SRI YERRAMILLI NARAYANA MURTHY

Re-Accredited by NAAC with 'A' grade collage with CGPA of 3.41

Narsapur-534275 West Godavari District

DEPARTMENT OF CHEMISTRY

A Project work on

" Valency Bond Theory "

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Submitted to :- D. Suresh sir

Department of chemistry

Submitted by:-

K. Divya sri 3rd Bsc. CBM

N. Sri Latha 3rd Bsc. CBM

D. Jahanavi 3rd Bsc. CBM

Md. Ayesha Fathima 3rd Bsc. CBM

J. Priyanka 3rd Bsc .CBM

VALENCE BOND THEORY

In the valence bond (VB) theory, proposed in large part by the American scientists Linus Pauling and John C. Slater, bonding is accounted for in terms of hybridized orbitals of the... The basis of VB theory is the Lewis concept of the electron-pair bond.

Many approaches have been put forth to explain the nature of bonding in coordination compounds. One of them is the Valence Bond (VB) Theory. The Valence Bond Theory was developed in order to explain chemical bonding using the method of quantum mechanics. This theory primarily focuses on the formation of individual bonds from the atomic orbitals of the participating atoms during the formation of a molecule.

According to the valence bond theory,

Electrons in a molecule occupy atomic orbitals rather than molecular orbitals. The atomic orbitals overlap on the bond formation and the larger the overlap the stronger the bond.

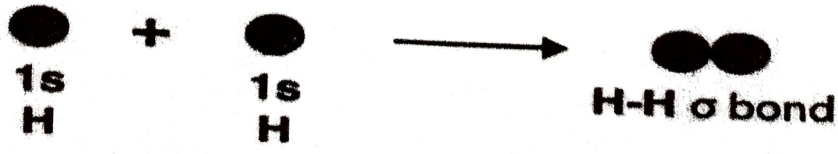
The metal bonding is essentially covalent in origin and metallic structure involves resonance of electron-pair bonds between each atom and its neighbors.

History of valence bond theory :

The Lewis approach to chemical bonding failed to shed light on the formation of chemical bonds. Also, valence shell electron pair repulsion theory (or VSEPR theory) had limited applications (and also failed in predicting the geometry corresponding to complex molecules).

In order to address these issues, the valence bond theory was put forth by the German physicists Walter Heinrich Heitler and Fritz Wolfgang London. The Schrodinger wave equation was also used to explain the formation of a covalent bond between two hydrogen atoms. The chemical bonding of two hydrogen atoms as per the valence bond theory is illustrated below.

This theory focuses on the concepts of electronic configuration, atomic orbitals (and



their overlapping) and the hybridization of these atomic orbitals. Chemical bonds are formed from the overlapping of atomic orbitals wherein the electrons are localized in the corresponding bond region.

The valence bond theory also goes on to explain the electronic structure of the molecules formed by this overlapping of atomic orbitals. It also emphasizes that the nucleus of one atom in a molecule is attracted to the electrons of the other atoms.

Postulates of Valence Bond Theory

The important postulates of the valence bond theory : *are listed below.*

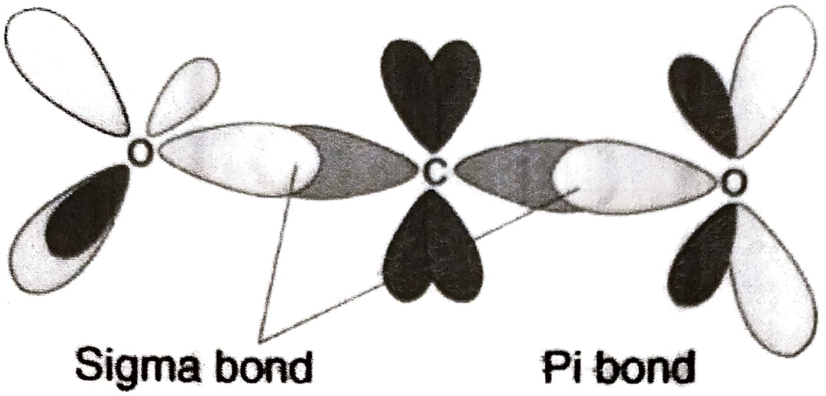
Covalent bonds are formed when two valence orbitals (half-filled) belonging to two different atoms overlap on each other. The electron density in the area between the two bonding atoms increases as a result of this overlapping, thereby increasing the stability of the resulting molecule.

