ATOMIC ENERGY CENTRAL SCHOOL-3 TARAPUR

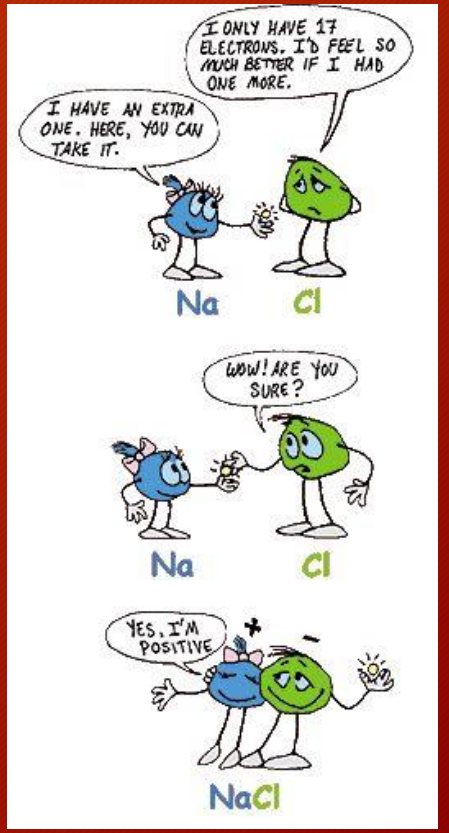
- MODULE-1
- UNIT- CHEMICAL BONDING

Syllabus

- Chemical Bonding and Molecular Structure 14 Periods : Valence electrons, ionic bond, covalent bond, bond parameters, Lewis structure, polar character of covalent bond, covalent character of ionic bond, valence bond theory, resonance, geometry of covalent molecules, VSEPR theory, concept of hybridization, involving s, p and d orbitals and shapes of some simple molecules, molecular orbital theory of homonuclear diatomic molecules(qualitative idea only), Hydrogen bond.

CHEMICAL BONDING

- Force of attraction which is capable to hold constituent particles of matter together is known as Chemical bond or chemical bonding.
- This is a one kind of relation established between particles when they come in the vicinity of each other.
- A chemical bond is a attraction between atoms, ions or molecules that enables the formation of chemical compounds. The bond may result from the electrostatic force of attraction between oppositely charged ions as in ionic bonds or through the sharing of electrons as in covalent bonds
- The attractive force which holds various constituents (atoms, ions, etc.) together in different chemical species is called a chemical bond.



Why do atoms combine?

Every system tends to be more stable by lowering its energy and bonding is nature's way of lowering the energy of the system to attain stability means atoms tend to reduce their potential energy therefore combine to convert in to most stable state of lower energy i.e. molecule.

Why do atoms combine?

To answer such questions different theories and concepts have been put forward from time to time. These are Kössel-Lewis approach, Valence Shell Electron Pair Repulsion (VSEPR) Theory, Valence Bond (VB) Theory and Molecular Orbital (MO) Theory.

Octet Rule

- Octet Rule(electronic theory of chemical bonding):
- Kössel 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.

Lewis Symbols

- 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.

For example,

● = Valency electrons

Li● ●Be●

Ionic bond

The bond formed, as a result of the electrostatic attraction between the positive and negative ions was termed as the electrovalent bond or ionic bond.

