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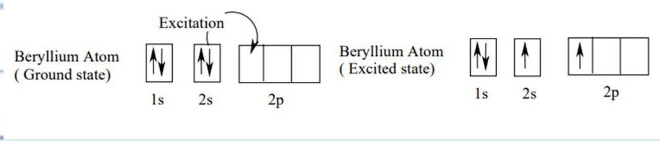
Modern Theories of Chemical Bonding

I. Valence Bond Theory (VBT)

VBT can be understood by the concept of hybridisation of orbitals. According to this two or more than two non-equivalent orbitals (having different energies and shapes) of comparable energies mix or hybridize and give rise to an equal number of equivalent (same energies and shapes) hybrid orbitals. For example, beryllium chloride (triatomic molecule ($BeCl_2$). The electronic configuration of

Be: $1s^2 2s^2$; Cl: $1s^2\ 2s^2 2p^6 3s^2 3p^5$



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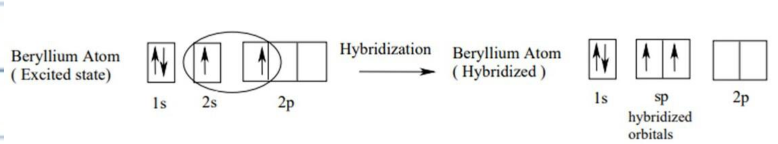
To form bonds with two Cl atoms, the valence electrons of Be atom must overlap with the 2p electrons of the two Cl atoms. Since the valence shell of Be atom contains both the electrons in the same orbital (i.e., 2s) it cannot overlap with the 2p orbital of Cl atoms containing 5 electrons. In the process of bond formation, an electron from the 2s orbital of Be atom gets momentarily excited to the empty 2p orbital as shown below.



Now the two valence electrons are in two singly occupied orbitals which can overlap with the 1s orbitals of the two hydrogen atoms and form two bonds. In case of $BeCl_2$ the two singly occupied orbitals (2s and 2p) hybridize to give two sp-hybrid orbitals. This is called **sp- hybridisation**. These hybrid orbitals lie along the z- direction and point in opposite directions.

Modern Theories of Chemical Bonding

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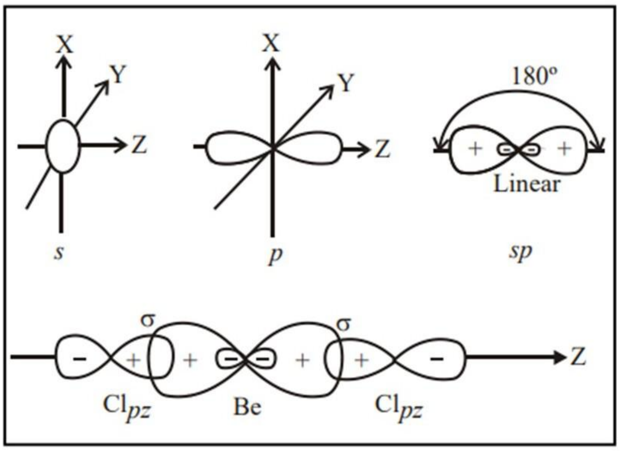
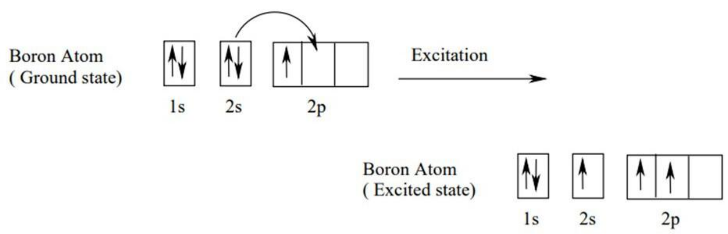
These hybrid orbitals can now overlap with the 2p orbitals of Cl atoms to give the linear molecule of $BeCl_2$. as shown in Figure below

