Inorganic Chemistry Paper - III

B.Sc Part-II, Group-B - 3

Valence bond Theory approach for Complex Compound

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Lecture Notes Series :-

Valance Bond theory

Valence bond theory is a Modern theory to explain the bonding and Properties of Coordination compound or complex compounds.

In 1931 Pauling (1931) Introduced this theory hence, It is also Known as Pauling's theory, based on revolutionary idea of hybridisation. According to him strong bonds are formed not by pure S-orbital or by pure P-Orbitals alone. but by a suitable combination of these two or three or More Known as hybrid orbitals. Thus with the combination of one S-orbital and three P-orbitals we obtain four equivalent hybrid orbitals sp^3 which are directed towards the four corners of a regular tetrahedron. This is known as sp^3 hybridisation. Besides this in complexes dsp^2 (Square Planar) and d^2sp^3 (octahedral) hybridisation are very common.

It has been observed that transition Metal atoms are capable of forming complex compounds. According to Pauling in such a State normal

is broken and new hybrid orbitals are formed. Hence we can get 4 or 6 or higher equivalent orbitals according to the number of vacant orbitals. Here different type of hybridisation have been discussed with their characteristic

Important feature of valence bond Theory.

(i) The central metal atom or ion provides hybrid orbitals as required by the ligands i.e coordination no to form complex.

(ii) Each ligand has at least one s-orbitals having the pair of electrons.

(iii) The lone pair of electrons of the ligand overlap with the empty hybrid orbital of the metal ions or atoms.

(iv) If d-orbitals are involved in the hybridisation that may be either inner viz (n-1) d-orbitals or the outer viz (n)-orbitals. The complexes formed in these two ways are known as low spin and high spin complexes respectively.

(v) If the complex does not contain unpaired electron is called diamagnetic while the complex having one or more unpaired electron is called Paramagnetic while

Illustration :- We discuss valence bond theory by taking some examples of metal co-ordination compounds. In these cases the orbitals are designated by squares and electrons are indicated by arrows.

In transition metal atoms d-electrons levels are partly filled, hence it is the number of d-electron in the central atom (forming complex) that determines the possible modes of hybridisation and the shape of the complex (octahedral, square planar or tetrahedral)

In complex formation Hund's rule of maximum multiplicity is strictly followed i.e. as many orbitals are singly occupied as possible before any pairing occurs. In complex formation redistribution of electrons and complete pairing takes places. In this way some orbitals are vacated and made available for hybridisation.

1. Octahedral complexes

Such complexes are most common and have been studied most extensively. Let us consider the formation of $[Fe(CN)_6]^{4-}$ complex ion. The electronic configuration of Fe atom is $1s^2, 2s^2, 2p^6, 3s^2, 3p^6 3d^{10}, 4s^2$ or the ferrous ion or the ferrous ion (Fe^{2+}) has $3d^6$ configuration.

When six CN^- ions approach to ferrous ion to form $[Fe(CN)_6]^{4-}$ complex ion. The pairing of electrons takes place (since CN^- ion is a strong ligand hence pairing is possible) in this way two empty orbitals are available for hybridisation.

Now d^2sp^3 hybridisation takes place in the ferrous ion which provides six equivalent d^2sp^3 hybrid orbitals to forms $[Fe(CN)_6]^{4-}$ ion as shown below.

Ground state configuration of Fe —

3d					4s	4p		
↑↓	↑	↑	↑	↑	↑↓			

Ground state configuration of Fe^{2+}

3d					4s	4p		
↑↓	↑	↑	↑	↑				

Due to strong ligand 3d electrons paired opposite hunds rule.

3d					4s	4p		
↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

Fe^{2+} having gained six electrons pairs in $[Fe(CN)_6]^{4-}$

d^2sp^3 hybridisation

CN CN CN CN CN CN

Each one has to find his peace from within. And peace to be real must be unaffected by outside circumstances

$[Fe(CN)_6]^{4-}$