

Schrodinger Wave Equation

According to Schrodinger wave equation electrons are treated as wave motion in three dimensional space around the nucleus having wave function, nodes and quantized energies from the classical wave mechanics wave function (ψ) is the amplitude or wave function of a wave moving in three dimensional space with velocity (v) and frequency (γ). The wave equation :-

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + 4\pi^2 \gamma^2 \psi = 0 \rightarrow (1)$$

According to non-classical de-broglie's equation

$$\lambda = \frac{h}{mv}$$

$$\frac{1}{\lambda} = \frac{mv}{h}$$

$$\frac{1}{\lambda} = \gamma$$

$$\left[\gamma = \frac{mv}{h} \right]$$

The above terms substitute in eqⁿ (1)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + 4\pi^2 \left(\frac{mv}{h} \right)^2 \psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + 4\pi^2 \left(\frac{m^2 v^2}{h^2} \right) \psi = 0 \rightarrow (2)$$

Kinetic energy of electron $KE = \frac{1}{2}mv^2$

Multiply above equation both sides with $2m$

$$2mKE = \frac{1}{2}mv^2(2m)$$

$$2mKE = m^2v^2$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + 4\pi^2 \frac{2mKE}{h^2} \psi = 0$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m K E}{h^2} \psi = 0 \rightarrow (3)$$

The total energy $E = K.E + P.E$

$$K.E = E - P.E \quad (\because P.E = V)$$

$$K.E = E - V$$

Substitute in eqⁿ (3)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

(or)

$$\text{Simply } \nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

The above equation is called as Schrodinger wave equation

∇^2 = Laplace operator

$$\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

ψ = Wave function

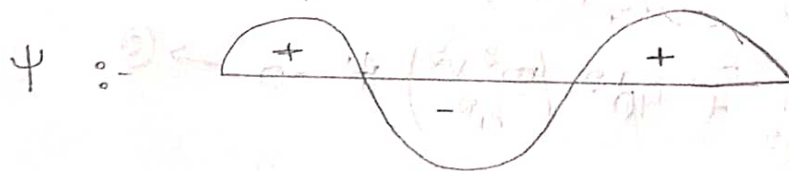
m = mass of electron

h = Planck's constant

E = Total Energy

V = Potential Energy

Significance of ψ and ψ^2 :



1. ψ is the amplitude (maximum displacement) of the wave is called the wave function
2. The wave function (ψ) takes the positive value
3. The wave function (ψ) takes the negative value
4. Wave function (ψ) takes zero while crossing (or) intercepting the axis
5. The wave function (ψ) is a state of function and

do not have any physical significance
5. Δ only represents the amplitude of electron wave.

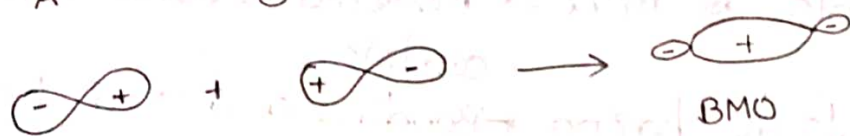
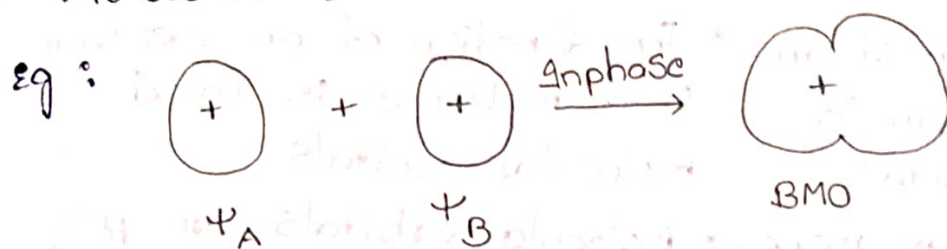
ψ^2 :-

1. ψ^2 is the probability function
2. ψ^2 is the probability of finding an electron around the nucleus and maximum is called the orbital
3. The value of ψ^2 is always positive

4. ψ^2 represents to find out the orbital of electron
5. ψ^2 could be interpreted as a probability density

