1. MOLECULAR ORBITAL THEORY

1. VALENCE BOND THEORY

The theory was developed by Hitler and London in 1927 and later extended by Pauling and Slater in 193. The theory is based on the following two principles.

(i) If $\psi_A$ and $\psi_B$ are the wave function for two isolated independent atoms A and B, then the total wave function $\psi$ of the system can be written as a product of the wave functions of the two atoms.

$\psi = \psi_A \cdot \psi_B$

(ii) If a system can be represented by wave functions such as $\psi_1$, $\psi_2$, $\psi_3$ ----, then the true wave function $\psi$ can be obtained by taking a linear combination of all these wave functions.

$\psi = N (C_1 \psi_1 + C_2 \psi_2 + C_3 \psi_3 + \ldots)$

Where, $N$ is the normalization constant and $C_1$, $C_2$, $C_3$ ---- are the various coefficients. These Coefficients are so adjusted as to give a state of lowest energy and maximum stability. The assumptions of valence bond approach based on the above principles may be given as follows.

1) Atoms maintain their individuality in a molecule.

2) The bond is formed due to interaction of valence electron as the atom approach each other.

3) When bond is formed between the atoms, only one electron from each bonded atom loses its identity.

4) The electrons forming the bond between the two atoms undergo exchange between them and thus bond is stabilized.
Main features of valence bond theory

1) Overlapping of atomic orbitals of the two atoms having unpaired electron forms bond and electron spins are mutually neutralized.
2) The electron pair is localized between the two bonded atoms.
3) Strength of the bond depends on the extent of overlapping. Larger the area of overlap, stronger is the bond formed.
4) It gives explanation for the presence of partial ionic nature in a covalent bond.
5) It introduced the concept of resonance and the connection between resonance energy and molecular stability.

2. Molecular Orbital Theory (M.O.T.)

This theory put forward by Hund and Mulliken. It treats the molecule in the same way as an atom. It is based on following assumption.

1) A molecule is made of atoms.
2) When a molecule is formed, atoms lose their individual character.
3) A molecular orbital is associated with a molecule as a whole.
4) Electrons in molecule are delocalised as compared to what they are in an isolated atom.
5) The quantised molecular orbitals of varying energy levels surround all the nuclei of the bonded atoms.
6) A molecular orbital is associated to be formed by the coalescence of the individual atomic orbitals when the atoms to be bonded come together.
7) The wave functions of a molecular orbital are obtained by linear combination of wave functions of atomic orbitals.
Comparison of V.B Theory and M.O. Theory

1) The valence bond theory considers an atom consisting of a nucleus and electrons present in an atomic orbital. Thus the atomic orbital is monocentric. The molecular orbital theory considers that an electron in a molecule moves in the field of more than one nucleus and one or more than one nucleus. Thus the molecular orbital is polycentric.

2) Just as there are atomic orbitals s, p, d and f in an atom, there are molecular orbitals σ, π, δ in a molecule.

3) Just as there are atomic orbitals possess different shapes and energies, molecular orbital possesses different shapes and energies.

4) Just as there are atomic orbitals can be arranged in their increasing order of energy, the molecular orbital can also be arranged in the increasing order of energy.

5) Just as \( \phi \) denotes the electron density in a particular orbital of an atom, \( \Psi \) denotes the electron density in a particular molecular orbital.

6) Just as we use aufbau principle for atoms, we can use it for molecule. Therefore, (a) each molecular orbital can accommodate two electrons with opposite spins and (b) the electrons are first filled into the lower energy orbital then the electron go to the higher energy available molecular orbital one at a time.

7) The atomic orbital of two or more atoms combine to form a molecular orbital only when they have i) close distance ii) similar energy iii) matching symmetry iv) matching geometry.

8) Fig 1.1(a) shows that when A and B combine, they do not lose their identity while forming a molecular orbital by V.B. Theory. Fig 1.1(b)
shows that when A and B combine, they lose their identity while forming a molecular orbital by M.O. Theory.

\[ \text{Fig 1.1 Formation of a molecular orbital by V.B. theory and M.O. theory.} \]

**Comparison of Atomic Orbital and Molecular Orbital**

<table>
<thead>
<tr>
<th>Atomic Orbital</th>
<th>Molecular Orbital</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. It contains a single nucleus i.e. it is monocentric</td>
<td>1. It contains more than two nucleus i.e. it is polycentric.</td>
</tr>
<tr>
<td>2. Nucleus of the atom is fixed in Space.</td>
<td>2. Nucleus of the constituent atoms of the molecule are Fixed in space at their proper relative orientation.</td>
</tr>
<tr>
<td>3. They are named as s, p, d and f.</td>
<td>3. They are named as σ, π and δ.</td>
</tr>
<tr>
<td>4. It is derived from a particular atom.</td>
<td>4. It is derived from the constituent atoms.</td>
</tr>
<tr>
<td>5. It has a definite shape, size and energy.</td>
<td>5. The shape, size and energy of a M.O. depends upon the shape, size and energy of orbital of constituent atoms.</td>
</tr>
</tbody>
</table>
Linear Combination of Atomic Orbitals (LCAO) Method

It is a simple and useful method of obtaining a wave function, which is described as follows: Consider two similar atoms H and H. These atoms with their atomic orbitals are described by some wave function say \( \phi_1 \) and \( \phi_2 \).

When these atoms form a bond the electrons in the atomic orbitals occupy molecular orbitals. The molecular orbital is formed by linear combination of the atomic orbitals \( \phi_1 \) and \( \phi_2 \) that is, by adding or subtracting the two wave functions.

\[
\Psi = \phi_1 \pm \lambda \phi_2
\]

Where, \( \Psi \) is the wave function of the molecular orbital, \( \phi_1 \) and \( \phi_2 \) are the wave functions of atomic orbitals of atom A and B and \( \lambda \) is the mixing coefficient which is the measure of ionic character of the bond formed between atom 1 and 2. For a homonuclear diatomic molecule, that is, Where atoms 1 and 2 are identical, \( \lambda \) is equal to 1 and wave function of the molecular orbital is written as

\[
\Psi = \phi_1 \pm \phi_2
\]

Let us take an example of \( \text{H}_2 \) molecule. The hydrogen molecule is formed by combination of two hydrogen atoms. Let us consider that \( \phi_1 \) and \( \phi_2 \) represents the wave function of atomic orbital 1s for hydrogen atom 1 and 2. Then there are two possible ways of combination of the wave function \( \phi_1 \) and \( \phi_2 \).

