Chemical Bonding-IV

Section (A) : Molecular Orbital Theory (MOT)

The molecular orbital theory was developed by F. Hund and R.S. Mulliken in 1932. The salient features are:

(i) Just as electrons of any atom are present in various atomic orbitals, electrons of the molecule are present in various molecular orbitals.

(ii) Molecular orbitals are formed by the combination of atomic orbitals of comparable energies and proper symmetry.

(iii) An electron in an atomic orbital is influenced by one nucleus, while in a molecular orbital it is influenced by two or more nuclei depending upon the number of the atoms in the molecule. **Thus an atomic orbital is monocentric while a molecular orbital is polycentric.**

(iv) The number of molecular orbitals formed is equal to the number of combining atomic orbitals. When two atomic orbitals combine, two molecular orbitals called **bonding molecular orbital** and **anti-bonding molecular orbital** are formed.

(v) The bonding molecular orbital has lower energy and hence greater stability than the corresponding antibonding molecular orbital.

(vi) Just as the electron probability distribution around a nucleus in an atom is given by an atomic orbital, the electron probability distribution around a group of nuclei in a molecule is given by molecular orbital.

(vii) The molecular orbitals like the atomic orbitals are filled in accordance with the **Aufbau principle** obeying the **Pauli Exclusion principle** and the **Hund's Rule of Maximum Multiplicity**. But the filling order of these molecular orbitals is always **experimentally decided**, there is no rule like (n + l) rule in case of atomic orbitals.

Formation of Molecular Orbitals : Linear Combination of Atomic Orbitals(LCAO)

- Consider the example of H_2 molecule and label both nucleis as H_A and H_B.
- Both nucleus will have a wave function Ψ_A & Ψ_B associated to it.
- Bonding molecular orbital will be formed when both wave functions will combine in same phase.
  $\psi_m = [\psi_A + \psi_B]$
- Antibonding molecular orbital will be formed when both wave functions will combine in opposite phase.
  $\psi^*_m = [\psi_A - \psi_B]$

Note: The above equation should be regarded as the summation of the wave functions not as the mathematical addition or subtraction of wave function.

The molecular wave functions ψ_m and ψ^*_m are bonding and antibonding molecular orbitals; orbitals of this type, in which the line joining the two nuclei is a symmetry axis for the electron distribution, are known as σ orbitals if bonding and σ^* orbitals if antibonding, so we may alternatively denote them σ_{1s} and σ^*_{1s} orbitals. When the two 1s wave functions are added, they reinforce one another everywhere, and especially in the region between the two nuclei; the build-up of electron density there diminishes the internuclear repulsion and a strong bond results. When one of the two 1s wave functions is subtracted from the other, they exactly cancel in a plane midway between the nuclei, and the molecular wave function changes sign at this nodal plane. This lack of electron density raises the internuclear repulsion, the total energy becomes higher, the two nuclei are not bonded together, and the orbital is described as antibonding.

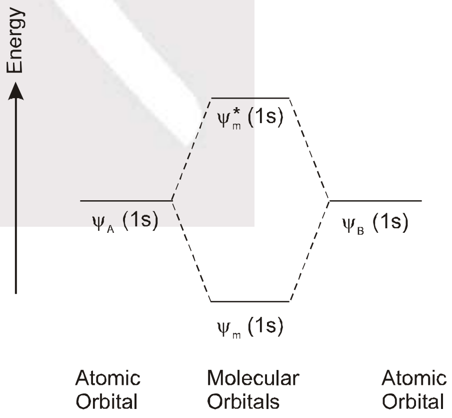

Figure: The relative energy levels of molecular orbitals and their constituent atomic orbitals for H_2.

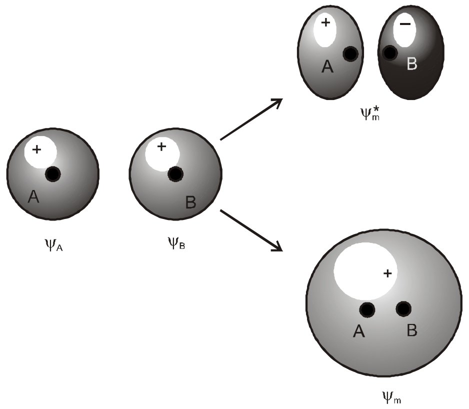

Figure : Another representation of the formation of molecular orbitals for H_2. Since the σ and σ^* orbitals are respectively centrosymmetric and non-centrosymmetric these orbitals may also be denoted by the symbols σ_g and σ^*_u.