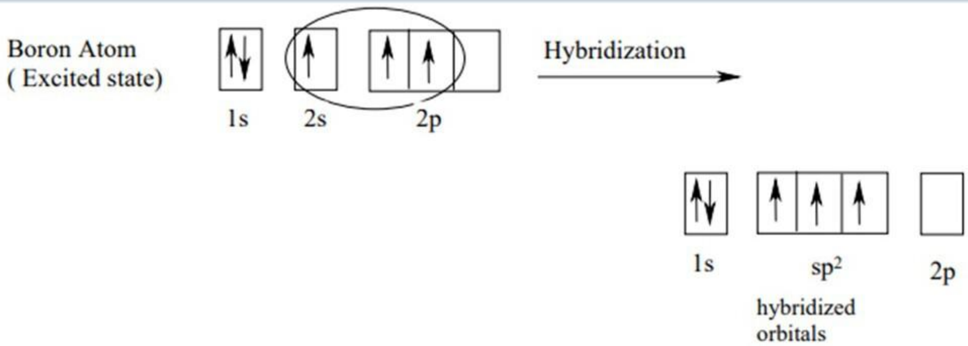


Eg 2. Boron trichloride, BF_3 (sp^2 hybridisation) :There are three electrons in the valence shell of B atom. In order to form bonds with three F atoms one of the electrons from the 2s orbital of boron atom is excited to its 2p orbital.

B: $1s^2 2s^2\ 2p^1$; F: $1s^2\ 2s^2 2p^5$

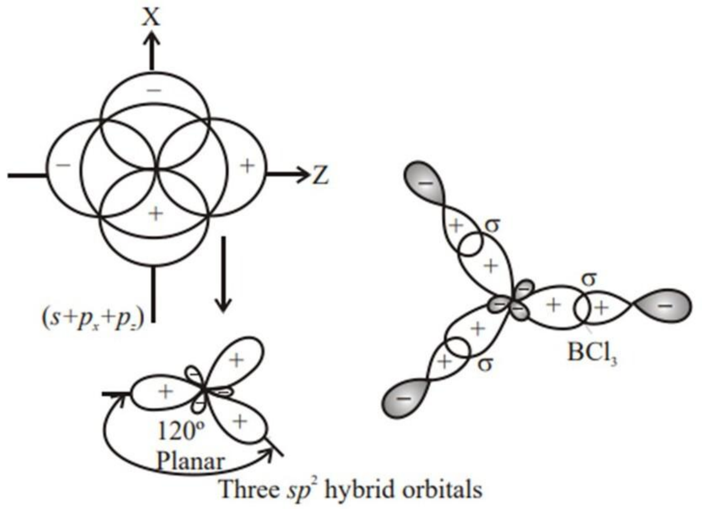


One 2s orbital and two 2p orbitals hybridise to give three sp2 hybridized orbitals. This is called **sp^2- hybridisation**.



Modern Theories of Chemical Bonding

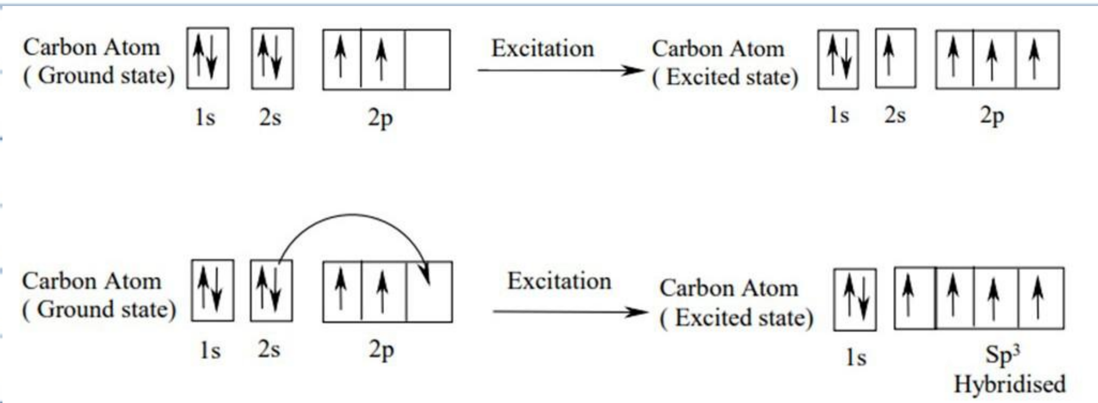
The three hybridized orbitals are coplanar and directed towards the corners of an equilateral triangle. These hybrid orbitals then form bonds with the p -orbitals of F atoms as shown below