1. In one way of combination, the signs of the two wave functions are same and in the other way of combination the signs of the two wave function are different.
2. The signs (+) and (-) refer to the sign of the wave functions. These signs determine the symmetry of the wave function. (The signs should not be confused with the signs of the charged bodies).

A wave function Ψ describes the probability of finding the electron and Ψ^2 describes the electron density.

Wave functions, which have the same sign, may be considered as waves that are in phase, which then combined add up to give a larger resultant wave as shown in figure 1.2.

Similarly, wave functions of different signs, correspond to wave that are completely out of phase and which cancel each other by destructive interface, as shown in fig. 1.3. Fig 1.2 and 1.3 show a graph of probability of
electron as a function of internuclear distance. The two ways of combination are

\[ \Psi (g) = \phi_1 + \phi_2 \quad \text{(2)} \]

\[ \Psi (u) = \phi_1 + (-\phi_2) \quad \text{(3)} \]

Equation 3 should be considered as the summation of the wave functions and not as the mathematical difference between them.

Thus, when a pair of atomic orbitals \( \phi_1 \) and \( \phi_2 \) combine, they produce a pair of MOs \( \Psi(g) \) and \( \Psi(u) \). Hence the number of MOs produced must always be equal to the number of AOs taking part in combination. That is, orbitals are not destroyed. Such type of addition and subtraction of wave functions of the AOs is termed as LCAO principle. In the MO theory, wave functions are designated as \( \Psi(g) \) and \( \Psi(u) \).

The letter \( g \) stands for gerade (even) and the letter \( u \) stands for ungerade (odd). The symbols \( g \) and \( u \) refer to the symmetry of the orbital about its center. The wave function is gerade, if the sign of \( \Psi \) remains unchanged, when the orbital is reflected about its center. The wave function is ungerade, if the sign of \( \Psi \) changed, when the orbital is reflected about its center. (i.e. \( x, y \) and \( z \) are replaced by \( -x, -y, \) and \( -z \)). The symmetry of the M.O. is also determined by another method. In this method, the molecular orbital is first rotated about the line joining the two nuclei and then rotated about a line perpendicular to the inter nuclear axis. The MO is gerade, if the sign of the lobes remains the same and the orbital is ungerade, if the sign changes.

The function \( \Psi(g) \) leads to increased electron density in between the nuclei and is, therefore, a Bonding Molecular Orbital (BMO) (attraction between the atoms). On the other hand, the wave functions \( \Psi(u) \) leads to
decreased electron density, that is, zero electron density in between the nuclei. This therefore an Anti Bonding Molecular Orbital (ABMO) (repulsion between the atoms). The ABMO is higher in energy and is indicated by *. The BMO is lower in energy. The gerade orbital Ψ (g) hereafter will be indicated by the symbol Ψ meaning thereby a bonding MO and the ungerade orbital Ψ(u) hereafter will be indicated by the symbol Ψ* meaning thereby an antibonding MO.

The electron distribution in a MO can be obtained by squaring the wave function. On squaring equation 2 and 3, we get

\[ \Psi_g^2 = \phi_1^2 + \phi_2^2 + 2\phi_1\phi_2 \quad (4) \]
\[ \Psi_u^2 = \phi_1^2 + \phi_2^2 - 2\phi_1\phi_2 \quad (5) \]

Equation (4) and (5) represent the probability functions for bonding Ψ and antibonding Ψ* MOs respectively. These two MOs differ by \(2\phi_1\phi_2\). The wave function \(\phi_1 + \phi_2\) increases the electron density in between the nuclei by the amount \(2\phi_1\phi_2\) and is, therefore, a bonding MO.

The wave functions \(\phi_1 - \phi_2\) decreases the electron density in between the nuclei by an amount \(2\phi_1\phi_2\) and is therefore, an antibonding MO.

**Formation of Bonding and Antibonding MOs (pictorial representation)**

Two atomic orbitals (say 1s) combine to give a pair of MOs Ψ bonding and Ψ* antibonding. The overlap of atomic orbital along the axis joining the nuclei forms a σ bond so these molecular orbital are further called σ bonding MOs and σ* antibonding MOs. Fig.1.4 shows formation of bonding and antibonding MOs.
1. MOLECULAR ORBITAL THEORY

When two 1S orbitals combine, they form a Ψ (or σ) Mo and a Ψ*(or σ*) MO. Fig.1.5 shows the energy level of atomic orbitals and molecular orbitals. In this diagram, the AOs are shown to the sides and the molecular orbitals formed are shown in the center. The two AOs $\phi_1$ and $\phi_2$ are of identical energy and hence the MOs Ψ and Ψ* or σ and σ* contain equal contribution from $\phi_1$ and $\phi_2$. The MO energy level diagram is symmetrical. The energy evolved during the formation of bonding MO, that is, Ψ or σ is shown as $-\Delta$ or $-\beta$ and the energy absorbed during the formation of antibonding MO, Ψ*or σ* is shown as $+\Delta$ or $+\beta$.

Fig: Energy diagram of sigma bond formation by orbital overlap

M.O. Energy Level Diagram

Fig 1.4 Formation of bonding and antibonding MOs
The energy of bonding MO is lower than that of the AO by an amount $\Delta$ or $\beta$ known as **stabilization energy**. Similarly, the energy of antibonding MO is greater than that of the AO by an amount $\Delta$ or $\beta$ known as **destabilization energy**. The decrease in energy is balanced by the increase in energy.