Molecular orbital wave functions are designated as ψ_g and ψ_u. g and u refer to the symmetry of the orbital about its centre. If the wave function is centrosymmetric, i.e. has the same sign at the same distance in opposite directions from the centre of symmetry. The orbital is said to gerade (German, even); if it changes sign on inversion about the centre it is said to ungerade (German, uneven).
Alternative method for determining the symmetry of the molecular orbital is to rotate the orbital about the line joining the two nuclei and then about a line perpendicular to this. If the sign of the lobes remain the same, the orbital is gerade, and if the sign changes, the orbital is ungerade.
Thus σ and π^* molecular orbitals are gerade and σ^* and π molecular orbitals are ungerade.

CONDITIONS FOR THE COMBINATION OF ATOMIC ORBITALS :

The linear combination of atomic orbitals to form molecular orbitals takes place only if the following conditions are satisfied :

1. **The combining atomic orbitals must have the same or nearly the same energy.** This means that 1s orbital can combine with another 1s orbital but not with 2s orbital because the energy of 2s orbital is appreciably higher than that of 1s orbital. It, therefore, means that only a limited number of combinations of atomic orbitals are possible.
2. **The combining atomic orbitals must have the same symmetry about the molecular axis.** By convention z-axis is taken as the molecular axis. It is important to note that atomic orbitals having same or nearly the same energy will not combine if they do not have the same symmetry. For example, $2p_z$ orbital of one atom can combine with $2p_z$ orbital of the other atom but not with the $2p_x$ or $2p_y$ orbitals because of their different symmetries.
3. **The combining atomic orbitals must overlap to the maximum extent.** Greater the extent of overlap, the greater will be the electron-density between the nuclei of a molecular orbital.

TYPES OF MOLECULAR ORBITALS :

Molecular orbitals of diatomic molecules are designated as σ(sigma), π(pie), δ(delta) etc.
In this nomenclature, the **sigma (σ) molecular orbitals are symmetrical around the bond-axis while pi (π) molecular orbitals are not symmetrical.** For example, the linear combination of 1s orbitals centered on two nuclei produces two molecular orbitals which are symmetrical around the bond-axis. Such molecular orbital's are of the σ type and are designated as $\sigma 1s$ and σ^*1s [Fig.(a)]. If internuclear axis is taken to be in the z-direction, it can be seen that a linear combination of $2p_z$-orbitals of two atoms also produces two sigma molecular orbitals designated as $\sigma 2p_z$ and $\sigma^* 2p_z$. [Fig. (b)] Molecular orbitals obtained from $2p_x$ and $2p_y$ orbitals are not symmetrical around the bond axis because of the presence of positive lobes plane. Such molecular orbitals, are labelled as π and π^* [Fig. (c)]. A π bonding MO has large electron density above and below the inter nuclear axis. The π^* antibonding MO has a node between the nuclei.
δ-type of molecular orbitals are obtained by involvement of d-orbitals into bonding.

Difference between π molecular orbitals and the σ orbitals.

(1) For π overlap the lobes of the atomic orbitals are perpendicular to the line joining the nuclei, while for σ overlap the lobes point along the line joining the two nuclei.

(2) For π molecular orbitals, ψ is zero along the internuclear line and consequently the electron density ψ^2 is also zero. This is in contrast to σ orbitals.

(3) The symmetry of π molecular orbitals is different from that shown by σ orbitals. If the bonding π MO is rotated about the inter nuclear line a change in the sign of lobe occurs. The π bonding orbitals are therefore ungerade, where as all σ bonding MO's are gerade. Conversely the antibonding π MO's are gerade while all σ antibonding MO's are ungerade.

ENERGY LEVEL DIAGRAM FOR MOLECULAR ORBITALS :

The energy levels of molecular orbitals have been determined experimentally from spectroscopic data for homonuclear diatomic molecules of second row elements of the periodic table. The increasing order of energies of various molecular orbitals for O_2 and F_2 is given below :

$\sigma 1s < \sigma^*1s < \sigma 2s < \sigma^*2s < \sigma 2p_z < (\pi 2p_x = \pi 2p_y) < (\pi^*2p_x = \pi^*2p_z) < \sigma^*2p_z$.

The increasing order of energies of various molecular orbitals for Be_2, B_2, C_2, N_2 etc., is :

$\sigma\ 1s < \sigma^*\ 1s < \sigma 2s < \sigma^*2s < (\pi 2p_x = \pi 2p_y) < \sigma 2p_z < (\pi^*2p_x = \pi^*2p_y) < \sigma^*2p_z$

The important characteristic feature of this order is that the **energy of $\sigma 2p_z$ molecular orbital is higher than that of $\pi 2p_x$ and $\pi 2p_y$ molecular orbitals.**

