Evaluate Yourself

6) Arrange the following in the decreasing order of Bond angle

i) CH_4, H_2O, NH_3 ii) C_2H_2, BF_3, CCl_4

10.7 Valence Bond Theory

Heitler and London gave a theoretical treatment to explain the formation of covalent bond in hydrogen molecule on the basis of wave mechanics of electrons. It was further developed by Pauling and Slater. The wave mechanical treatment of VB theory is beyond the scope of this textbook. A simple qualitative treatment of VB theory for the formation of hydrogen molecule is discussed below.

Consider a situation wherein two hydrogen atoms (H_a and H_b) are separated by infinite distance. At this stage there is no interaction between these two atoms and the potential energy of this system is arbitrarily taken as zero. As these two atoms approach each other, in addition to the electrostatic attractive force between the nucleus and its own electron (purple arrows), the following new forces begins to operate.

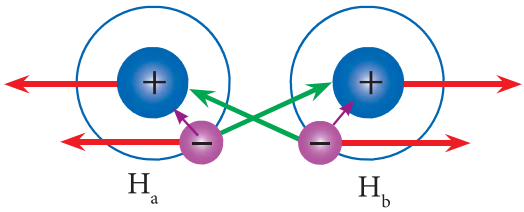


Fig 10. 17 (a) VB theory for the formation of hydrogen molecule

The new attractive forces (green arrows) arise between

(i) nucleus of H_a and valence electron of H_b

(ii) nucleus of H_b and the valence electron of H_a.

The new repulsive forces (red arrows) arise between

(i) the nucleus of H_a and H_b

(ii) valence electrons of H_a and H_b.

The attractive forces tend to bring H_a and H_b together whereas the repulsive forces tends to push them apart. At the initial stage, as the two hydrogen atoms approach each other, the attractive forces are stronger than the repulsive forces and the potential energy decreases. A stage is reached where the net attractive forces are exactly balanced by repulsive forces and the potential energy of the system acquires a minimum energy.

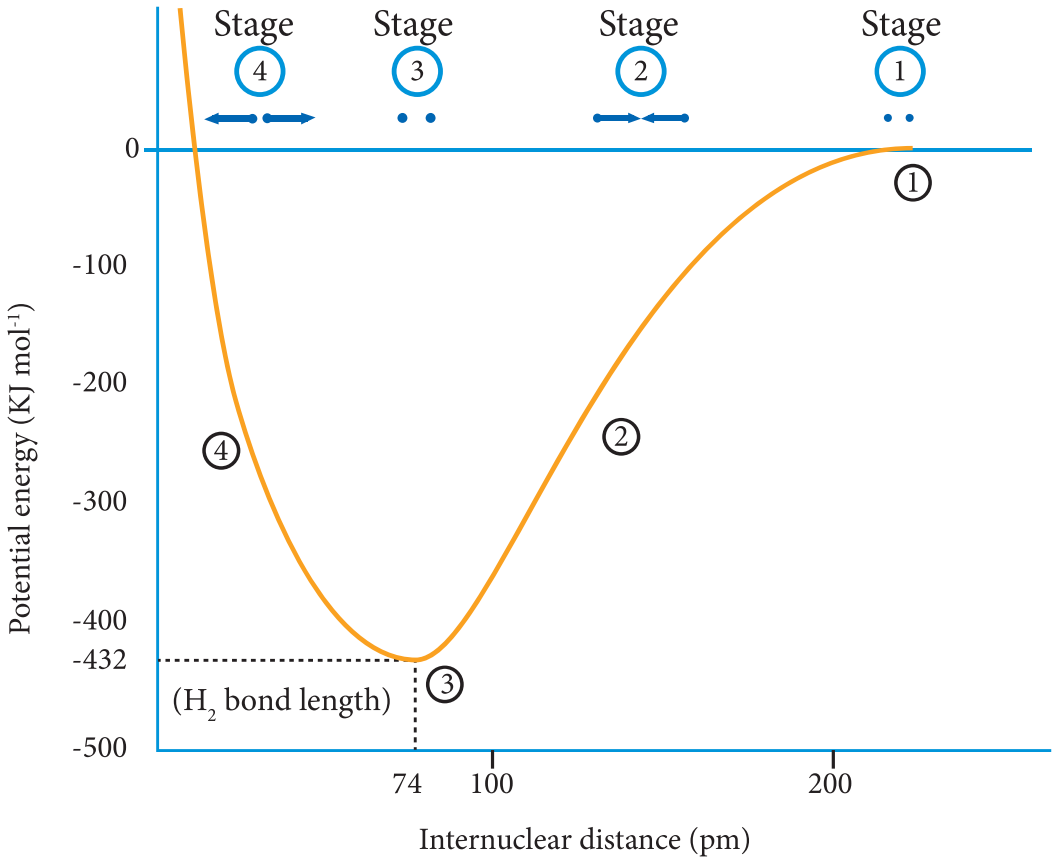


Fig 10. 17 (b) VB theory for the formation of hydrogen molecule

At this stage, there is a maximum overlap between the atomic orbitals of H_a and H_b, and the atoms H_a and H_b are now said to be bonded together by a covalent bond. The internuclear distance at this stage gives the H-H bond length and is equal to 74 pm. The liberated energy is 436 kJ mol^{-1} and is known as bond energy. Since the energy is released during the bond formation, the resultant molecule is more stable. If the distance between the two atoms is decreased further, the repulsive forces dominate the attractive forces and the potential energy of the system sharply increases

10.7.1 Salient features of VB Theory:

(i) When half filled orbitals of two atoms overlap, a covalent bond will be formed between them.

(ii) The resultant overlapping orbital is occupied by the two electrons with opposite spins. For example, when H_2 is formed, the two 1s electrons of two hydrogen atoms get paired up and occupy the overlapped orbital.

(iii) The strength of a covalent bond depends upon the extent of overlap of atomic orbitals. Greater the overlap, larger is the energy released and stronger will be the bond formed.

(iv) Each atomic orbital has a specific direction (except s-orbital which is spherical) and hence orbital overlap takes place in the direction that maximizes overlap

Let us explain the covalent bond formation in hydrogen, fluorine and hydrogen fluoride using VB theory.

10.8 Orbital Overlap

When atoms combines to form a covalent molecule, the atomic orbitals of the combining atoms overlap to form a covalent bond. The bond pair of electrons will occupy the overlapped region of the orbitals. Depending upon the nature of overlap we can classify the covalent bonding between the two atoms as sigma (σ) and pi (π) bonds.

10.8.1 Sigma and Pi bonds

When two atomic orbitals overlap linearly along the axis, the resultant bond is called a sigma (σ) bond. This overlap is also called 'head-on overlap' or 'axial overlap'. Overlap involves an s orbital (s-s and s-p overlaps) will always result in a sigma bond as the s orbital is spherical. Overlap between two p orbitals along the molecular axis will also result in sigma bond formation. When we consider x-axis as molecular axis, the p_x-p_x overlap will result in σ-bond.

When two atomic orbitals overlaps sideways, the resultant covalent bond is called a pi (π)bond. When we consider x-axis as molecular axis, the p_y-p_y and p_z-p_z overlaps will result in the formation of a π-bond.

Following examples will be useful to understand the overlap:

10.8.2 Formation of hydrogen (H_2) Molecule

Electronic configuration of hydrogen atom is $1s^1$

During the formation of H_2 molecule, the 1s orbitals of two hydrogen atoms containing one unpaired electron with opposite spin overlap with each other along the internuclear axis. This overlap is called s-s overlap. Such axial overlap results in the formation of a σ-covalent bond.