**Comparison between Bonding MO and Antibonding MO**

<table>
<thead>
<tr>
<th>BMO</th>
<th>ABMO</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. It is obtained by addition of wave function of AOs.</td>
<td>1. It is obtained by subtraction of wave function of AOs.</td>
</tr>
<tr>
<td>2. It has lower energy than that of combining AOs.</td>
<td>2. It has higher energy than that of combining AOs.</td>
</tr>
<tr>
<td>3. It is stable.</td>
<td>3. It is unstable.</td>
</tr>
<tr>
<td>4. Electron density is Concentrated in the region between the nuclei.</td>
<td>4. Electron density is away from Internuclear region.</td>
</tr>
<tr>
<td>5. It results in bonding.</td>
<td>5. It results in non-bonding.</td>
</tr>
<tr>
<td>6. Nuclear repulsion is shielded.</td>
<td>6. Nuclear repulsion is not shielded.</td>
</tr>
<tr>
<td>7. There is no node.</td>
<td>7. It has a node perpendicular to the bond axis.</td>
</tr>
</tbody>
</table>
Combination of s-s, s-p, p-p, p-d and d-d orbitals:

1. Combination of s and s atomic orbitals:

   In this case, s orbital of one atom combines with the s orbital of the other atom. This forms an \( \sigma \) bond and hence the \( \sigma \) MOs. This is shown in Fig.1.6

   ![Fig.1.6 Formation of \( \sigma \) bond by s-s overlap](image)

2. Combination of s and p atomic orbital:

   S orbital of one atom may combine with p orbital of the other atom. This combination takes place only when lobes of the p-orbital are pointing along the axis joining the nuclei. This forms \( \sigma \) bond and hence the \( \sigma \) MOs. It is shown in Fig.1.7

   ![Fig.1.7 s-p combination of atomic orbitals](image)

3. Combination of p and p atomic orbitals:

   The combination of p-orbital of one atom with the p-orbital of the other atom is called p-p combination. Overlapping of AOs produces MOs.
(i) Formation of $\sigma$ - MOs:

Let us first consider the combination of two p-orbitals both of which have lobes pointing along the axis joining the nuclei. This forms an $\sigma$ bond and hence the $\sigma$ MOs. This produces a bonding MO and an antibonding MO, as shown in Fig.1.8

![Fig.1.8 p-p combination of atomic orbitals](image)

Here X-axis has been assumed to be the molecular axis.

(ii) Formation of $\pi$ MOs:

Consider the combination of two p- orbitals both of which have lobes perpendicular to the axis joining the nuclei. This forms a $\pi$ bond and hence $\pi$ MOs. Lateral overlap of orbitals occur. This produces $\pi$ bonding and $\pi$ antibonding MOs, as shown in fig.1.9
Difference between $\sigma$ and $\pi$ MOs:

<table>
<thead>
<tr>
<th>$\sigma$ MOs</th>
<th>$\pi$ MOs</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Formed by the overlap of the lobes of AOs pointing along the internuclear line.</td>
<td>1. Formed by the overlap of the lobes of AOs perpendicular to the line joining to the nuclei.</td>
</tr>
<tr>
<td>2. The electron density is concentrated between the two nuclei.</td>
<td>2. The electron density is zero between the two nuclei.</td>
</tr>
<tr>
<td>3. All bonding MOs are symmetric about the internuclear axis. All $\sigma$ antibonding MOs are unsymmetric.</td>
<td>3. These have no symmetry about the internuclear axis. All $\pi$ antibonding MOs are symmetric.</td>
</tr>
</tbody>
</table>

4. Combination of p and d atomic orbitals

The combination of p-orbital of one atom with the d-orbital of another atom is called p-d combination. This produces one bonding MO and one antibonding MO. As shown in fig.1.10.

![Diagram of p-p AOs giving bonding and antibonding MOs](image-url)
1. MOLECULAR ORBITAL THEORY

In such a case, usually Py or Pz orbital of one atom overlap with d-orbital of the other atom to form a \( \pi \) bond. The lateral overlap of AOs produces \( \pi \) MOs.

5. Combination of d and d atomic orbitals

The combination of d-orbital of one atom with the d-orbital of the other atom is called d-d combination. This produces one bonding MO denoted as \( \delta \) and one anti bonding MO denoted by \( \delta^* \). The formation of \( \delta \) MO takes place by the overlap of two \( d_{xy} \) or \( d_{x^2-y^2} \) AOs.
These δ MOs have two nodal planes along the molecular axis, as shown by dashed lines in fig.1.11 since the figure becomes complicated, formation of anti bonding Mo is shown here.

**Rules for Linear Combination of Atomic Orbitals:**

1. If the two wave functions of the atomic orbitals have the same signs of the wave function, then it will result in the formation of a bonding MO.
2. If the two wave functions of the atomic orbitals have the different signs of the wave function, then it will result in the formation of an anti bonding MO.
3. The number of molecular orbitals formed will be equal to the number of atomic orbitals taking part in combination.
4. The atomic orbitals which are of lower energy or which do not have proper symmetry for combination will result in the formation of non-bonding MO.
5. If there are three atomic orbitals participating in the bond formation, they will result in the formation of one bonding, one anti bonding and one non-bonding MO.
6. The AOs which form the MO should have comparable energies.

**Non-bonding combination of orbitals:**

The orbitals which do not take part in bonding are called as non-bonding MOs. These orbitals of atoms are either very low in energy or they are not of proper symmetry hence they are not used for bonding. So they are called as non-bonding MOs. Fig1.12 shows the symmetries unsuitable for combination of orbitals. Hence they form non-bonding orbitals.
1. **H$_2^+$ ion:**

It consists of two H atoms and one electron. Two 1s orbitals give two MOs – one bonding, that is $\sigma$ and one anti bonding that is $\sigma^*$. Since the bonding orbital is lower in energy, the electron occupies the bonding MO. Fig.1.13 shows the MO energy level diagram of H$_2^+$ molecular ion.

![MO Energy level Diagram for Homonuclear Diatomic molecules of First Row Elements](image)

The molecular orbital electron configuration of H$_2^+$ ion is written as (1s)$^1$. The energy evolved during the formation of H$_2^+$ ion is given by the formula

**Energy evolved (E) =**

$$\text{[No.of electrons in BMO x } (-\beta) \text{ + No.of electrons in ABMO x } (+\beta)]$$

$$= (1) \times (-\beta) + (0) \times (+\beta) = -\beta$$
The energy evolved $-\beta$ is also called **stabilization energy**. The number of bonds between the two atoms is called bond order. The bond order of this ion is given by the formula

**Bond Order (B.O.) =**

$$\frac{1}{2} [\text{No. of electrons in BMO} - \text{No. of electrons in ABMO}] = \frac{1}{2} (1 - 0) = 1/2$$

The molecular ion is expected to be somewhat stable. This species can be detected spectroscopically when hydrogen under reduced pressure is subjected to an electric discharge. Since the $H_2^+$ ion has one unpaired electron, it is **paramagnetic**.

