimum in the gaseous state, Thus, the hydrogen bonds have strong influence on the structure and properties of the compounds.

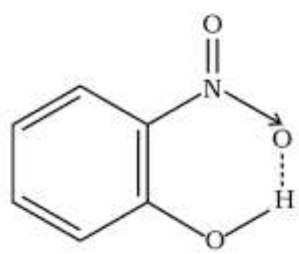
Types of H-Bonds

There are two types of H-bonds

(i) Intermolecular hydrogen bond
(ii) Intra-molecular hydrogen bond

(1) Intermolecular hydrogen bond: It is formed between two different molecules of the same or different compounds. For example, H-bond in case of HF molecule, alcohol or water molecules, etc.

(2) Intra-molecular hydrogen bond : It is formed when hydrogen atom is in between the two highly electronegative (F, O, N) atoms present within the same molecule. For example, in o-nitrophenol the hydrogen is in between the two oxygen atoms.



Intramolecular hydrogen bonding in o-nitrophenol molecule