

JEE Main Chemistry

Short Notes

Chemical Bonding and Molecular Structure-II

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Chemical Bonding and Molecular Structure

1. Quantum Mechanical approach to Covalent Bonding

Valence Bond Theory:

The valence bond theory was introduced by Heitler and London in 1927. Later on this theory was further developed by Pauling. This theory is based on the concept of atomic orbitals, overlapping of the atomic orbitals, and electronic configuration of the elements and hybridization of the orbitals. A chemical bond is formed due to the overlapping of the atomic orbitals. This is because of the overlapping, the electrons remain localized in the region where the bond is formed. The theory that explains about the bonding caused between two atoms due to the overlapping of the half-filled valence shell atomic orbitals and the sharing of an electron which results in the filling up of the orbitals is called as the valence bond theory.

Valence bond theory depends mainly on

- Overlapping theory
- Hybridization theory
-

Overlapping theory:

The overlapping theory depends on some important points which are cited below:

- Overlapping of the half-filled valence shell orbitals of the two atoms give rise to covalent bond.
- The bond that forms possess a pair of electrons with opposite spin in order to acquire stability.
- The orbitals possess directional character.
- More is the overlapping of the orbitals, more is the bond strength.
- The extent of overlapping is more in co-axial overlapping and less in collateral overlapping.
- A decrease in bond strength is observed with increasing value of 'n'.
So, $1s-2p > 2s-2p > 3s-3p$ and if 'n' possess the same value then, $2p-2p > 2s-2p > 2s-2s$.
- Sigma bond, pi bond and delta bonds are formed as a result of overlapping.

Sigma bond	Pi bond
<ol style="list-style-type: none">1. The axial overlapping of atomic orbitals forms a sigma(σ) bond.2. σ-bond formation involves overlapping of s-s, s-p and p-p orbitals.3. σ-bond is stronger because of larger extent of overlapping.4. Free rotation exists around a σ-bond.5. A sigma bond is present either alone or along with a π-bonds.6. In σ-bond there is the involvement of hybridised or unhybridised orbitals.	<ol style="list-style-type: none">1. The sidewise overlapping of atomic orbitals forms pi bond.2. It involves overlapping of p-p orbitals.3. Smaller extent of overlapping makes π-bond relatively weaker.4. Free rotation does not exist around π bonds.5. π-bond is always present along with a sigma-bond or along with π-bonds.6. In π-bond there is no involvement of hybridised orbitals.

Delta bond(δ) bond :



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The bond formed due to the lateral overlapping of all the four lobes of d orbital except the d_z^2 with another four lobes of d orbital is termed as the delta bond.

Hybridisation theory:

This theory was put forward by Slater and Pauling. The theory explains about the similar nature of covalent bonds in a molecule.

Hybridisation:

Hybridisation refers to the mixing of orbitals having different shapes and approximately equal energy where redistribution of energy takes place to form new orbitals possessing the same energy and shape.

Characteristics :

- It involves mixing of orbitals, not electrons.
- The new hybrid orbitals formed is equal to the number of atomic orbitals that takes part in hybridization.
- The hybrid orbitals consist of two lobes , one smaller and the other larger .The larger lobe forms a bond.
- The number of hybrid orbitals formed is equal to the number of sigma bonds and lone pair of electrons present.
- The order of directional properties of hybrid orbitals is: $sp < sp^2 < sp^3 < sp^3d < sp^3d^2 < sp^3d^3$
- Hybridized orbitals always form sigma bonds.


Types of hybridization:

sp hybridization	sp^2 hybridization	sp^3 hybridization	sp^3d hybridization	sp^3d^2 hybridization
one s and one p orbital mixes to form two new hybrid orbitals.	one s and two p orbitals mixes to form three new hybrid orbitals.	one s and three p orbitals mixes to form four new hybrid orbitals.	one s , three p and one d orbital mixes to form five new hybrid orbitals.	one s ,three p and two d orbital mixes to form six new hybrid orbitals.
s character in sp orbital =50%	s character in sp^2 orbital =33.3%	s character in sp^3 orbital =25%	s character in sp^3d orbital =20%	s character in sp^3d^2 orbital =16.67%
bond angle =180	bond angle =120	bond angle = 109	bond angle between three hybrid orbitals is 120 and that between two hybrid orbitals is 90	bond angle =90

Resonance:

Resonance is the phenomenon of describing a molecule accurately by a number of structures similar to the canonical structures of the hybrid orbitals possessing similar energy, position of nuclei, bonding and non-bonding pairs of electrons. Resonance provides stability to the molecule. This is because the energy of the resonance hybrid is less than that of a single canonical structure.