2) **$H_2$ Molecule:**

It consists of two H atoms and their two electrons. Two 1s orbitals give two MOs- one bonding that is $\sigma$ and one antibonding that is $\sigma^*$. Since the bonding orbital is lower in energy, the two electron occupies the bonding MO. Fig.1.14 shows the MO energy level diagram of $H_2$ Molecule. The MO electron configuration of $H_2$ molecule is written as $(\sigma 1s)^2$. The energy evolved during the formation of $H_2$ molecule is given by the formula.
Energy evolved =
\[ \text{Energy evolved} = (2) \times (-\beta) + (0) \times (+\beta) = -2\beta \]

The energy evolved \(-2\beta\) are also called stabilization energy. The number of bonds between the two atoms is called bond order. The bond order of this molecule is given by the formula

\[ \text{Bond Order} = \frac{1}{2} (\text{No. electrons in BMO} - \text{No. of electrons in ABMO}) \]

\[ = \frac{1}{2} (2 - 0) = 1 \]

The molecule is stable. Since the H\(_2\) molecule has all the electrons paired, it is diamagnetic.

3) He\(_2^+\) ion:

It consists of two He atoms and three electrons. One He atom gives 1s\(^2\) electrons and the other He atom gives 1s\(^1\) electron. Two 1s orbitals give two MOs – one bonding, that is \(\sigma\) and one anti bonding that is \(\sigma^*\). Since the bonding orbital is lower in energy, the electron occupies the bonding MO.

Fig. 1.15 shows the MO energy level diagram of He\(_2^+\) molecule. First two electrons occupy the BMO. Third electron go to ABMO.
Energy evolved =

\[ \text{[No. of electrons in BMO X (-}\beta) + \text{No. of electrons in ABMO X (+}\beta)]\]

\[ = (2) \times (-\beta) + (1) \times (+\beta) = -\beta \]

The energy evolved \(-\beta\) is also called stabilization energy. The number of bonds between the two atoms is called bond order. The bond order of this ion is given by the formula

**Bond Order** = \(\frac{1}{2}[\text{No. of electrons in BMO} - \text{No. of electrons in ABMO}]\)

\[ = \frac{1}{2} (2-1) = 1/2 \]

The molecular ion \(\text{He}_2^+\) is expected to be somewhat stable. Since the \(\text{He}_2^+\) ion has one unpaired electron, it is paramagnetic.

4) \(\text{He}_2\) Molecule:

It contains two He atoms and four electrons. Each He atom gives \(1s^2\) electrons. Two \(1s\) orbitals give two MOs - one bonding, that is \(\sigma\) and one anti bonding, that is \(\sigma^*\). First two electrons occupy the bonding MO.

The bonding MO can accommodate only two electrons. So the next two electrons go to the anti bonding MO. Fig.1.16 shows the MO energy level diagram of \(\text{He}_2\) molecule.

The MO electron configuration of \(\text{He}_2\) molecule is written as \((\sigma1s)^2, (\sigma^*1s)^2\).

Hence the bonding and anti bonding orbitals are equally occupied.
The two electrons in anti bonding orbital cancel the effect of the two bonding electrons. The energy evolved during the formation of $\text{He}_2$ molecule is given by the formula

$$\text{Energy evolved} = \left[ \text{No. of electrons in BMO} \times (-\beta) + \text{No. of electrons in ABMO} \times (+\beta) \right]$$

$$= (2) \times (-\beta) + (2) \times (+\beta) = 0$$

The energy evolved, that is, the stabilization energy is zero so the molecule is not stable.

$$\text{Bond Order} = \frac{1}{2} \left[ \text{No. of electrons in BMO} - \text{No. of electrons in ABMO} \right]$$

$$= \frac{1}{2} (2 - 2) = 0$$

This shows that there is no bond formed between two He atoms. Since the $\text{He}_2$ molecule is not stable. It does not exist. Thus He is found as a monoatomic gas.

**MO Energy level Diagram for Homonuclear Diatomic molecules of second Row Elements**

Second row element contains 2s and 2p orbitals.
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The s orbital gives σ and σ* MOs. The overlap of Px and Px orbital gives σ px and σ*px MOs. The overlap of py and py orbital gives πpy and π*py MOs. The overlap of pz and pz orbitals gives πpz and π*pz MOs. The πpy and πpz MOs and similarly the π*py and π*pz MOs have equivalent energies hence they are said to be degenerate. The magnitude of the overlap decreases in the order s-s = pσ – pσ > pπ – pπ. Hence the value of Δ or β also decreases in the same manner. The energy sequence of the MOs is

\[
σ1s < σ*1s < σ2px < π2py = π2pz < π*2py = π*2pz < σ*2px.
\]

The diagram 1.17 (a) and the sequence of energy level assumes that s atomic orbital overlap with only s atomic orbital, p atomic orbital overlap with only p atomic orbital i.e. there is no interaction between s and p orbitals of a given atom.

In practice, such an interaction does take place and the sequence of energy levels is changed.
In Li₂, Be₂, B₂, C₂ and N₂ the energy difference between 2s and 2p atomic orbitals is not large and they are likely to interact when permitted by symmetry. Consequently, s and px atomic orbitals interact with one another resulting in the repulsion between pairs of orbitals of the same type, i.e. σ₂s and σ₂px and two σ* orbitals, i.e. σ*₂s and σ*₂px. The new sequence of MOs for Li₂, Be₂, B₂, C₂ and N₂ thus becomes

σ₁s < σ*₁s < σ₂s < σ*₂s < \pi₂py = \pi₂pz < σ₂px < \pi*₂py = \pi*₂pz < σ*₂px.

After nitrogen the energy difference between S and p atomic orbitals becomes sufficiently large and such effect may be practically neglected. The occupancy of available homonuclear orbitals in energy order is easily understood from the energy level diagram Fig.1.17 (b)
5) Li₂ Molecule

This molecule is formed by the combination of two lithium atoms. Each lithium atom has electron configuration 1s², 2s¹. The 1s orbital is lower in energy so it does not take part in bonding. Thus 1s orbital remain as a non-bonding orbital. Only the 2s orbital with its one electron takes part in bonding. Since there are two atomic orbitals, they will form two MOs, σ and σ*. There are two electrons which enter the bonding MO i.e. σ.