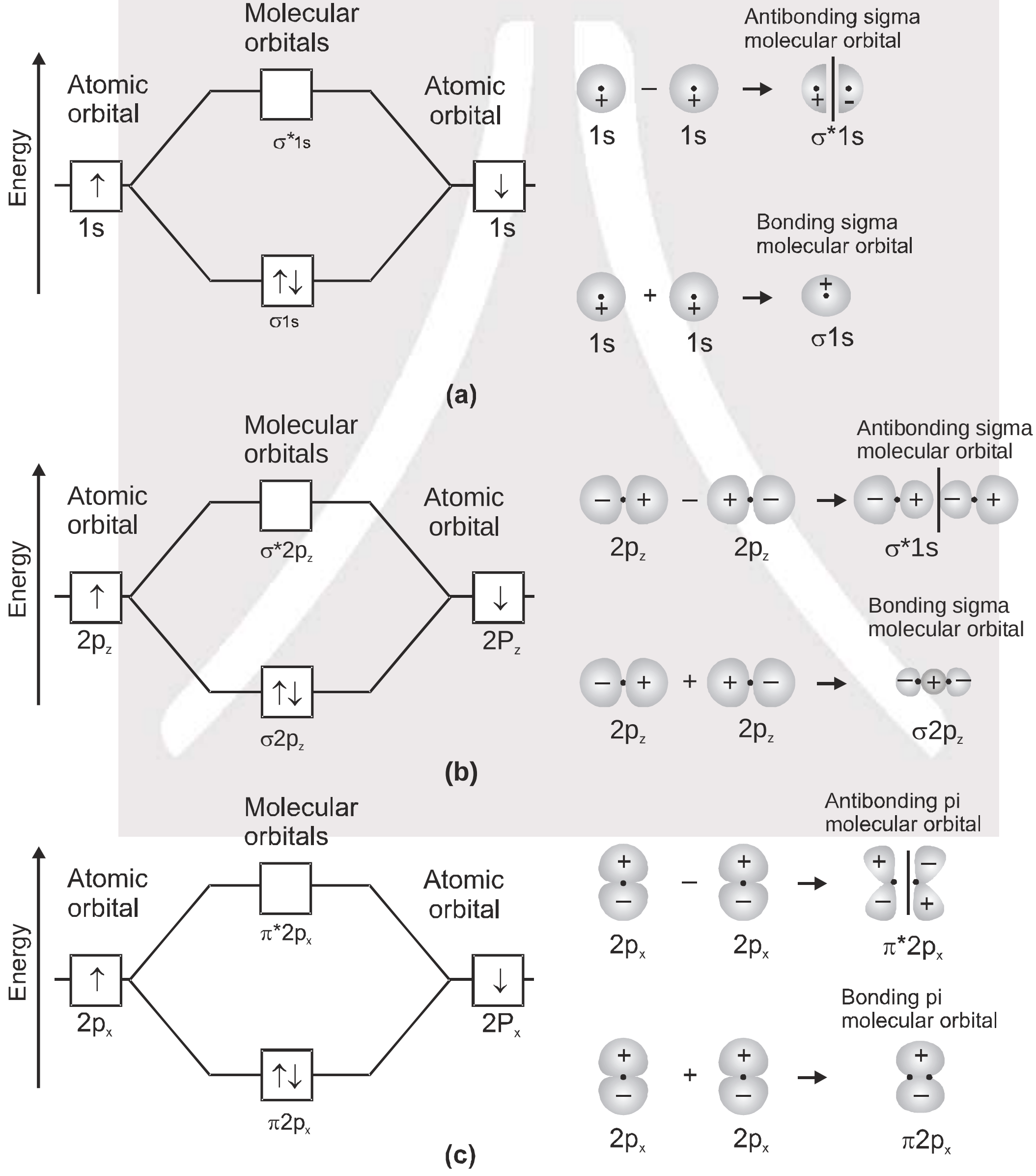

Figure : *Bonding and antibonding molecular orbitals formed through combinations of (a) 1s atomic orbitals; (b) $2p_z$ atomic orbitals and (c) $2p_x$ atomic orbitals.*

Section (B) : Application of MOT

ELECTRONIC CONFIGURATION AND MOLECULAR BEHAVIOUR

The distribution of electrons among various molecular orbitals is called the electronic configuration of the molecule. From the electronic configuration of the molecule, it is possible to get important information about the molecule as discussed below.

(i) The molecule is stable if N_b is greater than N_a, and (ii) The molecule is unstable if N_b is less than N_a

In (i) more bonding orbitals are occupied and so the bonding influence is stronger and a stable molecule results. In (ii) the antibonding influence is stronger and therefore the molecule is unstable.

N_b is number of electrons in bonding molecular orbitals and N_a is number of electrons in antibonding molecular orbitals.