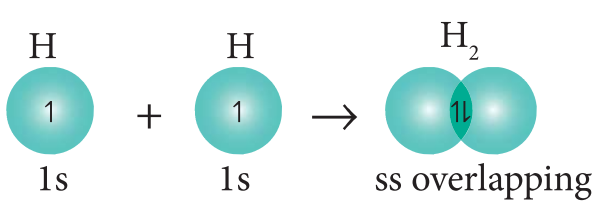


Fig 10. 18 Formation of hydrogen molecule

Formation of fluorine molecule (F_2):

Valence shell electronic configuration of fluorine atom : $2s^2\ 2p_x^2, 2p_y^2, 2p_z^1$

When the half filled p_z orbitals of two fluorine overlaps along the z-axis, a σ-covalent bond is formed between them.

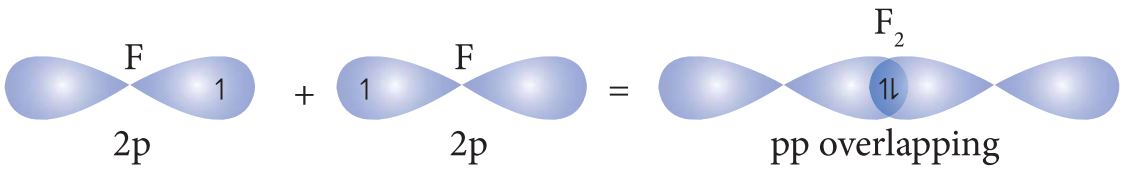


Fig 10. 19 Formation of F_2 Molecule

Formation of HF molecule:

Electronic configuration of hydrogen atom is $1s^1$

Valence shell electronic configuration of fluorine atom : $2s^2\ 2p_x^2, 2p_y^2, 2p_z^1$

When half filled 1s orbital of hydrogen linearly overlaps with a half filled $2p_z$ orbital of fluorine, a σ-covalent bond is formed between hydrogen and fluorine.

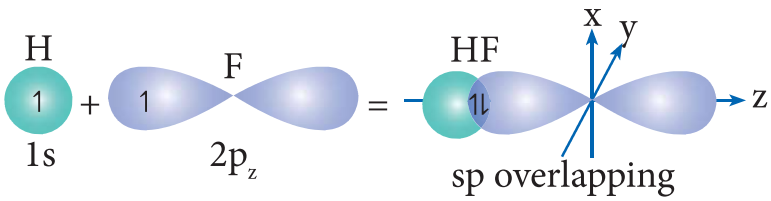


Fig 10.20 Formation of HF Molecule

Formation of oxygen molecule (O_2):

Valence shell electronic configuration of oxygen atom : $2s^2\ 2p_x^2, 2p_y^1, 2p_z^1$

			π bond	σ bond
Oxygen 1	1↿⇂	1↿⇂	1	1
	$2s^2$	$2p_x^2$	$2p_y^1$	$2p_z^1$
Oxygen 2	1↿⇂	1↿⇂	1	1
	$2s^2$	$2p_x^2$	$2p_y^1$	$2p_z^1$

When the half filled p_z orbitals of two oxygen overlaps along the z-axis (considering molecular axis as z axis), a σ-covalent bond is formed between them. Other two half filled p_y orbitals of two oxygen atoms overlap laterally (sideways) to form a π-covalent bond between

the oxygen atoms. Thus, in oxygen molecule, two oxygen atoms are connected by two covalent bonds (double bond). The other two pair of electrons present in the 2s and $2p_x$ orbital do not involve in bonding and remains as lone pairs on the respective oxygen.

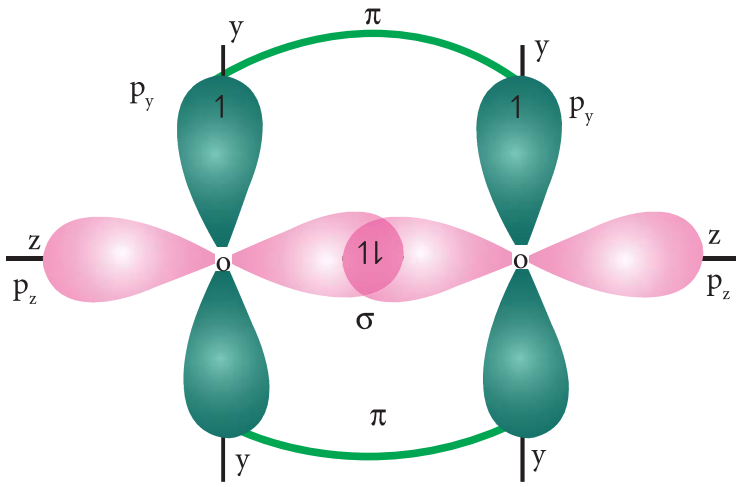


Fig 10. 21 Formation of π bond in O_2 Molecule

Evaluate Yourself

7) Bond angle in PH_4^+ is higher than in PH_3 why?

10.9 Hybridisation

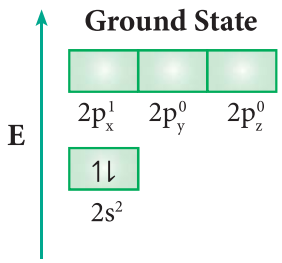
Bonding in simple molecules such as hydrogen and fluorine can easily be explained on the basis of overlap of the respective atomic orbitals of the combining atoms. But the observed properties of polyatomic molecules such as methane, ammonia, beryllium chloride etc... cannot be explained on the basis of simple overlap of atomic orbitals. For example, it was experimentally proved that methane has a tetrahedral structure and the four C-H bonds are equivalent. This fact cannot be explained on the basis of overlap of atomic orbitals of hydrogen (1s) and the atomic orbitals of carbon with different energies ($2s^2\ 2p_x^2\ 2p_y 2p_z$).

In order to explain these observed facts, Linus Pauling proposed that the valence atomic orbitals in the molecules are different from those in isolated atom and he introduced the concept of hybridisation. Hybridisation is the process of mixing of atomic orbitals of the same atom with comparable energy to form equal number of new equivalent orbitals with same energy. The resultant orbitals are called hybridised orbitals and they posses maximum symmetry and definite orientation in space so as to minimize the force of repulsion between their electrons .

10.9.1 Types of hybridisation and geometry of molecules

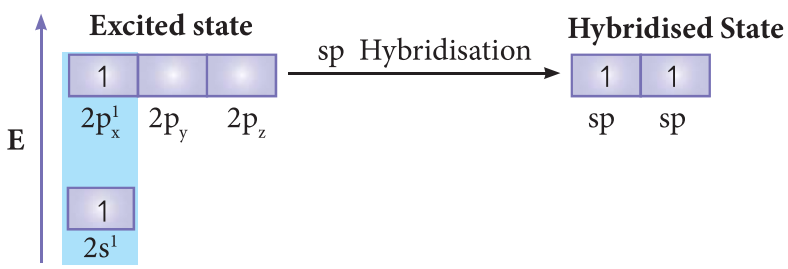
sp Hybridisation:

Consider the bond formation in beryllium chloride. The ground state valence shell electronic configuration of Beryllium atom is $[He]2s^2\ 2p^0$



In $BeCl_2$ both the Be-Cl bonds are equivalent and it was observed that the molecule is linear. VB theory explain this observed behaviour by sp hybridisation. One of the paired electrons in the 2s orbital gets excited to 2p orbital and the electronic configuration at the excited state is shown.