While writing the MO electron configuration of Li₂ Molecule, the presence of non-bonding 1s² electron is shown by capital letter K because these two electrons are present in the first shell i.e. K shell. There are two Li atoms taking part in bonding so the letter K is repeated. The remaining two electrons of the Li₂ Molecule go to the BMO. Fig. 1.18 shows the MO Energy level diagram of Li₂ Molecule. The MO electron configuration of Li₂ Molecule is written as [ KK (σ2s)²]. The stabilization energy is found out as follows.

\[
\text{Stabilisation Energy} = \left[ \text{No. of electrons in BMO} \times (-\beta) + \text{No. of electrons in ABMO} \times (+\beta) \right]
\]
\[
= (2) \times (-\beta) + (0) \times (+\beta) = -2 \beta
\]

**Bond Order** = \(\frac{1}{2} \left[ \text{No. of electrons in BMO} - \text{No. of electrons in ABMO} \right]
\]
\[
= \frac{1}{2} (2 - 0) = 1
\]

The bond order is one. The bond energy is 25 Kcal/mole. Li₂ Molecule exist in vapour state. Since all the electrons are paired, the molecule is diamagnetic. Li₂ Molecule is compared with H₂ Molecule, both these molecules are diamagnetic. They have bond order one.
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**H₂ Molecule** | **Li₂ Molecule**
---|---
1) Bond length = 0.74 Å0 | 1) Bond length = 2.67 Å0
2) Bond energy = 103 Kcal | 2) Bond energy = 25 Kcal

Bond energy of Li₂ Molecule is less than H₂ molecule because 2s and 2p orbitals of Li atom are much larger and more diffuse than the 1s orbital of hydrogen. They tend to overlap less effectively and at a greater internuclear distance than in case of 1s orbital of H.

The 1s electron of Li cause a repulsion between the atoms which loosens closer approach of the atoms. Due to above two reasons, bond length in Li₂ Molecule is more than that in H₂ Molecule and bond energy in Li₂ Molecule is less than that in H₂ Molecule.
6. Be₂ Molecule

This molecule is formed by the combination of two beryllium atoms. Each beryllium atom has electron configuration 1s², 2s². The 1s orbital is lower in energy so it does not take part in bonding. Thus 1s orbital remain as a non-bonding orbital. Only the 2s orbital with its one electron takes part in bonding. Since there are two atomic orbitals, they will form two MOs, σ and σ*. The first two electrons enter the BMO and the next two electrons enter the ABMO.

While writing the MO electron configuration of Be₂ Molecule, the presence of non-bonding 1s² electron is shown by capital letter K because these two electrons are present in the first shell i.e. K shell. There are two Be atoms taking part in bonding so the letter K is repeated. The two electrons of the Be₂ Molecule go to the BMO and two electrons in the ABMO. Fig. 1.19
shows the MO Energy level diagram of Be₂ Molecule. The MO electron configuration of Be₂ Molecule is written as [KK (σ2s)², (σ*2s)²]. The stabilization energy is found out as follows.

**Stabilization Energy =**

\[
\text{Stabilization Energy} = [\text{No. of electrons in BMO} \times (-\beta) + \text{No. of electrons in ABMO} \times (+\beta)]
\]

= \(2 \times (-\beta) + 2 \times (+\beta) = 0\)

**Bond Order =** \(\frac{1}{2} \left[ \text{No. of electrons in BMO} - \text{No. of electrons in ABMO} \right] \)

= \(\frac{1}{2} (2 - 2) = 0\)

The bond order is zero. The bond energy is zero. Be₂ Molecule is not in existence.

7. **B₂ Molecule**

This molecule is formed by the combination of two Boron atoms. Each Boron atom has electron configuration 1s², 2s², 2p¹. The 1s orbital is lower in energy so it does not take part in bonding. Thus 1s orbital remain as a non-bonding orbital. Only two 2s orbital and six 2p orbitals of two boron atoms i.e. total eight orbitals form total eight MOs. Here 2s and 2p orbitals of boron atom are close in energy so they interact and the sequence of energy levels of MOs is according to Fig. 1.17(b)

In B₂ Molecule While writing the MO electron configuration of B₂ Molecule, the presence of non-bonding 1s² electron is shown by capital letter K because these two electrons are present in the first shell i.e. K shell. There are two B atoms taking part in bonding so the letter K is repeated.

The remaining six electrons of the B₂ Molecular orbital following Aufbau principle and Hund’s rule of maximum multiplicity. First two electrons go to σ2s BMO, the next two go to the σ*2s BMO. The remaining
two electrons occupy the $\pi_2py$ and $\pi_2pz$ orbitals with parallel spins. These two orbitals are degenerate. Fig. 1.20 shows the MO Energy level diagram of $B_2$ Molecule.

The MO electron configuration of $B_2$ Molecule is written as 

$$[KK(\sigma_2s)^2, (\sigma^*2s)^2, (\pi_2py)^1, (\pi_2pz)^1].$$

The stabilization energy is found out as follows.

**Stabilisation Energy**

$$\text{Stabilisation Energy} = 
\text{[No.of electrons in BMO} \times (-\beta) + \text{No.of electrons in ABMO} \times (+\beta)]
$$

$$= (4) \times (-\beta) + (2) \times (+\beta) = -2\beta$$

**Bond Order**

$$\text{Bond Order} = \frac{1}{2} \text{ [No. of electrons in BMO} - \text{ No. of electrons in ABMO]}
$$

$$= \frac{1}{2} (4-2) = 1$$
The bond order is one. \( \text{B}_2 \) Molecule exist in vapour state. It has bond length 1.59 Å and bond energy 69 Kcal/mole. Since two electrons are unpaired, the molecule is paramagnetic.

8. \( \text{C}_2 \) Molecule

This molecule is formed by the combination of two carbon atoms. Each carbon atom has electron configuration \( 1s^2, 2s^2, 2p^2 \). The 1s orbital is lower in energy so it does not take part in bonding. Thus 1s orbital remains as a non-bonding orbital. Only two 2s orbital and six 2p orbitals of two carbon atoms i.e. total eight orbitals form total eight MOs. Here 2s and 2p orbitals of carbon atom are close in energy so they interact and the sequence of energy levels of MOs is according to Fig. 1.17(b) in \( \text{B}_2 \) Molecule.
While writing the MO electron configuration of C₂ Molecule, the presence of non-bonding 1s² electron is shown by capital letter K because these two electrons are present in the first shell i.e. K shell. There are two C atoms taking part in bonding so the letter K is repeated. The remaining eight electrons of the C₂ Molecular orbital following Aufbau principle and Hund’s rule of maximum multiplicity. First two electrons go to σ2s BMO, the next two go to the σ*2s BMO. The remaining four electrons occupy the π2py and π2pz orbitals. These two orbitals are degenerate. Fig. 1.21 shows the MO Energy level diagram of C₂ Molecule. The MO electron configuration of C₂ Molecule is written as [KK (σ2s)², (σ*2s)², (π2py)², (π2pz)²]. The stabilization energy is found out as follows.