- **BOND ORDER**

Bond order (B.O.) = ½(N_b – N_a)

A positive bond order (i.e., $N_b > N_a$) means a stable molecule while a negative (i.e., $N_b < N_a$) or zero (i.e., $N_b = N_a$) bond order means an unstable molecule.

- **BOND-LENGTH**

The bond order between two atoms in a molecule may be taken as an approximate measure of the bond length. The bond length decreases as bond order increases.

MAGNETIC NATURE

If all the molecular orbitals in a molecule are doubly occupied, the substance is diamagnetic (repelled by magnetic field) e.g., N_2 molecule. However if one or more molecular orbitals are singly occupied it is paramagnetic (attracted by magnetic field), e.g., O_2 molecule.

BONDING IN SOME HOMONUCLEAR DIATOMIC MOLECULES

1. **Hydrogen molecule (H_2) :** $(\sigma 1s)^2$

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

This means that the two hydrogen atoms are bonded together by a single covalent bond. The bond dissociation energy of hydrogen molecule has been found to be 438 kJ mol^{-1} and bond length equal to 74 pm. Since no unpaired electron is present in hydrogen molecule, therefore, it is diamagnetic.

2. **Helium molecule (He_2) :** $(\sigma 1s)^2\ (\sigma^*1s)^2$

Bond order of He_2 is ½(2 – 2) = 0

The molecular orbital description of He_2 predicts two electrons in a bonding orbital and two electrons in an antibonding orbital, with a bond order of zero - in other words, no bond. This is what is observed experimentally. The noble gas He has not significant tendency to form diatomic molecules and, like the other noble gases, exists in the form of free atoms. He_2 has a very low binding energy, approximately 0.01J/mol ; for comparison, H_2 has a bond energy of 436 kJ/mol.

3. **Lithium molecule (Li_2) :** $(\sigma 1s)^2\ (\sigma^*1s)^2\ (\sigma 2s)^2$

Its bond order, therefore, is 1/2(4 – 2) = 1. It means that Li_2 molecule is stable and since it has no unpaired electrons it should be diamagnetic. Indeed diamagnetic Li_2, the molecules are known to exist in the vapour phase. The MO model predicts a single Li-Li bond in Li_2, in agreement with gas phase observations of the molecule.

Beryllium (Be_2) : $(\sigma 1s)^2\ (\sigma^*1s)^2\ (\sigma 2s)^2\ (\sigma^*2s)^2$

Be_2 has the same number of antibonding and bonding electrons and consequently a bond order of zero. Hence, like He_2, Be_2 is not a stable chemical species.

Boron (B_2) : $(\sigma 1s)^2\ (\sigma^*1s)^2\ (\sigma 2s)^2\ (\sigma^*2s)^2\ (\pi 2p^1_x = \pi 2p^1_y)\ (\sigma p_z)^0$

Here is an example in which the Molecular orbital model has distinct advantage over the Lewis dot picture, B_2 is found only in the gas phase; solid boron is found in several very hard forms with complex bonding, primarily involving B_{12} icosahedra. B_2 is paramagnetic. This behaviour can be explained if its two highest energy electrons occupy separate p-orbitals. The Lewis dot model cannot account for the paramagnetic behaviour of this molecule.

B_2 is also a good example of the energy level shift caused by the mixing of s and p orbitals. In the absence of mixing, the σ_g (2p) orbital is expected to be lower in energy than the π_u(2p) orbitals and the resulting molecule would be diamagnetic. However, mixing of the σ_g(2s) orbital with the σ_g(2p) orbital lowers the energy of the σ_g(2s) orbital and increases the energy of the σ_g(2p) orbital to a higher level than the π orbitals, giving the order of energies shown above. As a result, the last two electrons are unpaired in the degenerate (having the same energy) π orbitals, and the molecule is paramagnetic. Overall, the bond order is 1, even though the two p electrons are in different orbitals. The bond order of B_2 is 1/2(6 – 4) = 1.

4. **Carbon molecule (C_2):** $(\sigma 1s)^2\ (\sigma^*1s)^2\ (\sigma 2s)^2\ (\sigma^*2s)^2\ (\pi 2p_x^2 = \pi 2p_y^2)$ or KK $(\sigma 2s)^2\ (\sigma^*2s)^2\ (\pi 2p_x^2 = \pi 2p_y^2)$
The simple MO picture of C_2 predicts a doubly bonded molecule with all electrons paired, but with both highest occupied molecular orbitals (HOMOs) having π symmetry. It is unusual because it has two π bonds and no σ bond. The bond dissociation energies of B_2, C_2 and N_2 increase steadily, indicating single, double, and triple bonds with increasing atomic number. Although C_2 is not a commonly encountered chemical species (carbon is more stable as diamond, graphite, and the fullerenes), the acetylide ion, C_2^{2-}, is well known, particularly in compounds with alkali metals, alkaline earths, and lanthanides. According to the molecular orbital model, C_2^{2-} should have a bond order of 3 (configuration $\pi_u^2 \pi_u^2 \sigma_g^2$). This is supported by the similar C–C distances in acetylene and calcium carbide (acetylide) :