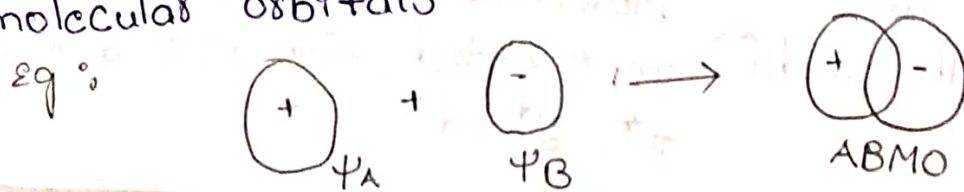
Molecular orbital Theory :

* Bonding Molecular orbital : when 2 atomic orbitals are in inphase or in constructive interference or an additive combination occurs new molecular orbitals hence these orbitals are called as Bonding molecular orbitals.



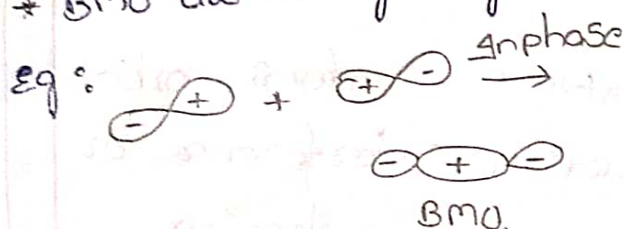
* Anti-Bonding molecular orbitals :

when 2 atomic orbitals in out of phase are destructive interference or a subtractive combination occurs a new molecular orbitals hence these molecular orbitals are called as Anti-Bonding molecular orbitals



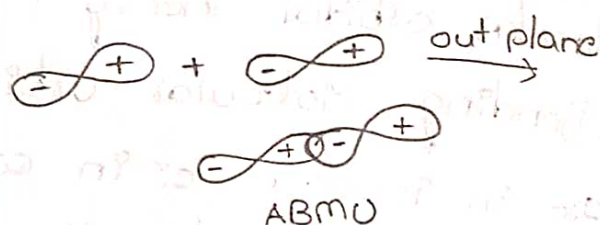
BMO

- * Bonding molecular orbitals are obtained by an additive combination of two atomic orbitals
- * BMO are represented with σ , π , δ etc.
- * BMO are lowestⁱⁿ energy
- * BMO are more stable
- * BMO are always symmetrical



A - BMO

- * Anti-Bonding molecular orbitals are obtained by a subtractive combination of two atomic orbitals
- * ABMO are represented by σ^* , π^* , δ^* etc.
- * ABMO are high in energy
- * ABMO are less stable
- * ABMO are unsymmetrical



Comparisons between orbitals and molecular orbitals

A.O

- * The wave function of an electron in an atom is called atomic orbitals
- * Atomic orbitals are mono-centric
- * Atomic orbitals are having non-bonding and Anti-Bonding molecular atomic orbitals
- * less in stable
- * Atomic orbitals are simple in shape

Atomic orbitals are represented with s, p, d, f

M.O

- * The function of an electron in a molecule is called molecular orbitals
 - * Molecular orbitals are poly-centric
 - * Bonding and anti-bonding molecular orbitals are present
 - * more in stable
 - * Molecular orbitals are more complex in shape
- Molecular orbitals are represented with σ , π , δ , σ^* , π^* , δ^* etc

Sarient features of Molecular orbital theory:

1. No. of atomic orbitals is equal to the number of molecular orbitals (Bonding molecular orbitals and Anti Bonding Molecular orbitals)
2. BMO are always lowest in energy when compared with atomic orbitals
3. ABMO are highest in energy when compared with atomic orbitals
4. BMO are more stable when compared with atomic orbitals
5. ABMO are less stable when compared with atomic orbitals
6. Molecular orbitals obeys Hund's principle
7. MOT obeys Pauli's exclusive principle
8. BMO are represented with σ , π , δ and ABMO are represented σ^* , π^* , δ^* etc...