**Stabilisation Energy =**

\[ \text{[No. of electrons in BMO x (-β) + No. of electrons in ABMO x (+β)]} \]

\[ = (6) \times (-β) + (2) \times (+β) = -4 \beta \]

**Bond Order =** \( \frac{1}{2} \times [\text{No. of electrons in BMO} - \text{No. of electrons in ABMO}] \)

\[ = \frac{1}{2} (6-2) = 2 \]

The bond order is two. C₂ Molecule exist in vapour state. It has bond length 1.31 Å and bond energy 150 Kcal/mole. Since all electrons are paired, the molecule is diamagnetic.

**9. N₂ Molecule**

This molecule is formed by the combination of two nitrogen atoms. Each nitrogen atom has electron configuration 1s², 2s², 2p³. The 1s orbital is lower in energy so it does not take part in bonding. Thus 1s orbital remain as a non-bonding orbital. Only two 2s orbital and six 2p orbitals of two nitrogen atoms i.e. total eight orbitals form total eight MOs. Here 2s and 2p orbitals
of nitrogen atom are close in energy so they interact and the sequence of energy levels of MOs is according to Fig.1.17 (b) in N₂ Molecule.

While writing the MO electron configuration of N₂ Molecule, the presence of non-bonding 1s² electron is shown by capital letter K because these two electrons are present in the first shell i.e.K shell. There are two N atoms taking part in bonding so the letter K is repeated. The remaining ten electrons of the N₂ Molecular orbital following Aufbau principle and Hund’s rule of maximum multiplicity. First two electrons go to σ2s BMO, the next two go to the σ*2s ABMO, four electrons go to the π2py and π2pz orbitals and the remaining two occupy the σ2px. Fig. 1.22 shows the MO Energy level diagram of N₂ Molecule.

![MO Energy Level diagram of N₂ Molecule](image-url)
The MO electron configuration of N₂ Molecule is written as \([KK (\sigma 2s)^2, (\sigma^* 2s)^2, (\pi 2py)^2, (\pi^* 2pz)^2 (\sigma 2px)^2]\). The stabilization energy is found out as follows.

**Stabilisation Energy =**

\[
\text{[No. of electrons in BMO \times (-\beta) + No. of electrons in ABMO \times (+\beta)]}
\]

\[
= (8) \times (-\beta) + (2) \times (+\beta) = -6\beta
\]

**Bond Order =** \(\frac{1}{2} \times \text{[No. of electrons in BMO – No. of electrons in ABMO]}\)

\[
= \frac{1}{2} (8 - 2) = 3
\]

The bond order is three. N₂ Molecule contains one \(\sigma\) and two \(\pi\) bonds. It has bond length 1.10 \(\text{Å}\) and bond energy 226 Kcal/mole. N₂ Molecule is highly stable and chemically inert. Since all electrons in N₂ Molecule are paired, the molecule is diamagnetic.

**10. O₂ Molecule**

This molecule is formed by the combination of two oxygen atoms. Each oxygen atom has electron configuration \(1s^2, 2s^2, 2p^4\). The \(1s\) orbital is lower in energy so it does not take part in bonding. Thus \(1s\) orbital remain as a non-bonding orbital. Only two \(2s\) orbital and six \(2p\) orbitals of two oxygen atoms i.e. total eight orbitals form total eight MOs. Here \(2s\) and \(2p\) orbitals of oxygen atom are well separated in energy so they do not interact and the sequence of energy levels of MOs in O₂ molecule is according to Fig. 1.17(a). While writing the MO electron configuration of O₂ Molecule, the presence of non-bonding \(1s^2\) electron is shown by capital letter K because these two electrons are present in the first shell i.e. K shell. There are two O atoms taking part in bonding so the letter K is repeated. The remaining twelve electrons of the O₂ Molecular orbital following Aufbau principle and Hund’s rule of maximum multiplicity.
1. MOLECULAR ORBITAL THEORY

First two electrons go to σ2s BMO, the next two go to the σ*2s ABMO, two electrons occupy the σ2px and the four electrons go to the \( \pi^*2py \) and \( \pi^*2pz \) orbitals and remaining two electrons go to the \( \pi^*2py \) and \( \pi^*2pz \) orbitals. Fig. 1.23 shows the MO Energy level diagram of O₂ Molecule.

The MO electron configuration of O₂ Molecule is written as [KK(σ2s)², (σ*2s)², (σ2px)², (π2py)², (π2pz)², (π*2py)¹, (π*2pz)¹]. The stabilization energy is found out as follows.

Stabilisation Energy =

\[
\text{[No. of electrons in BMO x (-\( \beta \)) + No. of electrons in ABMO x (+\( \beta \))]} \\
= (8) x (-\( \beta \)) + (4) x (+\( \beta \)) = -4 \beta
\]

Bond Order = \( \frac{1}{2} \) [No. of electrons in BMO – No. of electrons in ABMO]

\[
= \frac{1}{2} (8-4) = 2
\]
There is double bond in O₂ Molecule. It contains one σ and one π bond. It has bond length 1.21 Å and bond energy 118 Kcal/mole.

**Paramagnetism of O₂ Molecule:** In O₂ Molecule two unpaired electrons with parallel spins in the degenerate antibonding π MOs are shown in fig.1.23. This distribution of electrons in the antibonding π MOs is according to Hund’s rule. Oxygen molecule shows paramagnetic properties. MO theory gives a very simple explanation for the presence of two unpaired electrons and hence the paramagnetism of oxygen molecule.

It is very difficult to explain the paramagnetism of oxygen molecule with the help of VBT. The VBT assumes the sharing of electrons between the two oxygen atoms for the completion of octet configuration of each oxygen atom in the oxygen molecule. According to VBT oxygen molecule should be diamagnetic but in practice, it is paramagnetic. MO theory explains the paramagnetism of oxygen molecule.

**Effect of number of electrons in the antibonding MOs on bond lengths in diatomic species of oxygen:**

**O₂⁻ ion:**
O₂⁻ superoxide ion, is an example of molecular species. It has one electron more than the electrons of the O₂ molecule. Thus it has 17 electrons. Its MO representation is:

\[ O_2^- = [ KK(\sigma 2s)^2, (\sigma^*2s)^2, (\sigma 2px)^2 (\pi 2py)^2, (\pi^*2py)^2, (\pi^*2pz)^1] \]

It has one unpaired electron. The Bond order (BO) = ½(8- 5) = 1.5

Thus there is one σ bond and one three electron bond.