The presence of many unpaired electrons in the valence shell of an atom enables it to form multiple bonds with other atoms. The paired electrons present in the valence shell do not take participate in the formation of chemical bonds as per the valence bond theory.

Covalent chemical bonds are directional and are also parallel to the region corresponding to the atomic orbitals that are overlapping.

Sigma bonds and pi bonds differ in the pattern that the atomic orbitals overlap in, i.e. pi bonds are formed from sidewise overlapping whereas the overlapping along the axis containing the nuclei of the two atoms leads to the formation of sigma bonds.

The



Formation of Sigma and Pi Bonds – Valence Bond Theory (VBT)

formation of sigma and pi bonds is illustrated below.

It can be noted that sigma bonds involve the head-to-head overlapping of atomic orbitals whereas pi bonds involve parallel overlapping.

Number of orbitals and types of hybridization :

According to VBT theory the metal atom or ion under the influence of ligands can use its (n-1)d, ns, np, or ns, np, nd orbitals for hybridization to yield a set of equivalent orbitals of definite geometry such as octahedral, tetrahedral planar and so on. These hybrid orbitals are allowed to overlap with ligand orbitals that can donate electron pairs for bonding.

Coordination Number	Type of Hybridisation	Distribution of Hybrid Orbitals in Space
4	sp^3	Tetrahedral
4	dsp^2	Square planar
5	sp^3d	Trigonal bipyramidal
6	sp^3d^2	Octahedral
6	d^2sp^3	Octahedral

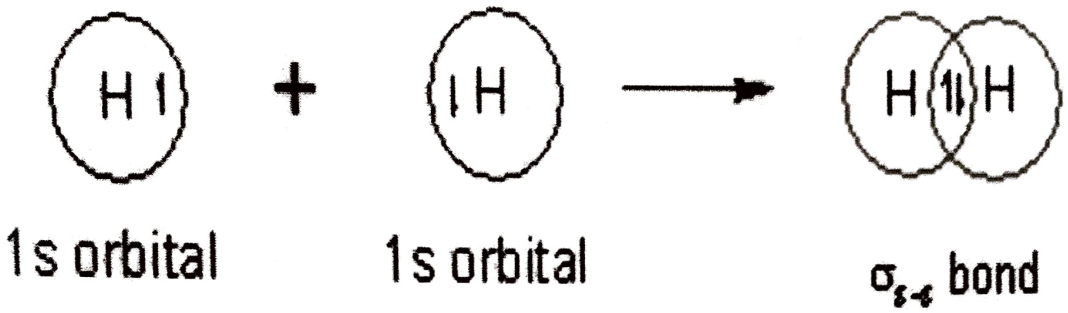
BONDING IN MOLECULES EXPLAINED BY VALENCE BOND THEORY

1) H2 molecule:

**** The electronic configuration of hydrogen atom in the ground state is 1s1.***

**** In the formation of hydrogen molecule, two half filled 1s orbitals of hydrogen atoms overlap along the inter-nuclear axis and thus by forming a σs-s bond.***

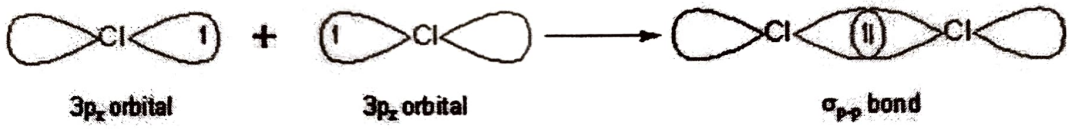
h2 molecule



2) Cl2 molecule:

**** The electronic configuration of Cl atom in the ground state is [Ne]3s2 3px2 3py2 3pz1.***

**** The two half filled 3pz atomic orbitals of two chlorine***



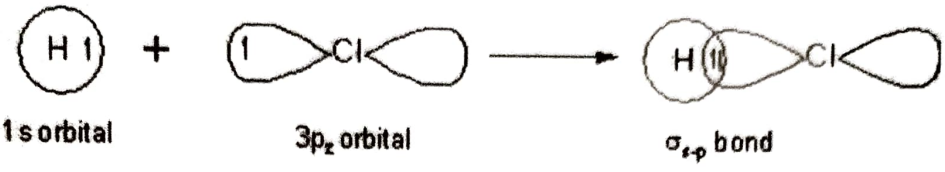
atoms overlap along the inter-nuclear axis and thus by forming a σp-p bond.cl2 molecule .