Molecular Orbital theory of N_2 (MOT of N_2)

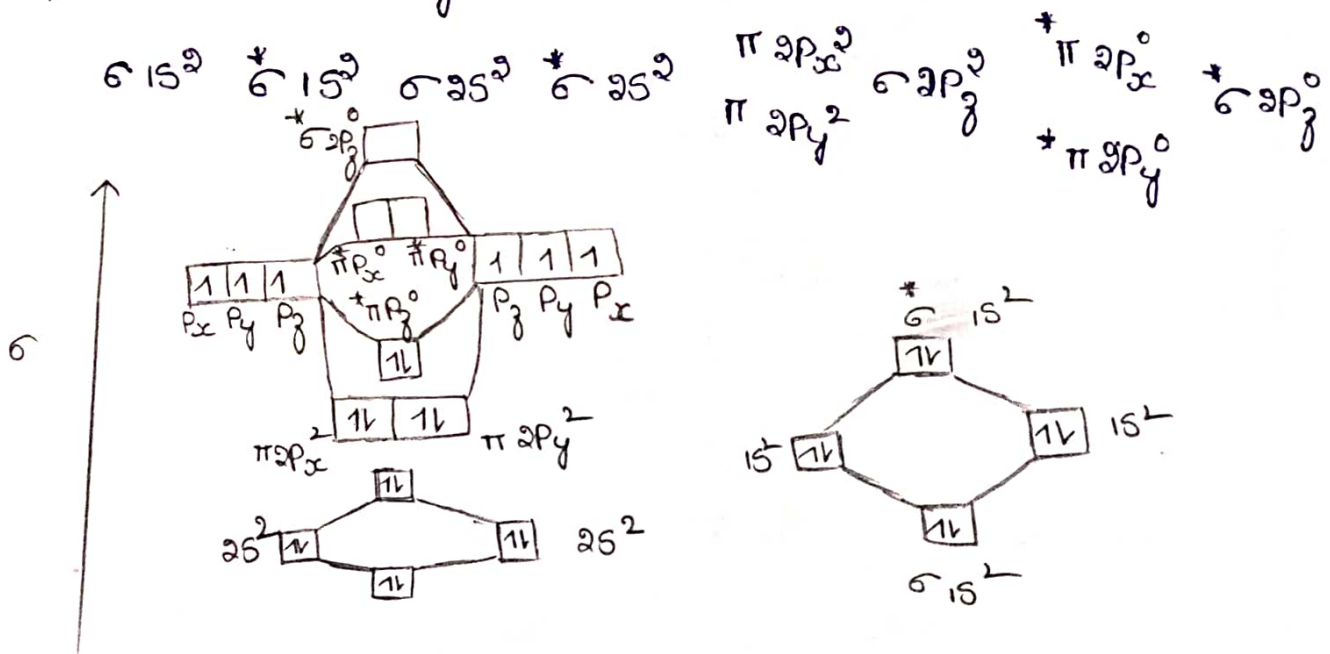
* Nitrogen molecule consists of N_2 two nitrogen atoms

The atomic number of nitrogen is 7

Electronic configuration of nitrogen $1s^2 2s^2 2p^3$

Total no. of electrons in nitrogen molecule equal to $14e^-$

The E.C of nitrogen molecule,



Bond order :

- * The half of the difference between total no. of electrons present in bonding molecular orbitals and Anti-Bonding molecular orbitals
- * Bond order indicates the number of covalent bonds present in the molecule