**O₂⁻² ion:** In a peroxide ion (O₂⁻²) there are two electrons more than the electrons in oxygen molecule. Thus it has 18 electrons and no unpaired electrons. Its MO representation is:
\[ \text{O}_2^{-2} = [KK(\sigma^2s)^2, (\sigma^*2s)^2, (\sigma^2px)^2, (\pi^2py)^2, (\pi^*2py)^2, (\pi^*2pz)^2] \]

The bond order (BO) = \( \frac{1}{2}(8-6) = 1 \) Thus there is one \( \sigma \) bond.

**\( \text{O}_2^+ \) ion:**

The \( \text{O}_2^+ \) positive ion is formed by losing one electron from the antibonding MO of the oxygen molecule. The bond order of \( \text{O}_2 \) is 2 while that of \( \text{O}_2^+ \) ion is 2.5 this results into the decrease of bond distance.

<table>
<thead>
<tr>
<th>Ion</th>
<th>Bond Order</th>
<th>Magnetic Property</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{O}_2^+ )</td>
<td>2.5</td>
<td>Paramagnetic</td>
</tr>
<tr>
<td>( \text{O}_2 )</td>
<td>2.0</td>
<td>Paramagnetic</td>
</tr>
<tr>
<td>( \text{O}_2^- )</td>
<td>1.5</td>
<td>Paramagnetic</td>
</tr>
<tr>
<td>( \text{O}_2^{-2} )</td>
<td>1.0</td>
<td>Dimagnetic</td>
</tr>
</tbody>
</table>

**11. \( \text{F}_2 \) molecule**

This molecule is formed by the combination of two fluorine atoms. Each fluorine atom has electron configuration 1s\(^2\), 2s\(^2\), 2p\(^5\). The 1s orbital is lower in energy so it does not take part in bonding. Thus 1s orbital remain as a non-bonding orbital. Only two 2s orbital and six 2p orbitals of two oxygen atoms i.e. total eight orbitals form total eight MOs. Here 2s and 2p orbitals of fluorine atom are well separated in energy so they do not interact and the sequence of energy levels of MOs in \( \text{F}_2 \) molecule is according to Fig.1.17(a).

While writing the MO electron configuration of \( \text{F}_2 \) Molecule, the presence of non-bonding 1s\(^2\) electron is shown by capital letter K because these two electrons are present in the first shell i.e.K shell. There are two F atoms taking part in bonding so the letter K is repeated. The remaining fourteen electrons of the \( \text{O}_2 \) Molecular orbital following Aufbau principle and Hund’s rule of maximum multiplicity.
First two electrons go to $\sigma$2s BMO, the next two go to the $\sigma^*$2s ABMO, two electrons occupy the $\sigma$2px four electrons go to the $\pi$2py and $\pi$2pz orbitals and the remaining four electrons go to the $\pi^*$2py and $\pi^*$2pz orbitals. Fig. 1.24 shows the MO Energy level diagram of F₂ Molecule.

![MO Energy Level Diagram of F₂ Molecule](image)

The MO electron configuration of F₂ Molecule is written as $\left[ KK(\sigma2s)^2, (\sigma^*2s)^2, (\sigma2px)^2, (\pi2py)^2, (\pi2pz)^2, (\pi^*2py)^2, (\pi^*2pz)^2 \right]$. The stabilization energy is found out as follows.

**Stabilisation Energy**

$$= [\text{No. of electrons in BMO} \times (-\beta) + \text{No. of electrons in ABMO} \times (+\beta)]$$

$$= (8) \times (-\beta) + (6) \times (+\beta) = -2 \beta$$

**Bond Order**

$$= \frac{1}{2} [\text{No. of electrons in BMO} - \text{No. of electrons in ABMO}]$$

$$= \frac{1}{2} (8-6) = 1$$
There is single bond in F₂ Molecule. It contains one σ bond. It has bond length 1.44 Å and bond energy 38 Kcal/mole. The molecule is stable.

12. Ne₂ Molecule

In this molecule all the orbitals are filled by electrons, so bond order is zero. Stabilization energy is also zero. Ne₂ Molecule is not stable so it does not exist. (Explanation is similar to that of He₂ Molecule)

MO Energy level Diagram for Heteronuclear Diatomic molecules:

1) Carbon monoxide Molecule (CO)

Carbon monoxide is a heteronuclear diatomic molecule. It is formed by the combination of carbon atom and oxygen atom. Here oxygen is more electronegative than carbon. The electron configuration of carbon is 1s², 2s², 2p² and that of oxygen is 1s², 2s², 2p⁴. The inner 1s electron of C and O don’t take part in bonding.
The Carbon monoxide Molecule is isoelectronic with N₂ molecule. Both of them have ten electron. The MO energy level diagram of N₂ molecule is similar to that of CO molecule. Except that the energy level of oxygen are lower than that of carbon atom. Fig 1.25 shows the energy level diagram of CO molecule. Since oxygen is more electronegative than carbon, its energy level is lower than those of carbon. The oxygen orbital contribute more to the antibonding MO. The eight electron in the bonding MO try to neutralize the greater nuclear charge on the oxygen core. Hence the polarity of CO is low. The MO electron configuration of CO molecule is

\[ \text{KK}(\sigma^2s)^2, (\sigma^*2s)^2,(\pi^2py)^2, (\pi^2pz)^2, (\sigma^2px)^2] \]

**Stabilisation Energy**

\[
\text{Stabilisation Energy} = (\text{No. of electrons in BMO x } (-\beta)) + \text{No.of electrons in ABMO x } (+\beta)
\]

\[
= (8) x (-\beta) + (2) x (+\beta) = -6\beta
\]

**Bond order**

\[
\text{Bond order} = \frac{1}{2} (8-2) = 3
\]

The CO molecule contains a triple bond. There is one \( \sigma \) and two \( \pi \) bonds. The bond length in CO molecule is 1.128 \( \text{Å} \) and bond energy 225 Kcal/mole.