Now, the 2s and 2p orbitals hybridise and produce two equivalent sp hybridised orbitals which have 50 % s-character and 50 % p-character. These sp hybridised orbitals are oriented in opposite direction as shown in the figure.



Overlap with orbital of chlorine

Each of the sp hybridized orbitals linearly overlap with $3p_z$ orbital of the chlorine to form a covalent bond between Be and Cl as shown in the Figure.

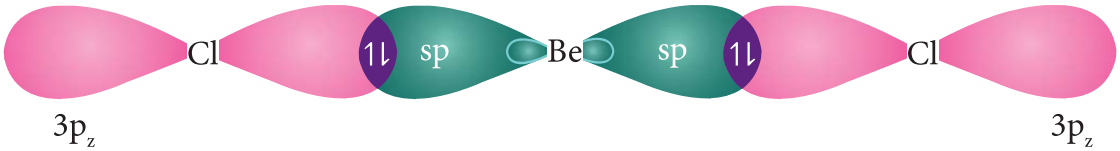
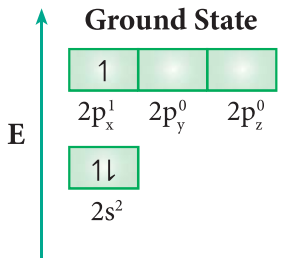


Fig 10.22 sp Hybridisation : $BeCl_2$

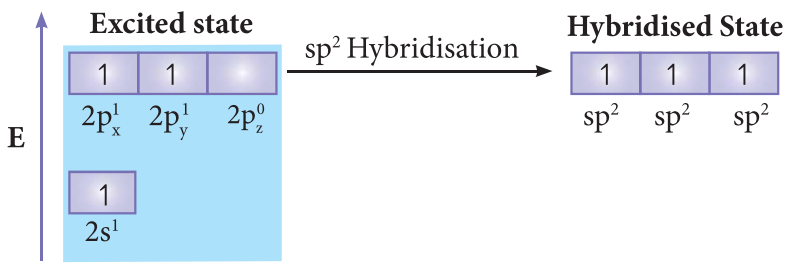
sp^2 Hybridisation:

Consider the bond formation in boron trifluoride.The ground state valence shell electronic configuration of Boron atom is $[He]2s^2\ 2p^1$.



In the ground state boron has only one unpaired electron in the valence shell. In order to form three covalent bonds with fluorine atoms, three unpaired electrons are required. To achieve this, one of the paired electrons in the 2s orbital is promoted to the $2p_y$ orbital in the excite state.

In boron, the s orbital and two p orbitals (p_x and p_y) in the valence shell hybridses, to generate three equivalent sp^2 orbitals as shown in the Figure. These three orbitals lie in the same xy plane and the angle between any two orbitals is equal to 120^0



Overlap with 2pz orbitals of fluorine:

The three sp^2 hybridised orbitals of boron now overlap with the $2p_z$ orbitals of fluorine (3 atoms). This overlap takes place along the axis as shown below.

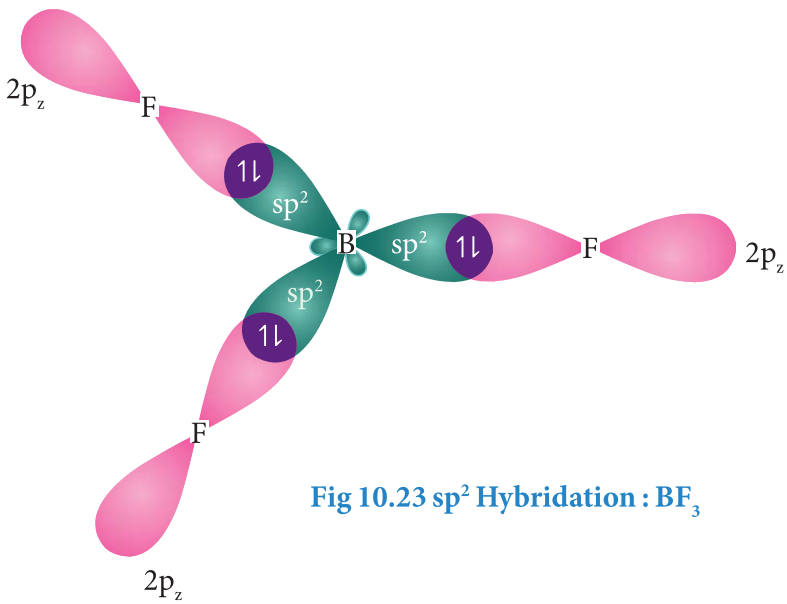
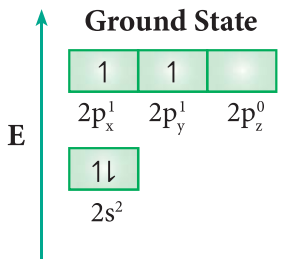


Fig 10.23 sp^2 Hybridation : BF_3

sp3 Hybridisation:

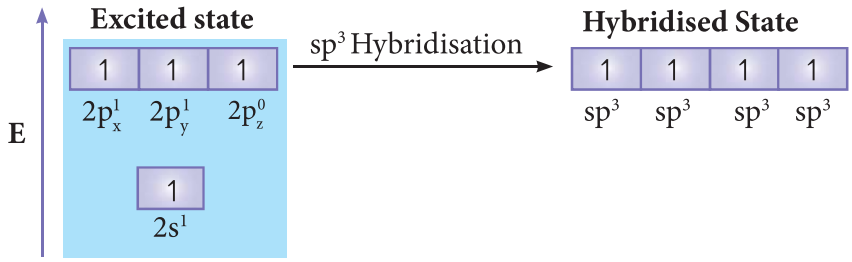
sp^3 hybridisation can be explained by considering methane as an example. In methane molecule the central carbon atom bound to four hydrogen atoms. The ground state valence shell electronic configuration of carbon is $[He]2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$.



In order to form four covalent bonds with the four hydrogen atoms, one of the paired electrons in the 2s orbital of carbon is promoted to its $2p_z$ orbital in the excite state. The one 2s orbital and the three 2p orbitals of carbon mixes to give four equivalent sp^3 hybridised orbitals. The angle between any two sp^3 hybridised orbitals is $109^0\ 28'$

Overlap with 1s orbitals of hydrogen:

The 1s orbitals of the four hydrogen atoms overlap linearly with the four sp^3 hybridised orbitals of carbon to form four C-H σ-bonds in the methane molecule, as shown below.