3) HCl molecule:

**** In the ground state, the electronic configuration of hydrogen atom is 1s1.***

**** And the ground state electronic configuration of Cl atom is [Ne]3s2 3px2 3py2 3pz1.***

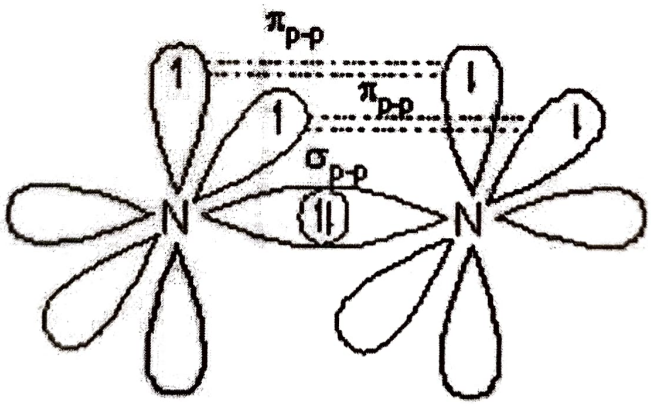
** The half filled 1s orbital of hydrogen overlap with the half filled 3pz atomic orbital of chlorine atom along the inter-nuclear axis to form a σs-p bond.*



4.N2 molecule:

** The ground state electronic configuration of N is [He] 2s2 2px1 2py1 2pz1.*

** A σp-p bond is formed between two nitrogen atoms due to overlapping of half filled 2px atomic orbitals along the inter-nuclear axis.*



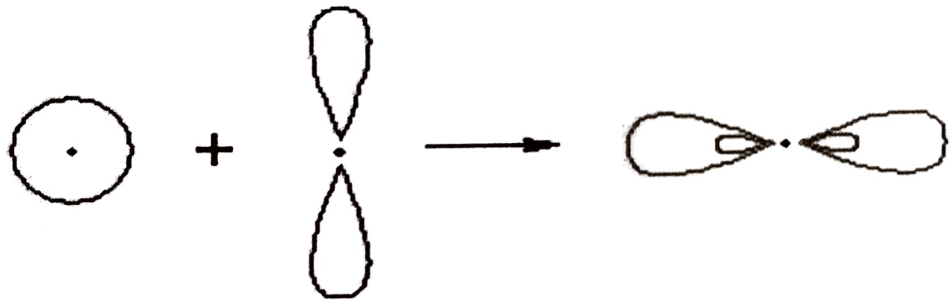
** The remaining half filled 2py and 2pz orbitals form two πp-p bonds due to lateral overlapping. Thus a triple bond (one and two) is formed between two nitrogen atoms.*

1.sp hybridization ;

** Intermixing of one 's' and one 'p' orbitals of almost equal energy to give two identical and degenerate hybrid orbitals is called 'sp' hybridization.*

** These sp-hybrid orbitals are arranged linearly at by making 180o of angle.*

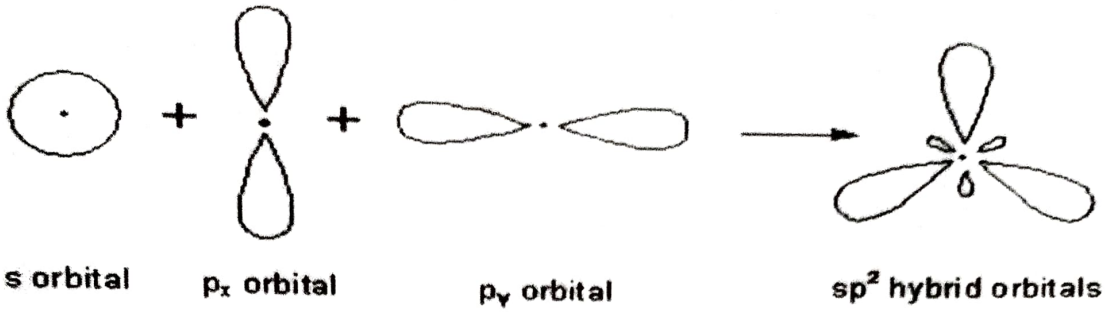
** They possess 50% 's' and 50% 'p' character.*