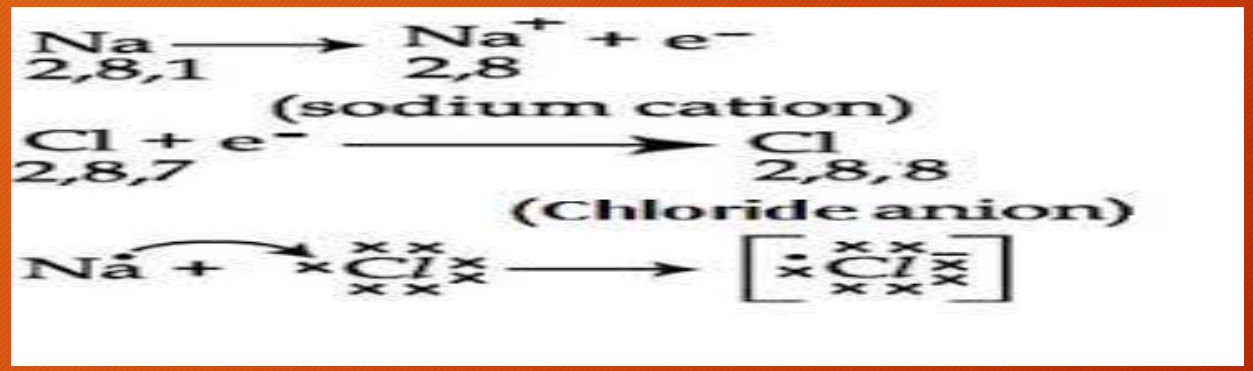
Or

The electrostatic force of attraction present between oppositely charged ions is known as ionic bond.

For example, the formation of NaCl or (formation of ionic bond) from sodium and chlorine can be explained as:

$_{11}Na$ = 2,8,1 and $_{17}Cl$ = 2,8,7

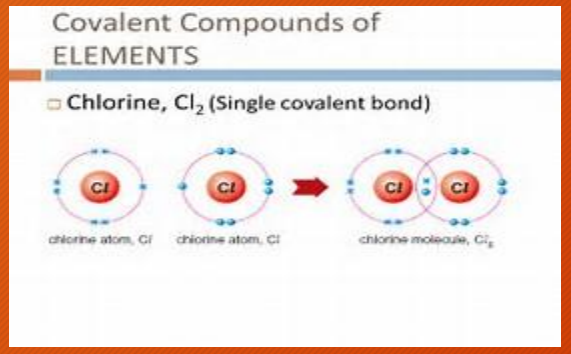
By exchanching 1e both Na and Cl atom got stable electronic configuration of nearest noble gases and octet of outermost shell is achieved.

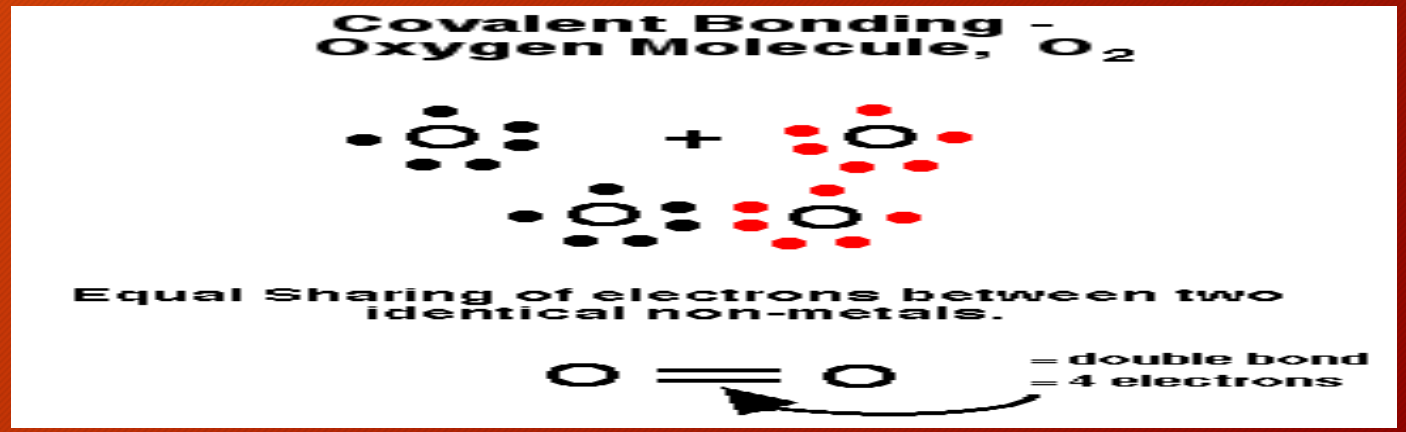


Covalent bond

Bond formed between the atoms by equal sharing of electrons is called as covalent bond.