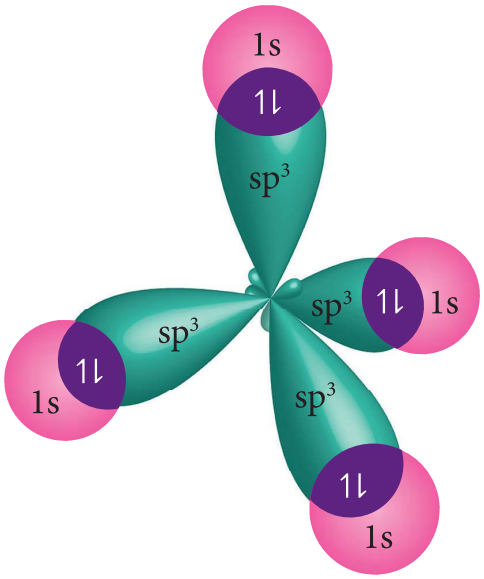
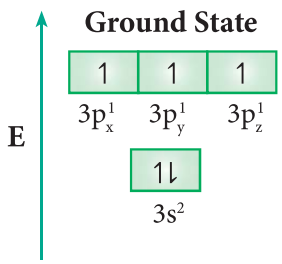


Fig 10.24 sp^3 Hybridisation : CH_4

sp^3d Hybridisation:

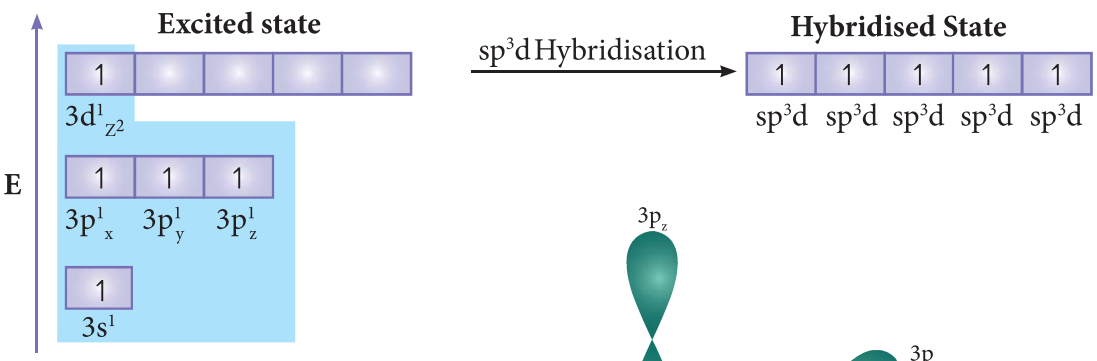
In the molecules such as PCl_5, the central atom phosphorus is covalently bound to five chlorine atoms. Here the atomic orbitals of phosphorous undergoes sp^3d hybridisation which involves its one 3s orbital, three 3p orbitals and one vacant 3d orbital (d_{z^2}). The ground state electronic configuration of phosphorous is [Ne]$3s^2\ 3p_x^1\ 3p_y^1\ 3p_z^1$ as shown below.



One of the paired electrons in the 3s orbital of phosphorous is promoted to one of its vacant 3d orbital (d_{z^2}) in the excite state. One 3s orbital, three 3p orbitals and one $3d_{z^2}$ orbital of phosphorus atom mixes to give five equivalent sp^3d hybridised orbitals. The orbital geometry of sp^3d hybridised orbitals is trigonal bi-pyramidal as shown in the figure 10.25.

Overlap with $3p_z$ orbitals of chlorine:

The $3p_z$ orbitals of the five chlorine atoms linearly overlap along the axis with the five sp^3d hybridised orbitals of phosphorous to form the five P-Cl σ-bonds, as shown below.



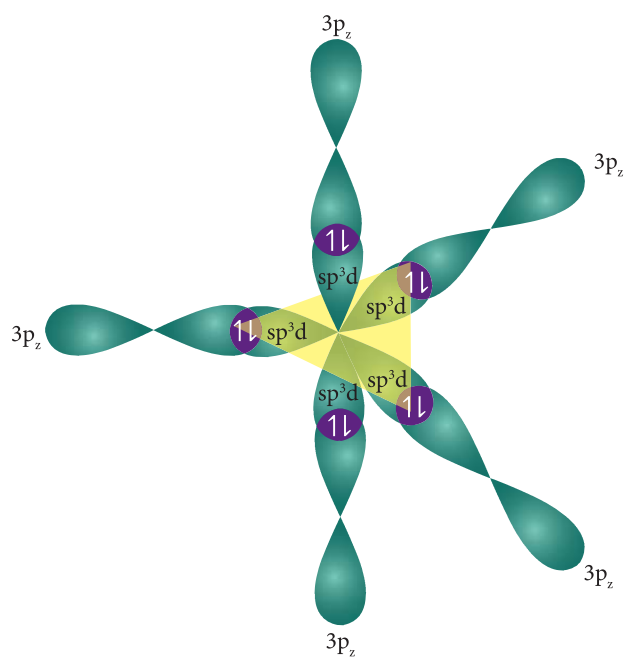
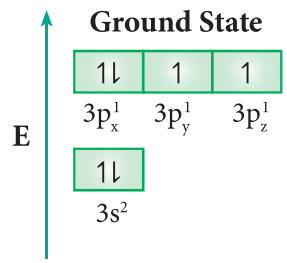


Fig 10.25 sp^3d Hybridisation : PCl_5

sp^3d^2 Hybridisation:

In sulphur hexafluoride (SF_6) the central atom sulphur extend its octet to undergo sp^3d^2 hybridisation to generate six sp^3d^2 hybridised orbitals which accounts for six equivalent S-F bonds. The ground state electronic configuration of sulphur is $[Ne]3s^2\ 3p_x^2\ 3p_y^1\ 3p_z^1$.



One electron each from 3s orbital and 3p orbital of sulphur is promoted to its two vacant 3d orbitals (d_{z^2} and $d_{x^2-y^2}$) in the excite state. A total of six valence orbitals from sulphur (one 3s orbital, three 3p orbitals and two 3d orbitals) mixes to give six equivalent sp^3d^2 hybridised orbitals. The orbital geometry is octahedral as shown in the figure.

Overlap with 2pz orbitals of fluorine:

The six sp^3d^2 hybridised orbitals of sulphur overlaps linearly with $2p_z$ orbitals of six fluorine atoms to form the six S-F bonds in the sulphur hexafluoride molecule.