Table-1

C – C Distance (pm)	
C = C (gas phase)	132
H – C ≡ C – H	120.5
CaC_2	119.1

The bond order of C_2 is 1/2 (8 – 4) = 2 and C_2 should be diamagnetic. Diamagnetic C_2 molecules have indeed been detected in vapour phase. It is important to note that double bond in C_2 consists of both pi bonds because of the presence of four electrons in two pi molecular orbitals. In most of the other molecules a double bond is made up of a sigma bond and a pi bond.

5. **Nitrogen molecule (N_2) :** $(\sigma 1s)^2\ (\sigma^*1s)^2\ (\sigma 2s)^2\ (\sigma^*2s)^2\ (\pi 2p_x^2 = \pi 2p_y^2)\ (\sigma 2p_z)^2$
N_2 has a triple bond according to both the Lewis and the molecular orbital models. This is in agreement with its very short N–N distance (109.8 pm) and extremely high bond dissociation energy (942kJ/mol.). Atomic orbitals decrease in energy with increasing nuclear charge Z ; as the effective nuclear charge increases, all orbitals are pulled to lower energies. The shielding effect and electron-electron interactions cause an increase in the difference between the 2s and 2p orbital energies as Z increases, from 5.7 eV for boron to 8.8 eV for carbon and 12.4 eV for nitrogen. As a result, the $\sigma_g(2s)$ and $\sigma_g(2p)$ levels of N_2 interact (mix) less than the B_2 and C_2 levels, and the σ_g (2p) and $\pi_u(2p)$ are very close in energy.
The bond order of N_2 is 1/2(10 – 4) = 3. It contains one sigma and two π bonds.

6. **Anionic nitrogen species (N_2^-) :** Though 15 electrons but derived from N_2, hence electronic configuration will be according to N_2
Electronic configuration : $(\sigma 1s)^2\ (\sigma^*1s)^2\ (\sigma 2s)^2\ (\sigma^*2s)^2\ (\pi 2p_x^2 = \pi 2p_y^2)\ (\sigma 2p_z)^2,\ (\pi^*2px)^1$
The bond order of N_2 is 1/2(10 – 5) = 2.5. It is paramagnetic species.

7. **N_2^+ :** Bond order = 2.5, out of N_2^+ and N_2^-, N_2^- is less stable though both have equal bond order but N_2^- has greater number of antibonding electrons.

8. **Oxygen molecule (O_2) :** $(\sigma 1s)^2\ (\sigma^*1s)^2\ (\sigma 2s)^2\ (\sigma^*2s)^2\ (\sigma 2p_z)^2\ (\pi 2p_x^2 = \pi 2p_y^2)\ (\pi^*2p_x^1 = \pi^*2p_y^1)$
O_2 is paramagnetic. This property, as for B_2, cannot be explained by the traditional Lewis dot structure $(\ddot{O}=\ddot{O})$, but is evident from the molecular orbital picture, which assigns two electrons to the degenerate π_g^* orbitals. The paramagnetism can be demonstrated by pouring liquid O_2 between the poles of a strong magnet; some of the O_2 will be held between the pole faces until it evaporates. The bond order of O_2 is $\frac{1}{2}\left[N_b - N_a\right] = \frac{1}{2}[10-6] = 2$. So in oxygen molecule, atoms are held by a double bond. Moreover, it may be noted that it contains two unpaired electrons in π^*2p_x and π^*2p_y molecular orbitals, therefore, **O_2 molecule should be paramagnetic, a prediction that corresponds to experimental observation.** Several ionic forms of diatomic oxygen are known, including O_2^+, and O_2^{2-}. The internuclear O–O distance can be conveniently correlated with the bond order predicated by the molecular orbital model, as shown in the following table.

Table-2

	Bond Order	**Internuclear Distance (pm)**	**Number of unpaired(s) Electrons**
O_2^+ (dioxygenyl)	2.5	112.3	1
O_2 (dioxygen)	2.0	120.07	2
O_2^- (superoxide)	1.5	128	1
O_2^{2-} (peroxide)	1.0	149	0
Note : Oxygen-oxygen distances in O_2^- and O_2^{2-} are influenced by the cation. This influence is especially strong in the case of O_2^{2-} and is one factor in its unsually long bond distance.			

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The extent of mixing is not sufficient in O_2 to push the $\sigma_g(2p)$ orbital to higher energy than the $\pi_g(2p)$ orbitals. The order of molecular orbitals shown is consistent with the photoelectron spectrum.