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

N_b = no. of electrons in BMO

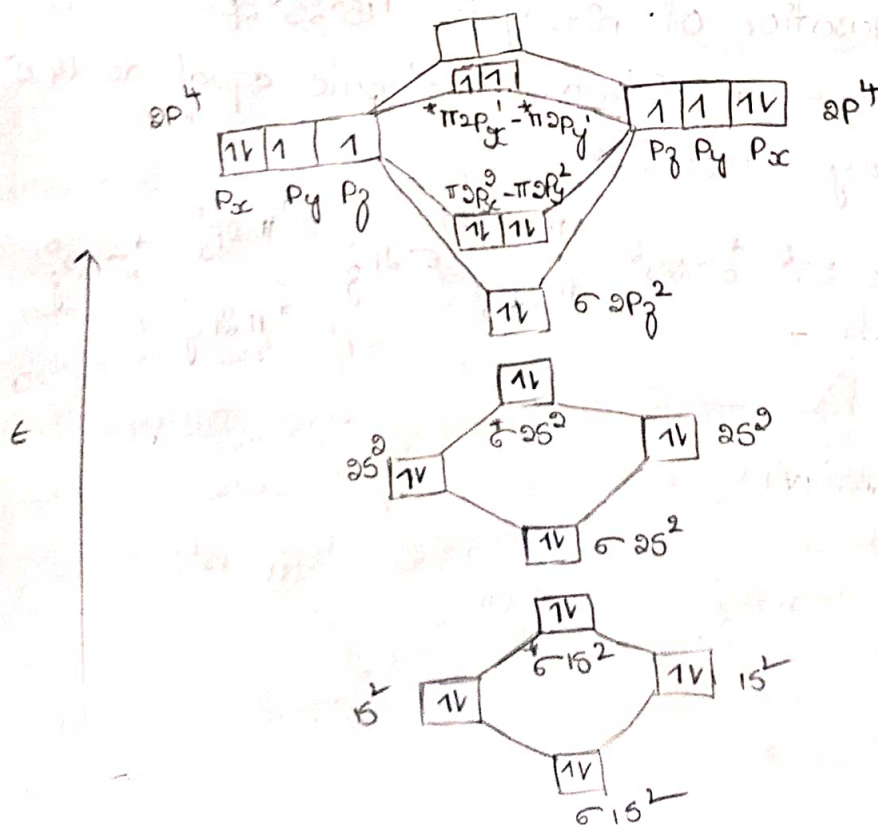
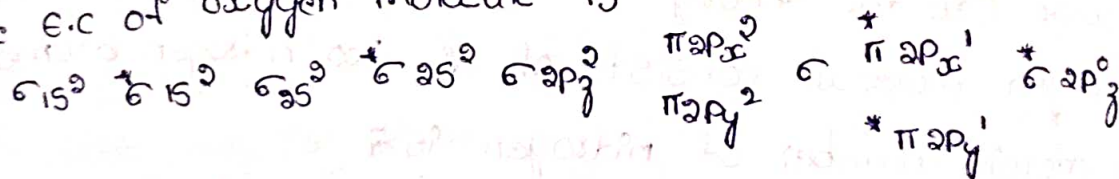
N_a = no. of electrons in ABMO

Bond order of N_2 :- $\frac{1}{2} [10 - 4] = \frac{1}{2} [6] = 3 \Rightarrow N \equiv N$

Molecular orbital Theory of O_2 :

- * Oxygen molecule consists of two oxygen atoms
- * The atomic no. of oxygen is 8
- * Electronic configuration of oxygen is $1s^2 2s^2 2p^4$
- * Total no. of electrons in oxygen molecule equal to $16e^-$