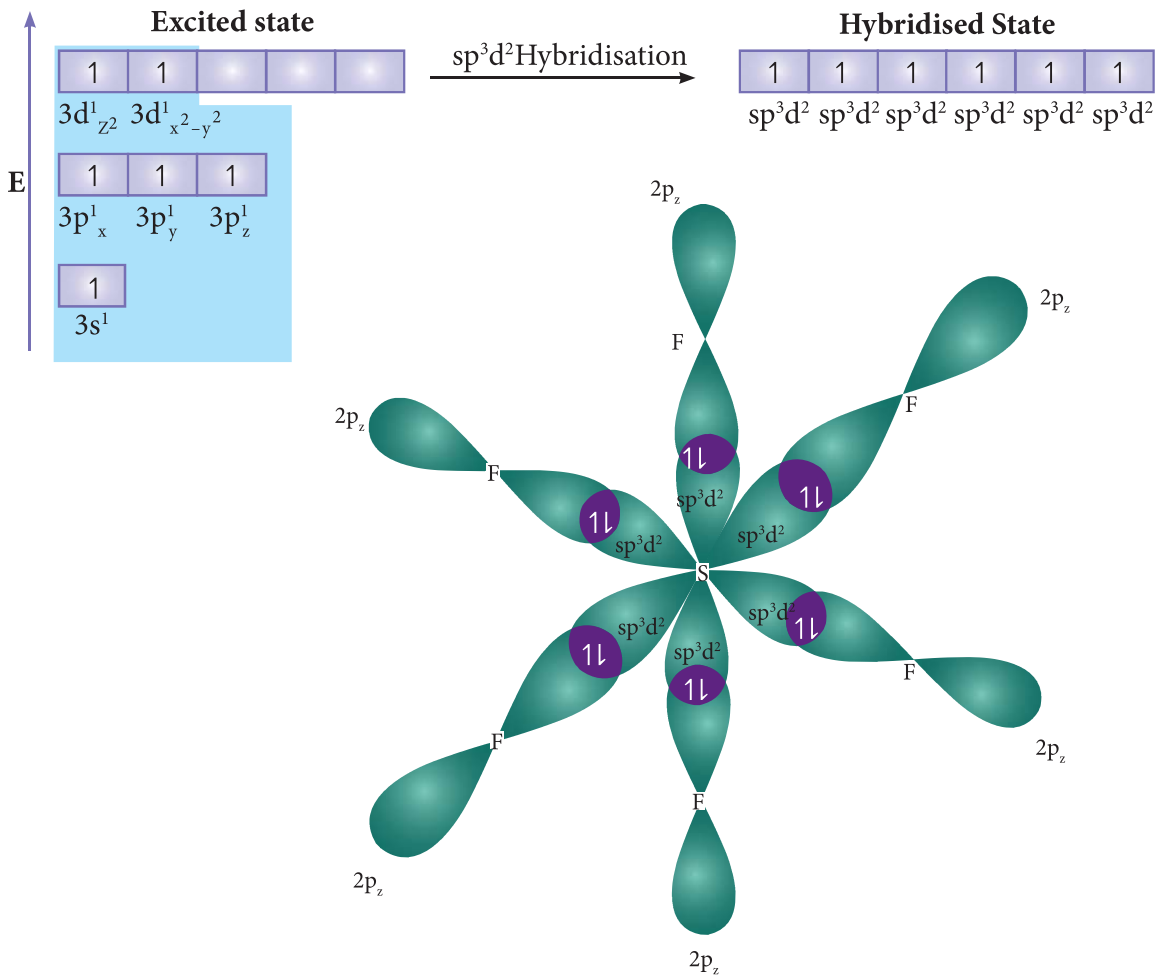
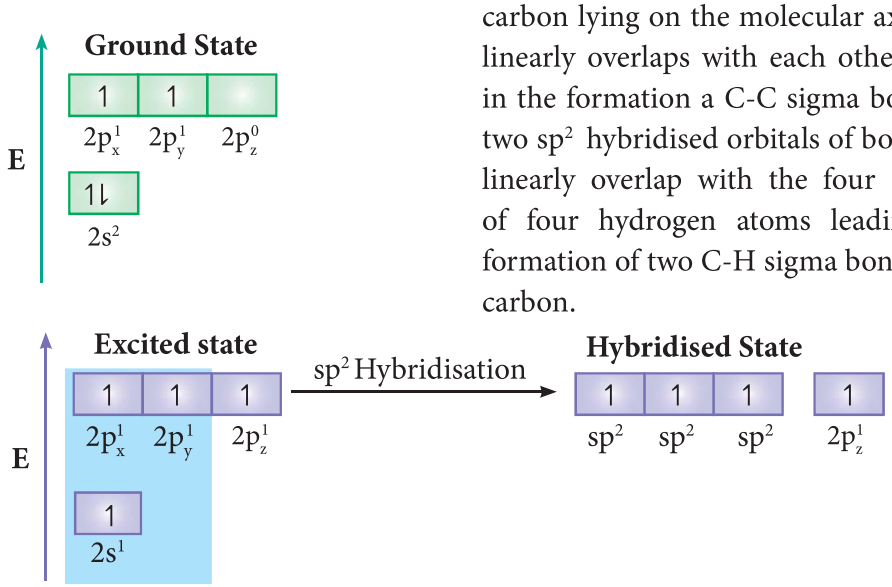


Fig 10.26 sp^3d^2 Hybridisation : SF_6

Bonding in Ethylene:

The bonding in ethylene can be explained using hybridisation concept. The molecular formula of ethylene is C_2H_4. The valency of carbon is 4. The electronic configuration of valence shell of carbon in ground state is $[He]2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$. To satisfy the valency of carbon promote an electron from 2s orbital to $2p_z$ orbital in the excited state.



In ethylene both the carbon atoms undergoes sp^2 hybridisation involving 2s, $2p_x$ and $2p_y$ orbitals, resulting in three equivalent sp^2 hybridised orbitals lying in the xy plane at an angle of 120^0 to each other. The unhybridised $2p_z$ orbital lies perpendicular to the xy plane.

Formation of sigma bond:

One of the sp^2 hybridised orbitals of each carbon lying on the molecular axis (x-axis) linearly overlaps with each other resulting in the formation a C-C sigma bond. Other two sp^2 hybridised orbitals of both carbons linearly overlap with the four 1s orbitals of four hydrogen atoms leading to the formation of two C-H sigma bonds on each carbon.

Formation of Pi (π) bond:

The unhybridised $2p_z$ orbital of both carbon atoms can overlap only sideways as they are not in the molecular axis. This lateral overlap results in the formation a pi(π) bond between the two carbon atoms as shown in the figure.

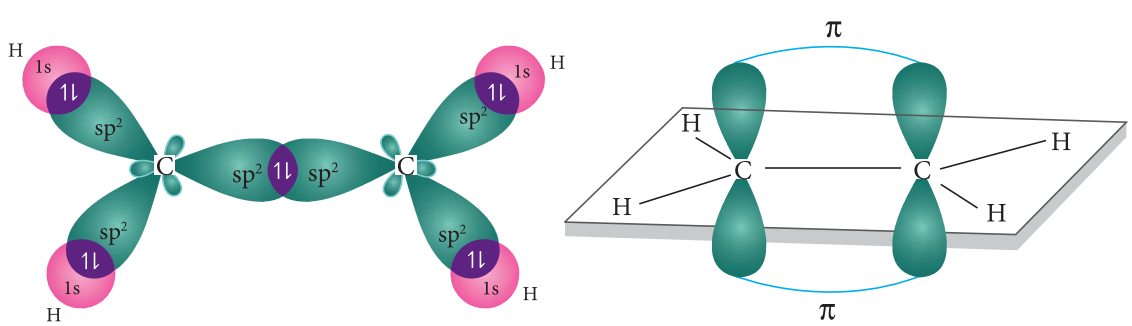


Fig 10.27 sp^2 Hybridisation : C_2H_4

Bonding in acetylene:

Similar to ethylene, the bonding in acetylene can also be explained using hybridisation concept. The molecular formula of acetylene is C_2H_2. The electronic configuration of valence shell of carbon in ground state is $[He]2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$. To satisfy the valency of carbon promote an electron from 2s orbital to $2p_z$ orbital in the excited state.

In acetylene molecule, both the carbon atoms are in sp hybridised state. The 2s and $2p_x$ orbitals, resulting in two equivalent sp hybridised orbitals lying in a straight line along the molecular axis (x-axis). The unhybridised $2p_y$ and $2p_z$ orbitals lie perpendicular to the molecular axis.

Formation of sigma bond:

One of the two sp hybridised orbitals of each carbon linearly overlaps with each other resulting in the formation a C-C sigma bond. The other sp hybridised orbital of both carbons linearly overlap with the two 1s orbitals of two hydrogen atoms leading to the formation of one C-H sigma bonds on each carbon.

Formation of pi bond:

The unhybridised $2p_y$ and $2p_z$ orbitals of each carbon overlap sideways. This lateral overlap results in the formation of two pi bonds (p_y-p_y and p_z-p_z) between the two carbon atoms as shown in the figure.