2. Molecular Orbital Theory :



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The MOT was proposed by Hund and Mullikan. According to this theory, two atomic orbitals come closer to each other and undergo overlapping to form two molecular orbitals. The combination of atomic orbitals gives rise to bonding and antibonding molecular orbitals respectively. The energy of the bonding molecular orbitals is greater than that of the antibonding molecular orbitals. Electrons in the orbitals are filled according to Aufbau's principle.

Formation of LCAO and Types of Molecular Orbitals:

Linear combination of atomic orbitals is a method used in quantum chemistry to calculate the molecular orbitals. In this method superimposition of the atomic orbitals takes place which leads to constructive and destructive interference. The constructive interference gives rise to bonding molecular orbitals whereas the destructive interference forms antibonding molecular orbital.

Conditions for Linear Combination of Atomic Orbitals (LCAO):

- The atomic orbitals that combine must possess almost equal energy.
- The symmetry of the combining atomic orbitals must be same.
- Extent of overlapping of the combining orbitals should be maximum.

Types of molecular orbitals:

The molecular orbitals of diatomic molecules are designated by sigma, pi and delta. The sigma molecular orbitals are symmetrical whereas the pi molecular orbitals are unsymmetrical. If the internuclear axis is assumed to be in the z direction, a linear combination of the 2pz orbitals of the atoms forms $2\sigma_p$ and σ^*2p_z . Moreover the presence of positive and negative lobes above and below the molecular plane makes the molecular orbitals of $2p_x$ and $2p_y$ unsymmetrical.

Electronic Configuration of Diatomic Molecules :

The order of energy in molecular orbitals of diatomic molecule is as:

- For H_2 to N_2
 $\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < n2p_x = n2p_y < \sigma 2p_z < n^* 2p_x = n^* 2p_y < \sigma^* 2p_z$
- For O_2 and F_2
 $\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_z < n2p_x = n2p_y < n^* 2p_x = n^* 2p_y < \sigma^* 2p_z$

σ^* , n^* are the antibonding orbitals and σ , n are the bonding orbitals.

$$\text{Bond order} = (N_b - N_a) / 2$$

N_b = number of electrons in bonding molecular orbital

N_a = number of electrons in nonbonding molecular orbitals.

If the value of bond order is 0, the species does not exist and the bond order value of 1,2,3 denotes single, double and triple bonds respectively.

Paramagnetic and Diamagnetic Behavior of Molecules:

Presence of unpaired electrons in a molecule means that the species is of paramagnetic nature and the presence of paired electrons means that the species is diamagnetic.

Concept of Bond Order, Bond Length and Bond Energy:

An increase in bond order increases the bond energy which further increases the stability and decreases the bond length of the molecule.

Formation of Hydrogen Bonding and its applications:

Hydrogen bond:



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The bond which is formed due to the linking of a hydrogen atom covalently with a strongly electronegative atom which may result in weak attraction with another electronegative atom in the same or different molecule is termed as the hydrogen bond. A broken line represents a hydrogen bond.

Conditions for the formation of hydrogen bonds:

- A highly electronegative atom attached to a hydrogen bond must be present in the molecule.
- The electronegative atom must be of smaller size. Smaller is the size, more is the force of attraction.

Effects of hydrogen bonding:

- Association of molecules is possible due to hydrogen bonding.
- Melting and boiling point of the molecules increases due to hydrogen bonding.
- Increase in viscosity and surface tension is observed due to hydrogen bonding.

Types of hydrogen bonding:

- Intermolecular hydrogen bonding: This type of hydrogen bonding occurs between two molecules. In such molecules, boiling and melting point are high.
- Intramolecular hydrogen bonding: This type of hydrogen bonding occurs within a molecule and such a bonding is also known as chelation. Melting and boiling point of such molecules decreases.

Applications of hydrogen bonding:

- DNA strands are held together by hydrogen bonds.
- Cleaning action of soaps and detergents
- In clothing material

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