The e.c of oxygen molecule is

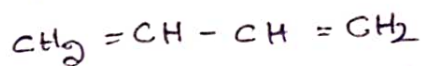


Bond order of O_2 is $= \frac{1}{2} (N_b - N_a)$

$= \frac{1}{2} (10 - 6)$

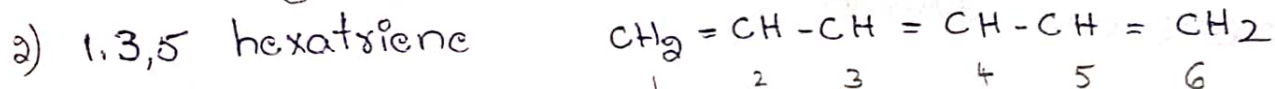
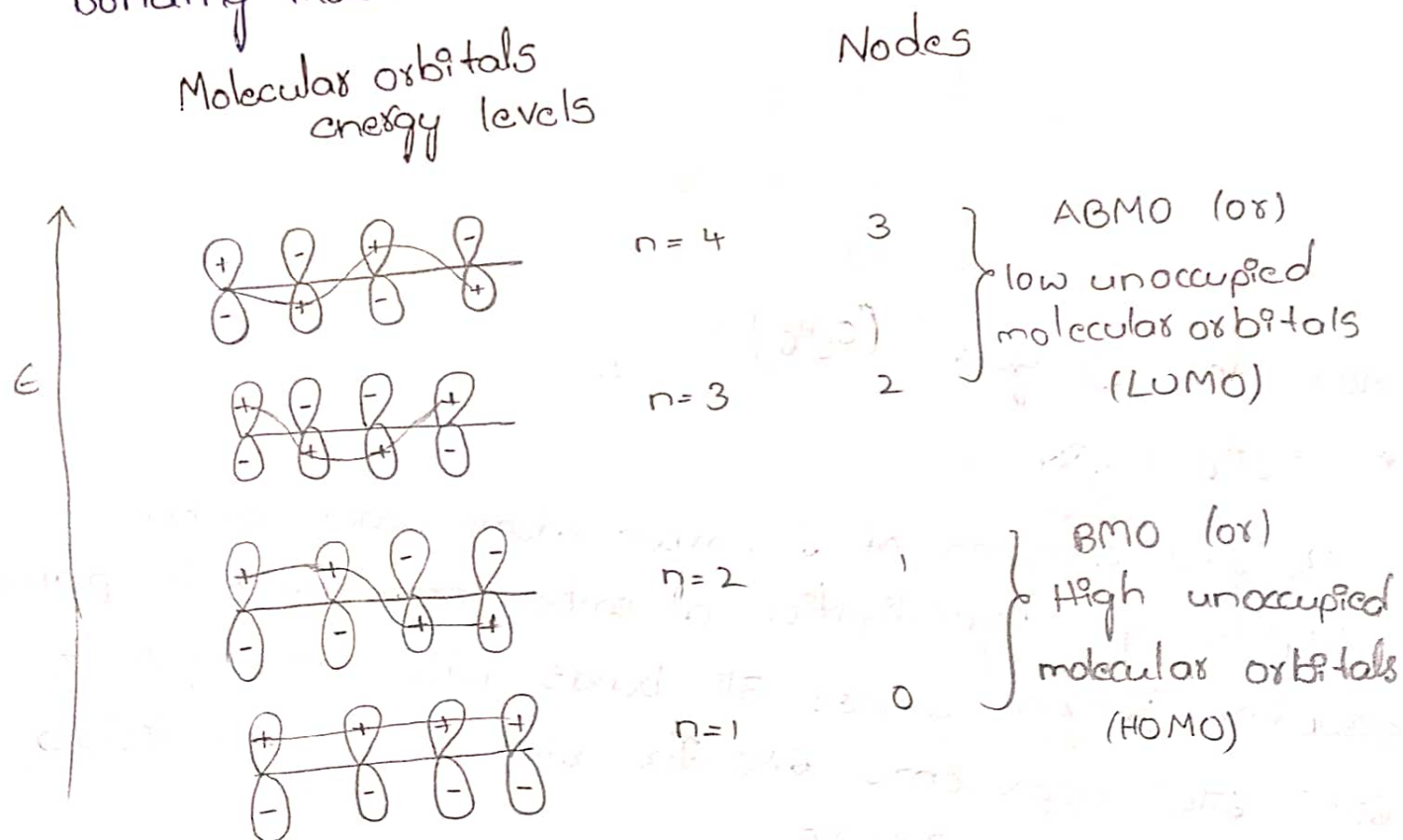
$= \frac{4}{2} = 2$

O_2 exhibits Paramagnetic and colour properties
not for conjugated πe^- system



- 1) 1,3 Butadiene consist of 4 carbon atoms, each carbon exhibits sp^2 hybridization, planar structures, 1,3 butadiene carry 2π bonds which is equal to 4π electrons
- 2) 4π electrons represents the no. of molecular orbitals ($k=4$) molecular orbitals. The 4 molecular orbitals are equal.