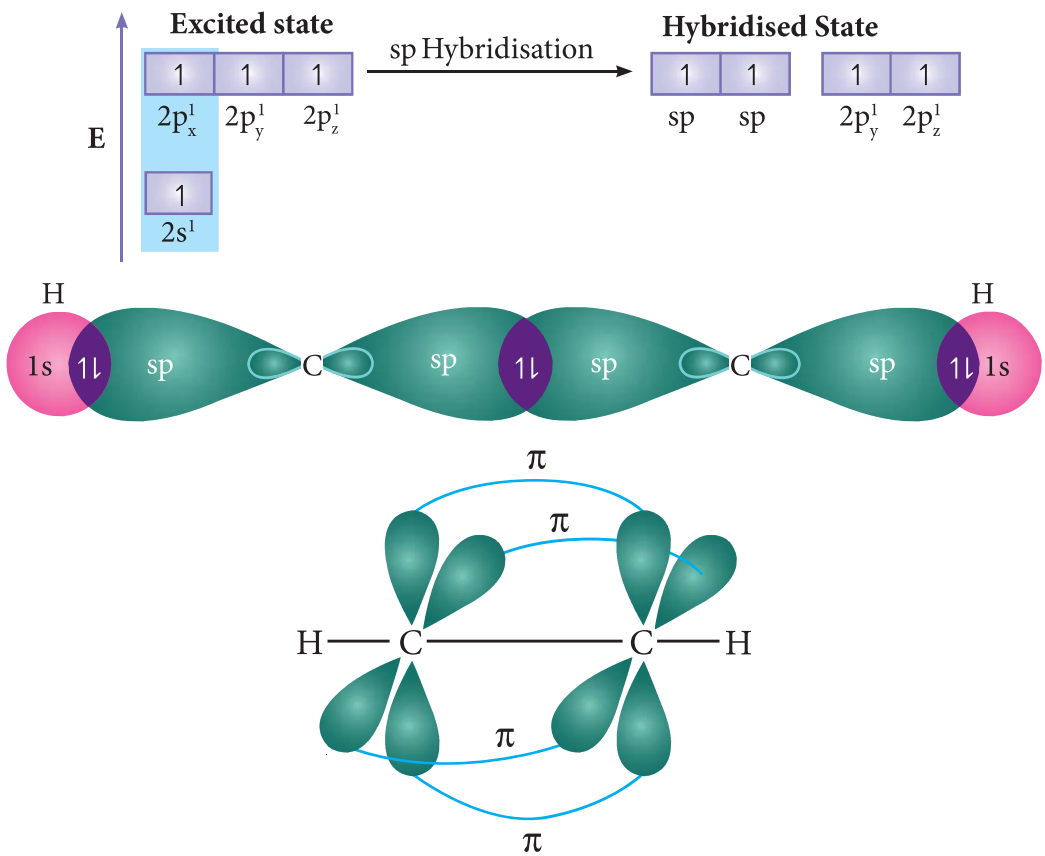


Fig 10.28 sp Hybridisation in acetylene: C_2H_2

Evaluate Yourself

8) Explain the bond formation in SF_4 and CCl_4 using hybridisation concept.

Evaluate Yourself

9) The observed bond length of N_2^+ is larger than N_2 while the bond length in NO^+ is less than in NO. Why?

10.10 Molecular orbital theory

Lewis concept and valence bond theory qualitatively explains the chemical bonding and molecular structure. Both approaches are inadequate to describe some of the observed properties of molecules. For example, these theories predict that oxygen is diamagnetic. However, it was observed that oxygen in liquid form was attracted towards the poles of strong magnet, indicating that oxygen is paramagnetic. As both these theories treated the bond formation in terms of electron pairs and hence they fail to explain the bonding nature of paramagnetic molecules. F. Hund and Robert. S. Mulliken developed a bonding theory called molecular orbital theory which explains the magnetic behaviour of molecules.

The salient features of Molecular orbital Theory (MOT):

1. When atoms combines to form molecules, their individual atomic orbitals lose their identity and forms new orbitals called molecular orbitals.

2. The shapes of molecular orbitals depend upon the shapes of combining atomic orbitals.

3. The number of molecular orbitals formed is the same as the number of combining atomic orbitals. Half the number of molecular orbitals formed will have lower energy than the corresponding atomic orbital, while the remaining molecular orbitals will have higher energy. The molecular orbital with lower energy is called bonding molecular orbital and the one with higher energy is called anti-bonding molecular orbital. The bonding molecular orbitals are represented as σ (Sigma), π (pi), δ (delta) and the corresponding antibonding orbitals are denoted as σ*, π* and δ*.

4. The electrons in a molecule are accommodated in the newly formed molecular orbitals. The filling of electrons in these orbitals follows Aufbau's principle, Pauli's exclusion principle and Hund's rule as in the case of filling of electrons in atomic orbitals.

5. Bond order gives the number of covalent bonds between the two combining atoms. The bond order of a molecule can be calculated using the following equation

$$\text{Bond order} = \frac{N_b - N_a}{2}$$

Where,

N_b = Total number of electrons present in the bonding molecular orbitals

N_a = Total number of electrons present in the antibonding molecular orbitals and

A bond order of zero value indicates that the molecule doesn't exist.

10.10.1 Linear combination of atomic orbitals

The wave functions for the molecular orbitals can be obtained by solving Schrödinger wave equation for the molecule. Since solving the Schrödinger equation is too complex, approximation methods are used to obtain the wave function for molecular orbitals. The most common method is the linear combination of atomic orbitals (LCAO).

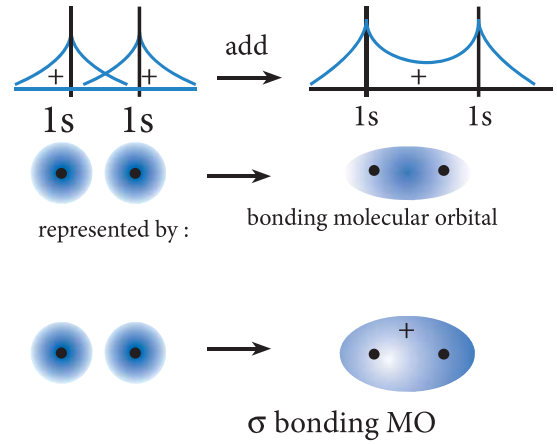
We know that the atomic orbitals are represented by the wave function Ψ. Let us consider two atomic orbitals represented by the wave function ψ_A and ψ_B with comparable energy, combines to form two molecular orbitals. One is bonding molecular orbital($\psi_{bonding}$) and the other is antibonding molecular orbital($\psi_{antibonding}$). The wave functions for these two molecular orbitals can be obtained by the linear combination of the atomic orbitals ψ_A and ψ_B as below.

$$\psi_{bonding} = \psi_A + \psi_B$$

$$\psi_{antibonding} = \psi_A - \psi_B$$

The formation of bonding molecular orbital can be considered as the result of constructive interference of the atomic orbitals and the formation of anti-bonding molecular orbital can be the result of the destructive interference of the atomic orbitals. The formation of the two molecular orbitals from two 1s orbitals is shown below.

Constructive interaction: The two 1s orbitals are in phase and have the same sign.