- when two atoms share one one electron(one electron pair) they are said to be joined by a single covalent bond.
- If two atoms share two two electrons(two electron pairs),the covalent bond between them is called a double bond.





Bond parameters

- **Bond Length:** Bond length is defined as the equilibrium distance between the nuclei of two bonded atoms in a molecule.
- **Bond Angle :** It is defined as the angle between the orbitals containing bonding electron pairs around the central atom in a molecule/complex ion. Bond angle is expressed in degree.
- **Bond Enthalpy :** It is defined as the amount of energy required

  to break one mole of bonds of a particular type between two atoms in a gaseous state. The unit of bond enthalpy is kJ mol^{-1} .
- **Bond Order :** the Bond Order is the number of bonds between the two atoms in a molecule.

Lewis Representation of Simple Molecules (the Lewis Structures)

- The Lewis dot structures provide a picture of bonding in molecules and ions in terms of the shared pairs of electrons and the octet rule.
- The Lewis dot structures can be written by adopting the following steps:

(1) The total number of electrons required for writing the structures are obtained by adding the valence electrons of the combining atoms.

(2)For anions, each negative charge would mean addition of one electron. For cations, each positive charge would result in subtraction of one electron from the total number of valence electrons.

(3) Having knowledge of the skeletal structure of the compound (known or guessed intelligently), it is easy to distribute the total number of electrons as bonding shared pairs between the atoms in proportion to the total bonds.

(4) In general the least electronegative atom occupies the central position in the molecule/ion.

(5)After accounting for the shared pairs of electrons for single bonds, the remaining electron pairs are either utilized for multiple bonding or remain as the lone pairs.

(6) The basic requirement being that each bonded atom gets an octet of electrons.

Lewis Representation of Simple Molecules (the Lewis Structures)

For Ex: CO_3^{2-}

(i) Total number of electrons for writing Lewis structure = C + 3 O + $2e^-$

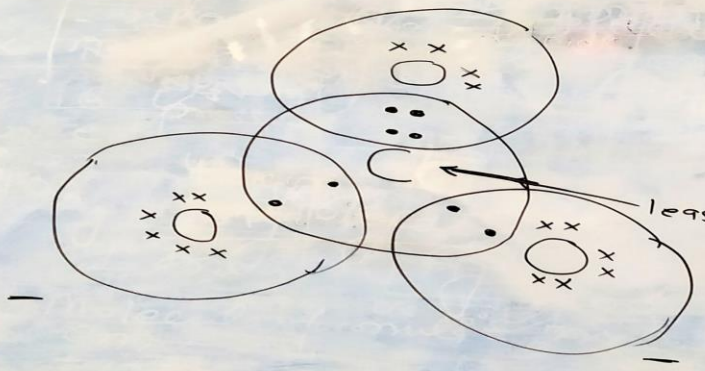
C: 6 (2,4) ; O: 8 (2,6)

= $\underbrace{4 + 3 \times 6}_{\text{valency electrons}} + 2e^-$ ← (2- negative charge)

= 24 electrons.

•• = bond pairs

×× = lone pairs



Polar character of covalent bond

- The existence of a hundred percent ionic orcovalent bond represents an ideal situation.In reality no bond or a compound is either completely covalent or ionic. When covalent bond is formed between two similar atoms, for example in H_2, O_2, Cl_2,N_2 or F_2, the shared pair of attracted by the two atoms. As a result electron pair is situated exactly between the two identical nuclei. The bond so formed is called nonpolar covalent bond. Contrary to this incase of a hetero nuclear molecule like HF, the shared electron pair between the two atoms gets displaced more towards fluorine since the electronegativity of fluorine is far greater than that of hydrogen. The resultant covalent bond is a polar covalent bond.
- As a result of polarisation, the molecule possesses the dipole moment.

