**Chemical Bonding and Molecular Structure**

**Chemical Bond:** It is the force which keeps atoms together in a molecule. The causes of formation of a chemical bond are:

* Tendency of atoms to complete their octets or duplets by rearrangement of their valence electrons (octet theory).
* The system acquires minimum energy when atoms are at some equilibrium distance where attractive forces dominate over repulsive forces.

**Types of Chemical Bonds:**

* Ionic bond
* Covalent bond
* Metallic bond
* Co-ordinate bond

**Ionic Bond:**

**a) Favourable conditions to form Ionic Bond:**

* Formed between electro positive element (group 1,2,13) and electro negative element (group 15,16,17)
* http://www.tutors4you.com/delta.jpgE.N >=2
* Lower I.E of one atom and high E.A of second atom
* Higher lattice energy
* Larger cations, smaller anions

**b) Properties:** Crystaline, stronger force of attraction, thermally stable, low volatality, high density, high melting point and boiling point, highly soluble in polar solvent, good conductor of electricity in molten or solution state, nondirectional bond.

**Covalent Bond:**

**a) Favourable conditions to form Covalent Bond:**

* Formed between two electronegative elements (group 14,15,16,17)
* http://www.tutors4you.com/delta.jpgE.N < 1.9
* Small cations, larger anions (Fajan's Rule)
* High charges on cation and anion (Fajan's Rule)
* Covalent bond is formed by sharing of electrons by two atoms to complete their octet or duplet

**b) Properties:**

* Compounds containing covalent bonds under normal condition of pressure and temperature exist as gases or liquids of low boiling point due to weak Vander Wall's force
* Relatively low melting point and boiling point, generally non-conductor, and soluble in non-polar solvent
* As the bond is rigid and directional, compounds with covalent bond show isomerism
* Covalency of the atom is equal to the number of covalent bonds formed by the atom

**Bond Length:** It is the average distance between the nuclei of two bonded atoms. It depends upon:

* Size of the atom: Bond length increases with increase in the size of atom (HI > HBr > HCl > HF)
* Multiplicity of bond: Bond length decreases with multiplicity of bond (C-C > C=C )
* Type of hybridisation: More s-character, shorter is the bond length, greater is the acidity with comparable compound

**Bond Energy:** It is the energy required to break one mole of bonds of a particular type of substance in gaseous state.

**Bond Angle:** It is the internal angle between the orbitals containing electron pairs in the valence shell of the central atom in a molecule:

* More the lone pairs on the central atom, smaller is the bond angle due to bp repulsion
* More electronegative the central atom, more is the bond angle
* More electronegative the surrounding atoms, lesser is the bond angle

**VBT:** Proposed by Heitler and London and extended by Pauling and State. The postulates are:

* Overlapping of atomic orbitals of valence shells of two atoms leads to the formation of a covalent bond
* Half filled orbital and opposite spin electrons are used
* http://www.tutors4you.com/symbolsigma.jpg- bond is formed by head on overlapping, http://www.tutors4you.com/symbolpie.jpg- bond is formed by lateral overlapping
* Greater the overlapping, stronger is the bond
* http://www.tutors4you.com/symbolsigma.jpg- bond is stronger than http://www.tutors4you.com/symbolpie.jpg- bond and http://www.tutors4you.com/symbolsigma.jpg- bond is directional while http://www.tutors4you.com/symbolpie.jpg- bond is non-directional
* The directon of the bond is the same as the direction of overlapping of orbitals
* The strength of http://www.tutors4you.com/symbolsigma.jpg- bond follows the order s -s < s - p < p - p
* Paired electrons are shifted to higher energy levels while forming a bond
* VBT cannot explain paramagnetic behaviour of O2

**Hybridization:**

* Number of hybrid orbitals = number of atomic orbitals intermixed
* Hybrid orbitals form http://www.tutors4you.com/symbolsigma.jpg-bond on overlapping
* It does not take place in and isolated atom. It occurs only during bond formation
* Hybrid orbitals tend to remain far apart therefore repulsion order is lp-lp>lp-bp>bp-bp
* Total number of hybrid orbitals of central atom = Number of its http://www.tutors4you.com/symbolsigma.jpg- bond pairs + Number of lone pair of electrons around the central atom
* Different types of hybridization are sp, sp2 , sp3 , sp3d ,sp3 d2 ,sp3 d3

**MOT:** The theory was developed by Hund & Mulliken. The basic postulates are:

* All atomic orbitals are mixed up to form molecular orbitals
* Total M.O = Total A.O
* Two A.O. combine to form tow M.Os. One is anti bonding M.O. and the other is bonding M.O.
* The filling up of electrons must follow Aufbau's principle., Pauli exclusion principle and Hund's rule.
* Bond order = (Nb - Na )/2 where Nb = Number of electrons in bonding M.O and Nb = Number of electrons in antibonding M.O
* Bond order http://www.tutors4you.com/sybolalpha.jpgBond energy http://www.tutors4you.com/sybolalpha.jpg1/Bond length

**Dipole Moment(µ):**

* Common in covalent compounds when formed between two dissimilar atoms
* Used to predict the extent of polarity in a molecule
* A vector quantity so follows vector addition or subtraction rule in predicting net dipole moment of a molecule
* Can predict the shape of molecules, H2 O - bent, BeF2 - linear

**Metallic Bond:**

**a) Favourable conditions to form Metallic Bond:**

* Formed between Electro positive ions packed in one of the 3 arrangements (1.CCP(or FCC), 2.HCP, 3 BCC)

**b) Properties:**

* Negatively charged electrons hold the ion together
* Highly conducting becauls the mobility of these electrons through the lattice
* High m.p and b.p
* If soluble, then soluble only in polar solvents of high dielectric constant

**Co-ordinate Bond:**

**a) Favourable conditions to form Metallic Bond:**

* One of the group or or atom must have a lone pair of electrons whereas the other must have the incomplete octet or duplet.
* Also known as dative bond

**b) Properties:**

* Intermediate between ionic and covalent compounds
* Sparingly soluble in water, not forming ions, largely soluble in non-polar solvents
* Melting and boiling points are higher than purely covalent compounds but less than purely ionic compounds
* Stable as covalent compounds, addition compounds are very stable
* Non conductor
* Bond is rigid and directional
* High value of dielectric constant

**Other Bonds:**

**a) H-bonding:** When H is attached to N, O, F

* It's strength is about one tenth of a covalent bond
* Small size and high electronegativity of atoms forms a strong H-bond
* They are of twor types; intermolecular (between two molecules) and intramolecular (within a molecule)
* Used to predict boiling point and density of water, solubility of alcohols and carboxylic acids in water.

**b) Dipole-dipole interactions:**

* These exist between molecules having permanent dipoles e.g. H-Cl, I-F etc

**c) Ion-dipole interactions:**

* Between and ion and a polar molecule eg hydration of ions like Na+ , Mg2+ etc
* Smaller the ion, more the dipole moment, stronger will be these interactions

**d) Ion-induced dipole interactions:**

* Between an Ion and a dipole induced by the ion in a nonpolar molecule

**e) Dipole-induced dipole interactions:**

* Between a dipole and and induced dipole in a non polar molecule

**f) Dispersion forces:**

* Between two nonpolar substances. The forces are between an instantaneous dipole and and induced dipole eg in O2 , N2 , He, Ne, Ar etc

**Note:** Dipole-dipole, dipole-induced dipole and dispersion forces are called Van der Wall's forces