Destructive interaction The two 1s Orbitals are out phase

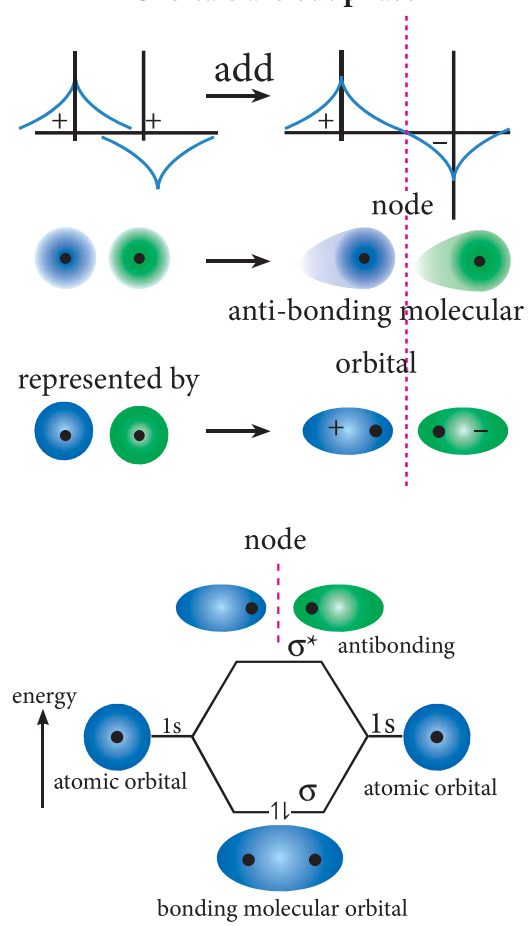


Fig 10.29 Linear Combination of atomic orbitals

10.10.2 Bonding in some Homonuclear di-atomic molecules:

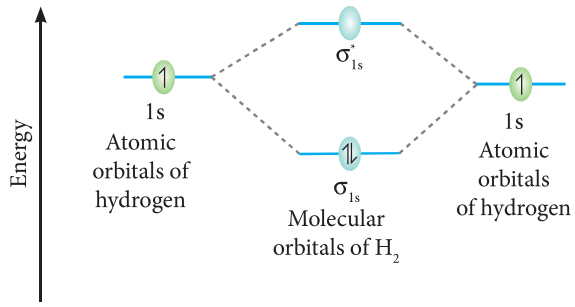


Fig 10.30 MO Diagram for H_2 molecule

Molecular orbital diagram of hydrogen molecule (H_2)

Electronic configuration of H atom is **$1s^1$**

Electronic configuration of H_2 molecule σ_{1s}^2

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{2-0}{2} = 1$$

Molecule has *no unpaired electrons.* Hence, it is **diamagnetic**.

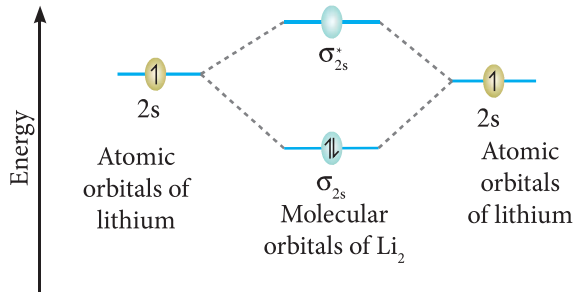


Fig 10.31 MO Diagram for Li_2 molecule

Molecular orbital diagram of lithium molecule (Li_2)

Electronic configuration of Li atom is **$1s^2\,2s^1$**

Electronic configuration of Li_2 molecule $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{4-2}{2} = 1$$

Molecule has *no unpaired electrons.* Hence it is **diamagnetic**.

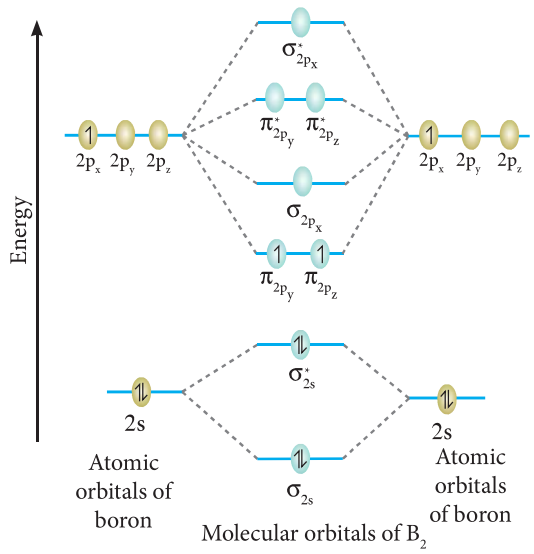


Fig 10.32 MO Diagram for B_2 molecule

Molecular orbital diagram of boron molecule (B_2)

Electronic configuration of B atom is **$1s^2\,2s^2\,2p^1$**

Electronic configuration of B_2 molecule $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi^1_{2p_y}, \pi^1_{2p_z}$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{6-4}{2} = 1$$

Molecule has *two unpaired electrons. Hence* it is **paramagnetic.**

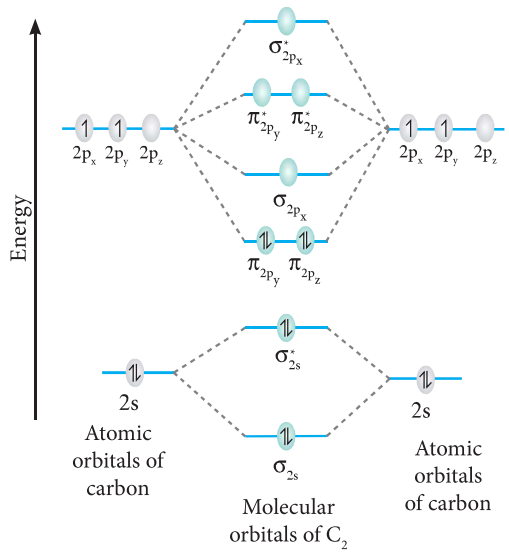


Fig 10.33 MO Diagram for C_2 molecule

Molecular orbital diagram of carbon molecule (C_2)

Electronic configuration of C atom is

$1s^2\,2s^2\,2p^2$

Electronic configuration of C_2 molecule $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi^2_{2p_y}, \pi^2_{2p_z}$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{8-4}{2} = 2$$

Molecule has *no unpaired electrons.* Hence, it is **diamagnetic.**

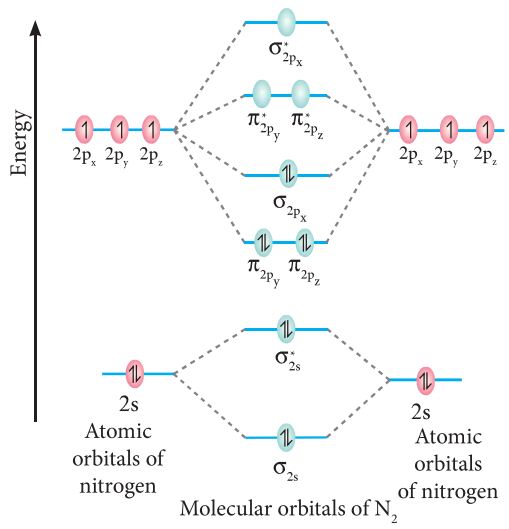


Fig 10.34 MO Diagram for N_2 molecule

Molecular orbital diagram of nitrogen molecule (N_2)

Electronic configuration of N atom is **$1s^2\,2s^2\,2p^3$**

Electronic configuration of N_2 molecule $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi^2_{2p_y}, \pi^2_{2p_z}\sigma_2^2 px$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{10-4}{2} = 3$$