**2. Nitric Oxide (NO) Molecule**

Nitric oxide is a heteronuclear diatomic molecule. It is formed by the combination of nitrogen atom and oxygen atom. Here oxygen is more electronegative than nitrogen. The electron configuration of nitrogen is \( 1s^2, 2s^2, 2p^3 \) and that of oxygen is \( 1s^2, 2s^2, 2p^4 \)

The inner 1s electron of N and O do not take part in bonding. The MO electron configuration of NO Molecule can be qualitatively obtained either by removing one electron from the configuration of O₂ molecule or by adding one electron to the configuration of N₂ molecule.
The MO energy level diagram of NO molecule is shown in fig 1.26 since oxygen is more electronegative than nitrogen, its energy level are lower than those of carbon.

\[ \text{MO electron configuration of NO molecule is } [\text{KK} (\sigma 2s)^2, (\sigma^* 2s)^2, (\sigma 2px)^2, (\pi 2py)^2, (\pi^* 2py)^1] \]

**Stabilisation Energy**

\[ \text{Stabilisation Energy} = (\text{No. of electrons in BMO} \times (-\beta)) + (\text{No. of electrons in ABMO} \times (+\beta)) \]

\[ = (8) \times (-\beta) + (3) \times (+\beta) = -5\beta \]

**Bond order**

\[ = \frac{1}{2} (8-3) = 2.5 \]
The bond length in NO molecule is 1.15 Å and bond energy 162 Kcal/mole, which is considerably less than that of O₂ or N₂ molecule. There is one unpaired electron in the (π*) orbital so the molecule is paramagnetic.

Nitrosyl Ion (NO⁺)

In the process of ionization, NO loses one electron and forms NO⁺ ion. The electron is removed from the antibonding (π*2py) orbital. The MO electron configuration of NO⁺ ion is

\[ [\text{K K}, (\sigma 2s)^2, (\sigma^* 2s)^2, (\sigma 2px)^2, (\pi 2py)^2, (\pi 2pz)^2] \]

The bond order of NO⁺ ion is \( \text{Bond order} = \frac{1}{2} (8-2) = 3 \)

Thus the bond in NO⁺ ion stronger and shorter than that in NO. The NO⁺ forms stable compound like NO, HSO₄(NO⁺, HSO₄⁻).

Hydrogen chloride (HCl) Molecule

It is a heteronuclear diatomic molecule in which chlorine atom is much more electronegative than hydrogen. The electron configuration of H is 1s¹ and that of Cl is 1s², 2s², 2p⁶, 3s², 3p⁵

The atomic orbitals of more electronegative element contribute more to the formation of bonding MO and less to the antibonding MO. Similarly, the atomic orbital of less electronegative element contribute more to the formation of antibonding MO and less to the bonding MO. That is the electron in the MO spent more time round one atom than the other. This causes charge separation and on the atoms and develops a dipole, thus the covalent bond in HCl molecule has partial ionic character.

Let us consider the formation of MO in HCl molecule. It is shown that the filled 1s, 2s, 2p and 3s orbitals of chlorine atom are lower in energy and
hence can not participate in bonding. Only the 3p orbitals of chlorine atom of suitable energy and can combine with the 1s orbital of hydrogen. If we assume H-Cl axis as the x-axis, then only the 3Px orbital of chlorine atom is of correct symmetry pointing along H-Cl axis. Thus out of the three 3Px orbitals only 3Px orbital of chlorine will be the most suitable one for bonding because it matches in symmetry and energy with the 1s orbital of hydrogen.

The other two 3p orbitals viz. 3py and 3pz being perpendicular to the bond axis are not of correct symmetry and hence remain nonbonding. The overlapping of 1s orbital of hydrogen and 3px orbital of chlorine gives rise to σ a bonding MO and σ* MO. Fig.1.27 shows the MO energy level diagram of HCl molecule.

While writing the electron configuration of HCl molecule, for H atom there are no electrons to be written as k shell. However, for Cl atom, for 1s² electrons we write k and for 2s² and 2p⁶ electrons we write L. Neglecting the 3s², 3pₓ² and 3pᵧ² electrons of chlorine atom, the MO electron configuration of HCL molecule is written as [K L (σsp)²]. The two electron occupy the bonding MO.

**Bond order** = ½ (2-1) = 1
The bond order is one. The molecule is diamagnetic. The bonding MO is closer to 3p_x orbital of chlorine atom hence it has more character of 3px orbital. the antibonding MO is closer to 1s orbital of hydrogen atom so it has more character of 1s orbital. H-Cl molecule is a polar and H-Cl bond is a polar covalent bond. The bond length in HCl molecule is 1.27Å° and bond energy is 103 kcal/mole.

**Molecular Orbitals in Heteronuclear Triatomic Molecules**

The molecules formed by three atoms of two different elements are called heteronuclear triatomic molecules. E.g. CO_2, NO_2, NO_2^- (nitrite molecule). These molecules may contain only sigma bond or both sigma and pi bonds.

**Molecular orbital diagram for carbon dioxide CO_2**

It is linear triatomic molecule. It is represented as \[ \text{O}^\sigma \pi \text{C}^\sigma \pi \text{O} \]

The outer electron configuration of C is 2s^2, 2p^2 and that of O is 2s^2, 2p^4. The molecular orbitals for CO_2 molecule are obtained from valence orbitals. Thus, the molecule contain 16 outer shell electrons, made up from six electrons from each of the two oxygen atoms and four electrons from the C atom. However the 2s orbitals of oxygen and the electrons therein are too low in energy so they do not take part in bonding. The MO diagram for CO_2 molecule is shown in figure 1.29.
Molecular orbital theory

1. MOLECULAR ORBITAL THEORY

Molecular orbital diagram for nitrogen dioxide molecule – NO₂
It is an angular triatomic molecule. It is represented as

\[
\begin{align*}
\text{N} & \quad \text{O} \quad \text{O} \\
\end{align*}
\]

The outer electron configuration of N is 2s² 2p³ and that of O is 2s² 2p⁴. The MOs for NO₂ molecule are obtained from these valence orbitals. Thus, the molecule NO₂ contain 17 outer shell electrons, made up from six electrons from each of the two O atoms and five electrons from the N atom. However
the 2s orbitals of oxygen and the electrons therein are too low in energy so they do not take part in bonding. The MO diagram for NO$_2$ molecule is shown in figure 1.30.

**Molecular orbital energy level diagram for NO$_2$**

![Molecular orbital energy level diagram for NO$_2$](image)

**Fig. 1.30 MO energy level diagram for NO$_2$ molecule**