Fluorine molecule (F_2) : $(\sigma 1s)^2$ $(\sigma^*1s)^2$ $(\sigma 2s)^2$ $(\sigma^*2s)^2$ $(\sigma 2p_z)^2$ $(\pi 2p^2_x = \pi 2p^2_y)$ $(\pi^*2p_x^2 = \pi^*2p^2_y)$

The molecular orbital picture of F_2 shows a diamagnetic molecule having a single fluorine-fluorine bond, in agreement with experimental data on this very reactive molecule.

The net bond order in N_2, O_2, and F_2 is the same whether or not mixing is taken into account, but the order of the filled orbitals is different. The switching of the order of the $\sigma_g(2p)$ and $\pi_u(2p)$ orbitals can occur because these orbitals are so close in energy ; minor changes in either orbital can switch their order. The energy difference between the 2s and 2p orbitals of the atoms increases with increasing nuclear charge, from 5.7 eV in boron to 27.7 eV in fluorine. Because the difference becomes greater, the s-p interaction decreases and the "normal" order of molecular returns in O_2 and F_2. The higher σ_g orbital is seen again in CO.

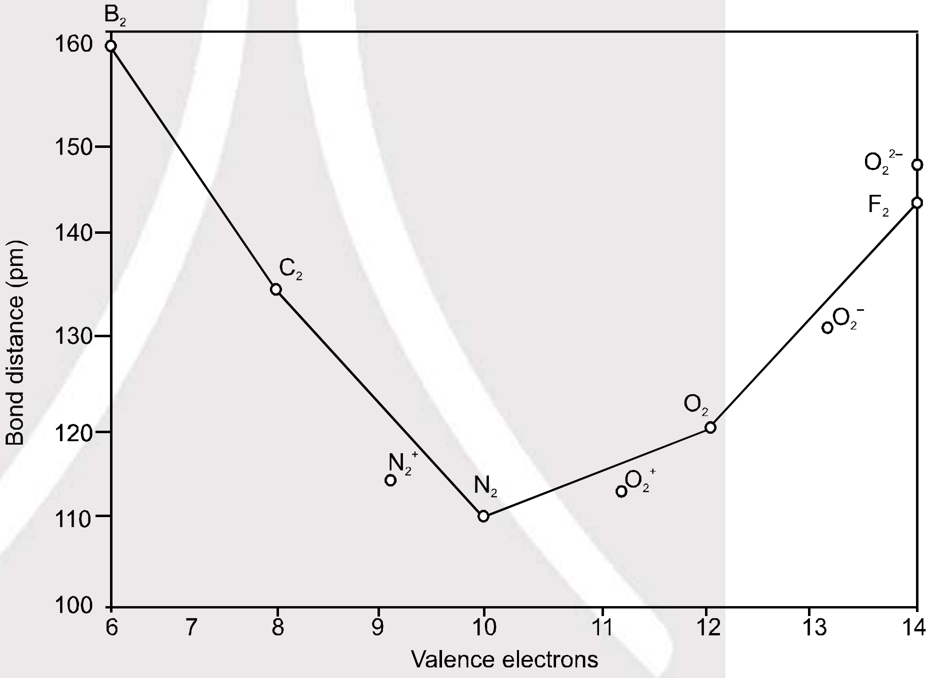
Neon molecule (Ne_2) : $(\sigma 1s)^2$ $(\sigma^*1s)^2$ $(\sigma 2s)^2$ $(\sigma^*2s)^2$ $(\sigma 2p_z)^2$ $(\pi 2p^2_x = \pi 2p^2_y)$ $(\pi^*2p_x^2 = \pi^*2p^2_y)$ $(\sigma^*2p_z)^2$

All the molecular orbitals are filled, there are equal numbers of bonding and antibonding electrons and the bond order is therefore zero. The Ne_2 molecule is a transient species, if it exists at all.

Note : **HOMO :** Highest Occupied Molecular Orbital., **LUMO :** Lowest Unoccupied Molecular Orbital

Bond lengths in homonuclear diatomic molecules

Figure shows the variation of bond distance with the number of valence electrons in second-period p block homonuclear diatomic molecules. As the number of electrons increases, the number in bonding orbitals also increases, the bond strength becomes greater, and the bond length becomes shorter. This continues up to 10 valence electrons in N_2 and then the trend reverses because the additional electrons occupy antibonding orbitals. The ions N_2^+, O_2^+, O_2^{2+} are also shown in the figure and follow a similar trend.



Figure

Solved Examples

Ex-1. Though O_2 molecule is paramagnetic yet it is a colourless gas. Why ?