Molecule has *no unpaired electrons.* Hence, it is **diamagnetic.**

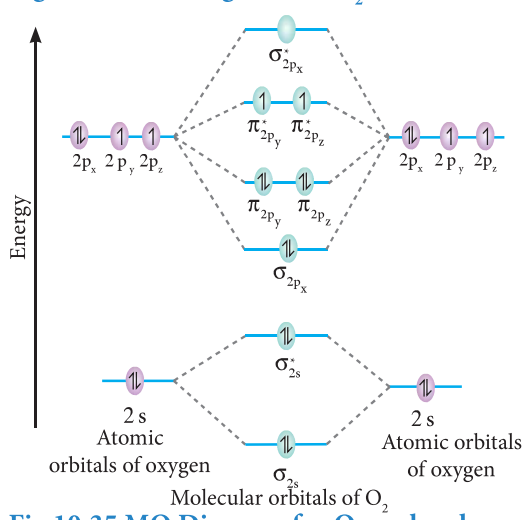


Fig 10.35 MO Diagram for O_2 molecule

Molecular orbital diagram of oxygen molecule (O_2)

Electronic configuration of O atom is **$1s^2\,2s^2\,2p^4$**

Electronic configuration of O_2 molecule $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \sigma^2_{2p_x}\ \pi^2_{2p_y}, \pi^2_{2p_z}, \pi^{*1}_{2p_y}, \pi^{*1}_{2p_z},$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{10-6}{2} = 2$$

Molecule has *two unpaired electrons.* Hence, it is **paramagnetic**.

10.10.3 Bonding in some Heteronucleardi-atomic molecules

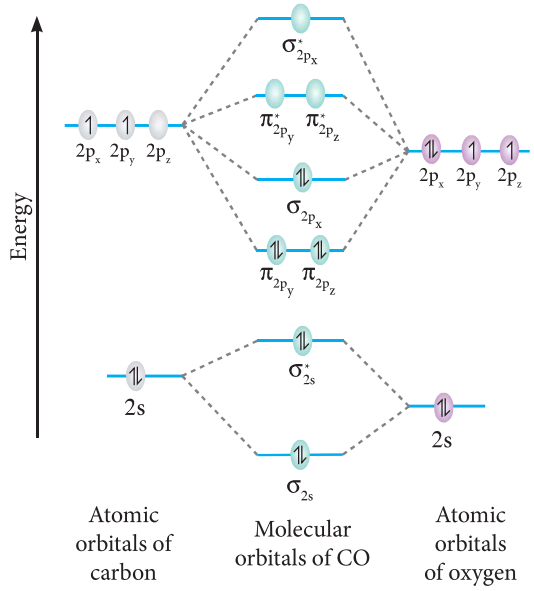


Fig 10.36 MO Diagram for CO molecule

Molecular orbital diagram of Carbon monoxide molecule (CO)

Electronic configuration of C atom is **$1s^2 2s^2 2p^2$**

Electronic configuration of O atom is **$1s^2 2s^2 2p^4$**

Electronic configuration of CO molecule $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi^2_{2p_y}, \pi^2_{2p_z}, \sigma^2_{2p_x}$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{10-4}{2} = 3$$

Molecule has *no unpaired electrons*. Hence, it is **diamagnetic**.

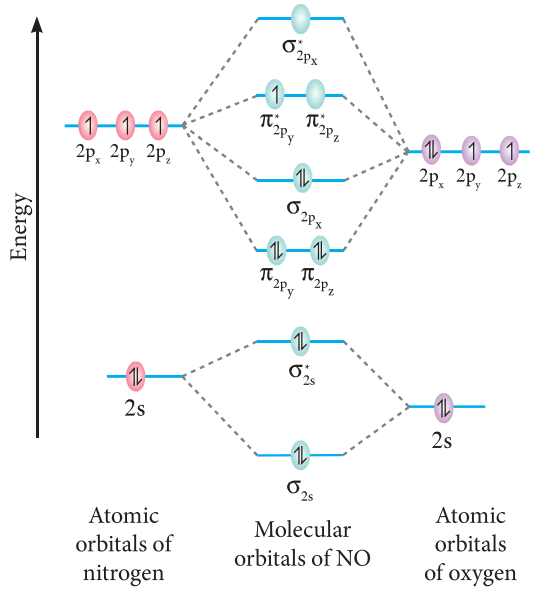


Fig 10.36 MO Diagram for NO molecule

Molecular orbital diagram of Nitric oxide molecule (NO)

Electronic configuration of N atom is **$1s^2 2s^2 2p^3$**

Electronic configuration of O atom is **$1s^2 2s^2 2p^4$**

Electronic configuration of NO molecule $\sigma_{1s}^2, \sigma_{1s}^{*2}, \sigma_{2s}^2, \sigma_{2s}^{*2}, \pi^2_{2p_y}, \pi^2_{2p_z}, \sigma^2_{2p_x}\ \pi^{*1}_{2p_y}$

$$\text{Bond order} = \frac{N_b - N_a}{2} = \frac{10-5}{2} = 2.5$$

Molecule has *one unpaired electron*. Hence, it is **paramagnetic**.

Evaluate Yourself

10) Draw the MO diagram for acetylide ion C_2^{2-} and calculate its bond order.

Metallic bonding

Metals have some special properties of lustre, high density, high electrical and thermal conductivity, malleability and ductility, and high melting and boiling points. The forces that keep the atoms of the metal so closely in a metallic crystal constitute what is generally known as the metallic bond. The metallic bond is not just an electrovalent bond(ionic bond), as the latter is formed between atoms of different electro negativities. Similarly, the metallic bond is not a covalent bond,as the metal atoms do not have sufficient number of valence electrons for mutual sharing with 8 or 12 neighboring metal atoms in a crystal. So, we have to search for a new theory to explain metallic bond. The first successful theory is due to Drude and Lorentz, which regards metallic crystal as an assemblage of positive ions immersed in a gas of free electrons. The free electrons are due to ionization of the valence electrons of the atoms of the metal. As the valence electrons of the atoms are freely shared by all the ions in the crystal, the metallic bonding is also referred to as electronic bonding. As the free electrons repel each other, they are uniformly distributed around the metal ions. Many physical properties of the metals can be explained by this theory, nevertheless there are exceptions.

The electrostatic attraction between the metal ions and the free electrons yields a three-dimensional close packed crystal with a large number of nearest metal ions. So, metals have high density. As the close packed structure contains many slip planes along which movement can occur during mechanical loading, the metal acquires ductility. Pure metals can undergo 40 to 60% elongation prior to rupturing under mechanical loading. As each metal ion is surrounded by electron cloud in all directions, the metallic bonding has no directional properties.

As the electrons are free to move around the positive ions, the metals exhibit high electrical and thermal conductivity. The metallic luster is due to reflection of light by the electron cloud. As the metallic bond is strong enough, the metal atoms are reluctant to break apart into a liquid or gas, so the metals have high melting and boiling points.

The bonding in metal is better treated by Molecular orbital theory. As per this theory, the atomic orbitals of large number of atoms in a crystal overlap to form numerous bonding and antibonding molecular orbitals without any band gap. The bonding molecular orbitals are completely filled with an electron pair in each, and the antibonding molecular orbitals are empty. Absence of band gap accounts for high electrical conductivity of metals. High thermal conductivity is due to thermal excitation of many electrons from the valence band to the conductance band. With an increase in temperature, the electrical conductivity decreases due to vigorous thermal motion of lattice ions that disrupts the uniform lattice structure, that is required for free motion of electrons within the crystal. Most metals are black except copper, silver and gold. It is due to absorption of light of all wavelengths. Absorption of light of all wavelengths is due to absence of bandgap in metals.