2.sp2 hybridization ;

** Intermixing of one 's' and two 'p' orbitals of almost equal energy to give three identical and degenerate hybrid orbitals is known as sp2 hybridization.*

** The three sp2 hybrid orbitals are oriented in trigonal planar symmetry at angles of 120o to each other.*



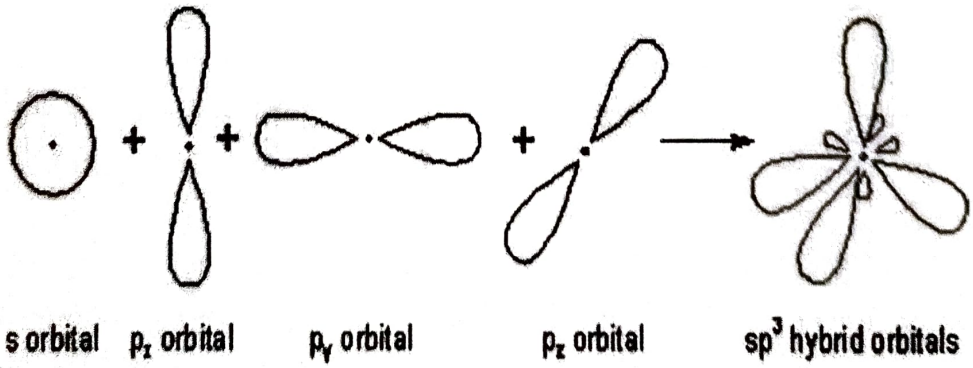
**** The sp2 hybrid orbitals have 33.3% 's' character and 66.6% 'p' character.***

3.sp3 hybridization :

**** In sp3 hybridization, one 's' and three 'p' orbitals of almost equal energy intermix to give four identical and degenerate hybrid orbitals.***

**** These four sp3 hybrid orbitals are oriented in tetrahedral symmetry with 109o28' angle with each other.***

**** The sp3 hybrid orbitals have 25% 's' character and 75% 'p' character.***

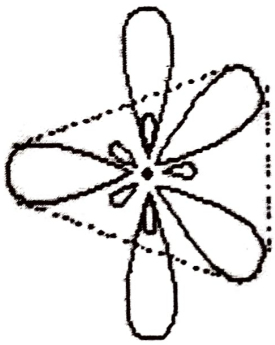


4.sp3d hybridization :

** In sp3d hybridization, one 's', three 'p' and one 'd' orbitals of almost equal energy intermix to give five identical and degenerate hybrid orbitals, which are arranged in trigonal bipyramidal symmetry.*

Among them, three are arranged in trigonal plane and the remaining two orbitals are present above and below the trigonal plane at right angles.

** The sp3d hybrid orbitals have 20% 's', 60% 'p' and 20% 'd' characters.*



sp^3d hybrid orbitals

Applications of Valence Bond Theory :

- *The maximum overlap condition which is described by the valence bond theory can explain the formation of covalent bonds in several molecules.*
- *This is one of its most important applications. For example, the difference in the length and strength of the chemical bonds in H2 and F2 molecules can be explained by the difference in the overlapping orbitals in these molecules.*
- *The covalent bond in an HF molecule is formed from the overlap of the 1s orbital of the hydrogen atom and a 2p orbital belonging to the fluorine atom, which is explained by the valence bond theory.*

Limitations of valence bond theory:

- *The shortcomings of the valence bond theory include*

- *Failure to explain the tetravalency exhibited by carbon.*

- No insight offered on the energies of the electrons.
- The theory assumes that electrons are localized in specific areas.
- It does not give a quantitative interpretation of the thermodynamic or kinetic stabilities of coordination compounds.
- No distinction between weak and strong ligands.
- No explanation for the colour exhibited by coordination compounds.