Sol. It is because the energy gap between HOMO and LUMO levels in O_2 molecule is so large that radiations of visible light cannot excite a e^- from HOMO to LUMO. In fact O_2 gas shows absorption in UV zone. So it is colourless.

Ex-2. Correct order of bond energy is:

(A) $N_2 > N_2^+ > N_2^- > N_2^{2-}$ (B) $N_2^+ > N_2^- > N_2^{2-} > N_2$ (C) $N_2 > N_2^- = N_2^+ > N_2^{2-}$ (D) $N_2^- > N_2 = N_2^+ > N_2^{2-}$

Sol. **(A)** Bond order is directly proportional to the bond energy.

Bond order of $N_2 = 3$, N_2^+, $N_2^- = 2.5$, $N_2^{2-} = 2$

But N_2^- has more electrons in antibonding MO's and thus N_2^+ is more stable than N_2^-. So correct order of bond energy will be $N_2 > N_2^+ > N_2^- > N_2^{2-}$

Ex-3. Which of the following species have a bond order of 3 ?

(A) CO (B) CN^- (C) NO^+ (D) O_2^+

Sol. **(A,B,C)** Species CO, CN^-, NO^+ are isoelectronic with 14 electrons to N_2 which has bond order of 3 (i.e. $\frac{10-4}{3}$ = 3), so their bond order will be equal to three.

Ex-4. Which of the following are diamagnetic ?

(A) C_2 (B) O_2^{2-} (C) Li_2 (D) N_2^+

Sol. **(A,B,C)** Species C_2, O_2^{2-}, Li_2 have all the electrons paired but N_2^+ has one unpaired electron in bonding molecular orbital so it is paramagnetic.

Section (C) : Metallic bonding

Most metals crystallise in close-packed structures. The ability of metals to conduct electricity and heat must result from strong electrons interactions among 8 to 12 nearest neighbours (which is also called coordination number). Bonding in metals is called metallic bonding. It results from the electrical attractions among positively charged metal ions and mobile, delocalised electrons belonging to the crystal as a whole.

Two models are considered to explain metallic bonding: (A) Band model (B) Electron-sea model

(A) Band Model :

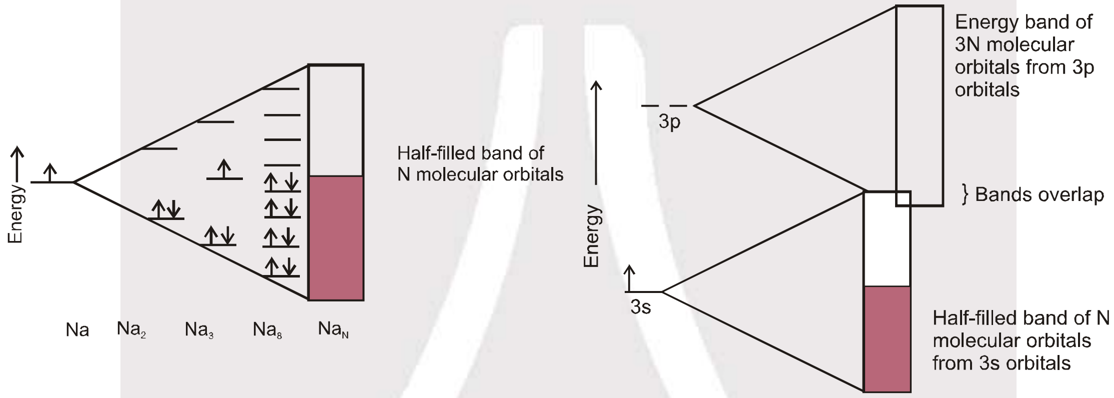


Figure : Band of orbital in crystal of sodium and overlapping of a half–filled "3s" band with an empty "3p" band of Na_N crystal

- According to band theory, the highest-energy electrons of metallic crystals occupy either a partially filled band or a filled band that overlaps an empty band.
- A band within which (or into which) electrons must move to allow electrical conduction is called a conduction band.
- The electrical conductivity of a metal decreases as temperature increases. The increase in temperature causes thermal agitation of the metal ions. This impedes the flow of electrons when an electric field is applied.
- Crystalline non-metals, such as diamond and phosphorus, are insulators, they do not conduct electricity. It is due to the fact that their highest-energy electrons occupy filled bands of molecular orbitals that are separated from the lowest empty bond (conduction band) by an energy difference called the band gap.
- In an insulator, this band gap is an energy difference that is too large for electrons to jump to get to the conduction band.