Eg3. Methane, CH_4 (sp^3 hybridisation)

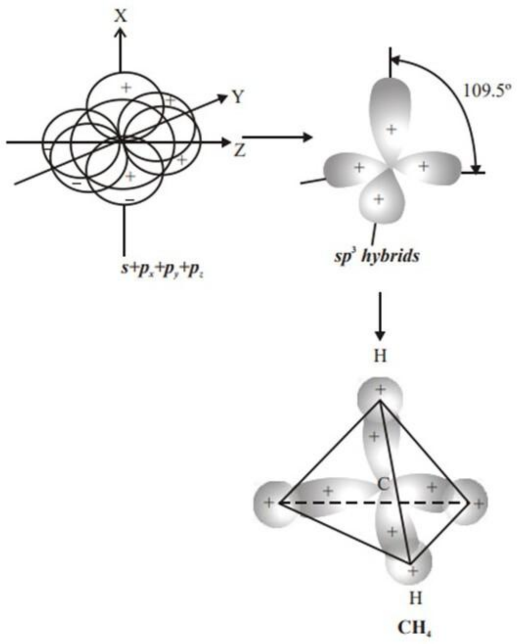
Electronic configuration H: $1s^1$; C:$1s^2 2s^2 2p^2$

In order to form bonds with four H atoms one of the electrons from the 2s orbital of C atom is excited to the 2p orbital. One 2s orbital and three 2p orbitals of the C atom then hybridize to give four sp^3 hybridized orbitals. This is called sp^3- hybridisation.



Modern Theories of Chemical Bonding

These four sp^3 hybrid orbitals are directed towards the corners of a regular tetrahedron. These hybrid orbitals then form bonds with the 1s orbitals of H atoms to give a CH_4 molecule as shown below

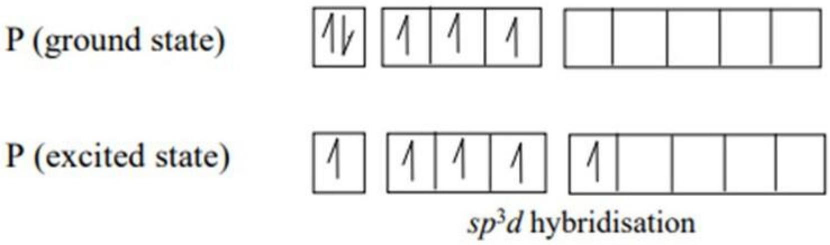


Eg4. Phosphorus pentachloride, PCl_5 (sp^3d hybridisation)

Electronic configuration P: $1s^2 2s^2 2p^6 3s^2 3p^3\ 3d^0$; Cl: $1s^2 2s^2 2p^6 3s^2 3p^5$

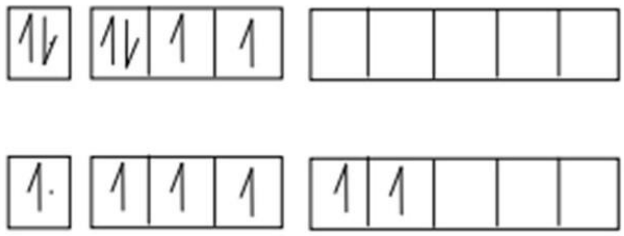
Five sp^3d hybrid orbitals are formed which are directed towards the corners of a trigonal bipyramidal. These orbitals overlap with singly filled p-orbitals of five Cl atoms and five bonds are formed. Thus PCl_5 molecule has a trigonal bipyramidal geometry.

Three P–Cl bonds (equatorial) make an angle of 120° with each other and lie in one plane. The other two P–Cl bonds (axial) are at 90° to the equatorial plane, one lying above and the other lying below the plane.



Modern Theories of Chemical Bonding

Eg.5. SF_6 (sp^3d^2 hybridisation):



sp^3d^2 hybridisation

Six sp^3d^2 hybrid orbitals are formed which are directed towards the corners of a regular octahedron. These orbitals overlap with singly filled orbitals of six F atoms and form sigma bonds giving a regular octahedral geometry.