Dipole moment

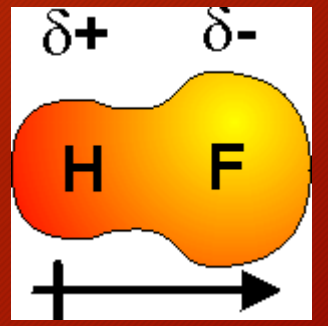
- Which can be defined as the product of the magnitude of the charge and the distance between the centres of positive and negative charge. It is usually designated by a Greek letter ‘μ’.

Mathematically, it is expressed as follows :

- Dipole moment (μ) = charge (Q) × distance of separation (r)

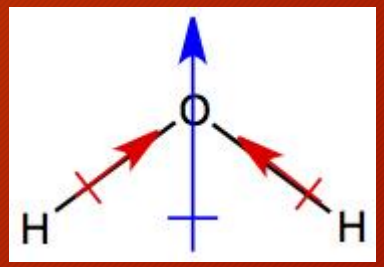
Dipole moment

- But in chemistry presence of dipole moment is represented by the crossed arrow (+--->) put on Lewis structure of the molecule. The cross is on positive end and arrow head is on negative end. For example the dipole moment of HF may be represented as in Fig.
- This arrow symbolises the direction of the shift of electron density in the molecule.
- In case of polyatomic molecules the dipole moment not only depend upon the individual dipole moments of bonds known as bond dipoles but also on the spatial arrangement of various bonds in the molecule. In such case, the dipole moment of a molecule is the vector sum of the dipole moments of various bonds.

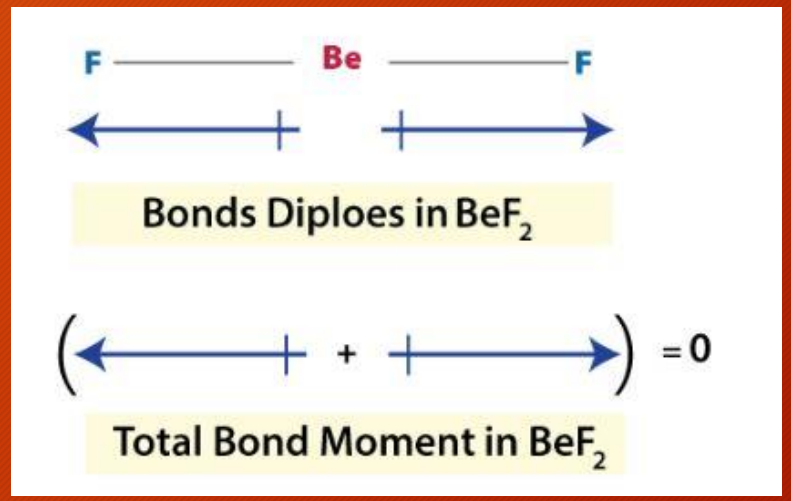


Dipole moment

- For example in H_2O molecule, which has a bent structure, the two O–H bonds are oriented at an angle of 104.50. Net Dipole moment, μ = 1.85 D is the resultant of the dipole moments of two O–H bonds.



- The dipole moment in case of BeF_2 is zero. This is because the two equal bond dipoles point in opposite directions and cancel the effect of each other.



Covalent character of ionic bond

- Just as all the covalent bonds have some partial ionic character, the ionic bonds also have partial covalent character. The partial covalent character of ionic bonds was discussed by Fajans.
- **Fajan's rule** : The cation polarises the anion, pulling the electronic cloud of anion toward itself and thereby increasing the electronic density between the two leading to the covalent character to the ionic bond.

(1) The smaller the size of the cation and the larger the size of the anion, the greater the covalent character of an ionic bond.

(2) The greater the charge on the cation, the greater the covalent character of the ionic bond.


THE-END