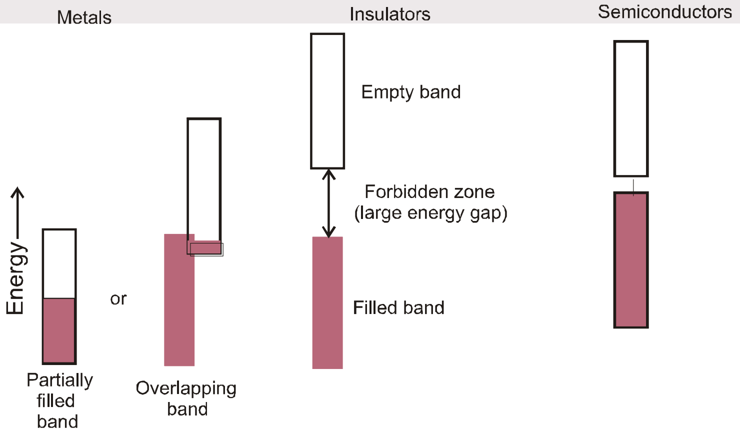


Figure : Distinction among metals, insulators and semiconductors. In each case an unshaded area represents a conduction band.

- Elements that are semiconductors have filled bands that are only slightly below, but do not overlap with empty bands.
- They do not conduct electricity at low temperatures, but a small increase in temperature is sufficient to excite some of the highest-energy electrons into the empty conduction band.

(B) Electron-Sea Model

- In lithium the ions would be Li^+ and one electron per atom would be contributed to the sea. These free electrons account for the characteristic metallic properties.
- If the ends of a bar of metal are connected to a source of electric current, electrons from the external source enter the bar at one end. Free electrons pass through the metal and leave the other end at the same rate.
- In thermal conductivity no electrons leave or enter the metal but those in the region being heated gain kinetic energy and transfer this to other electrons.
- According to the electron-sea model, the case of deformation of metals can be thought of in this way: If one layer of metal ions is forced across another, perhaps by hammering, the internal structure remains unchanged as the sea of electrons rapidly adjusts to the new situation.

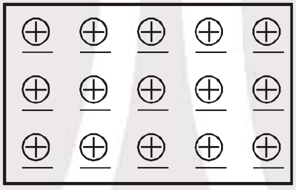


Fig. Metallic Bonding in Electron-Sea Model

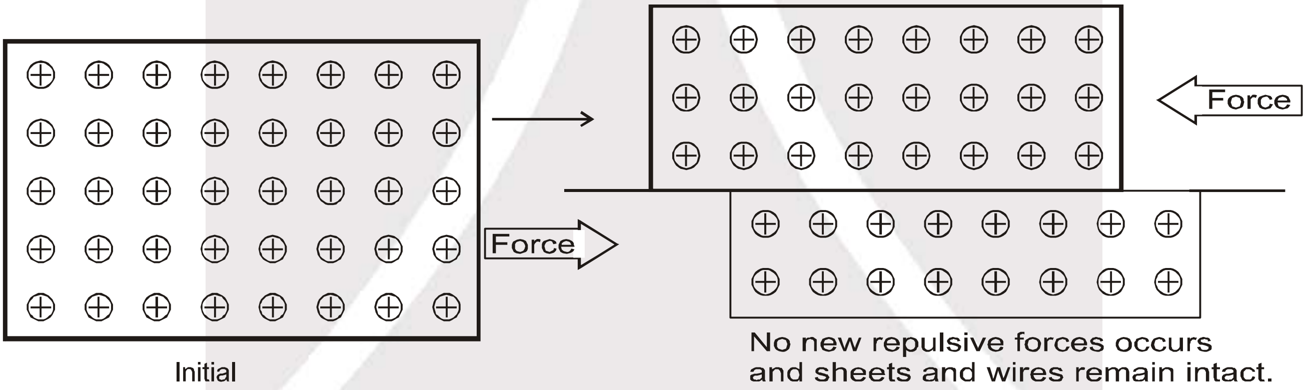


Figure : Effect of Distortion (by hammering) on Metal Sheet (assuming Electron Sea Model)

Solved Examples

Ex-5. Why transition element have high heat of atomization.

Sol. Transition metals may use inner -d-electrons along with the outer s-electrons for bonding as (n–1) d and ns have nearly same energy. So in them number of metallic bonds per atoms is quite large (more than two always). Hence element have high heat of atomization.

MISCELLANEOUS SOLVED PROBLEMS (MSPS)

Ex-1. Super oxides are coloured and paramagnetic why ?

Sol. Super oxides contain one unpaired electron in anti bonding molecular orbital and are coloured due to transition of HOMO orbital electron within visible region.

Ex-2. Of the species O_2^+, O_2^-, O_2 and O_2^{2-} which would have the maximum bond strength ?

Sol. O_2^+ has higher bond order i.e. 2.5 than O_2(2) and O_2^- (1.5) and bond strength is directly proportional to bond order.