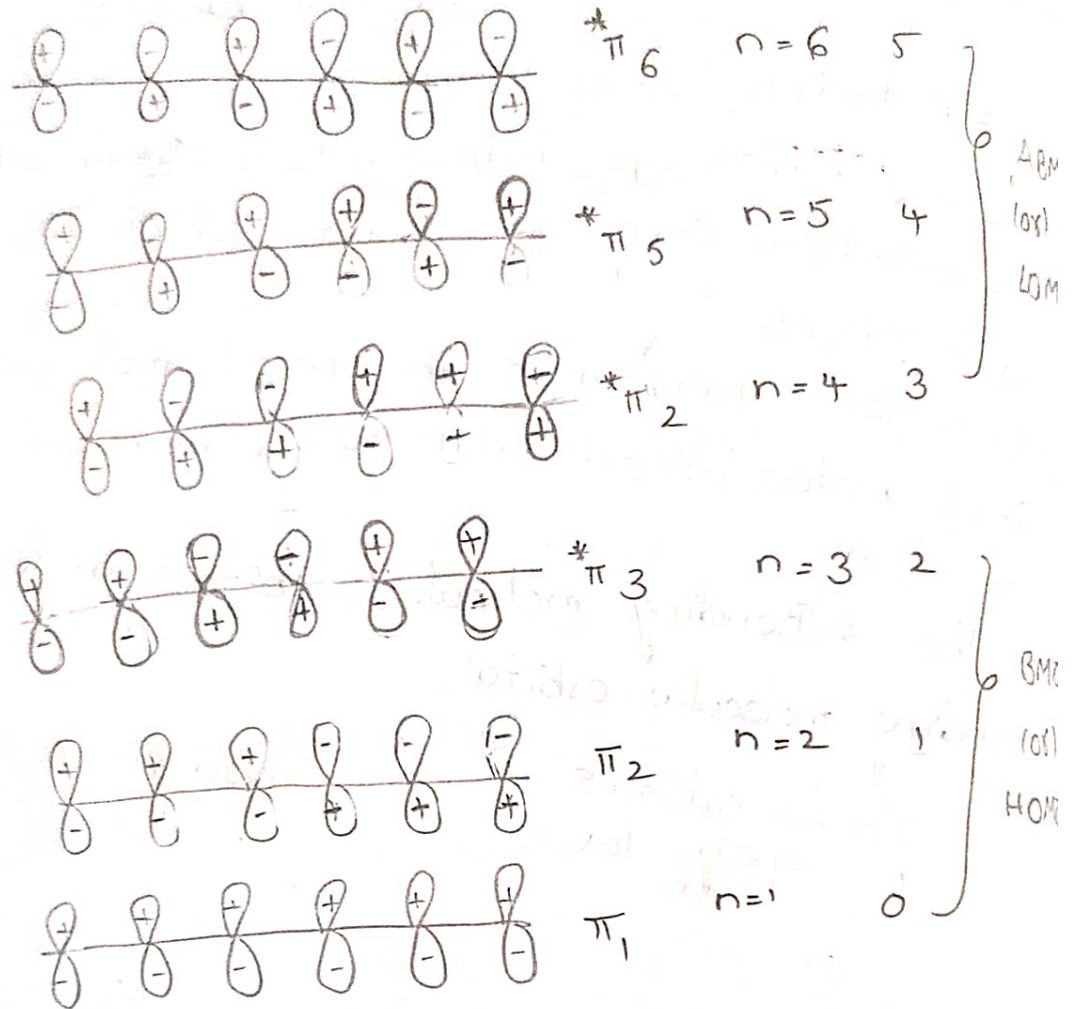
To the 2 Bonding molecules orbitals and 2 anti-bonding molecular orbital



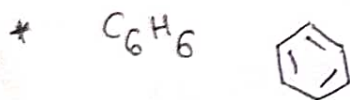
1,3,5 hexatriene consist of 6 carbons, each carbon exhibits sp^2 hybridisation, all carbon atoms exhibiting

planar structure, which is equal to $6\pi e^-$

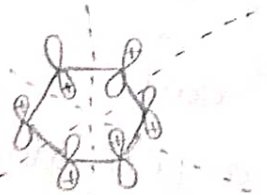
$6\pi e^-$ represents 6 molecular orbitals. The 6 MO are equal to 3 Bonding molecular orbitals and 3 antibonding molecular orbitals.



MOT for Benzene (C_6H_6)



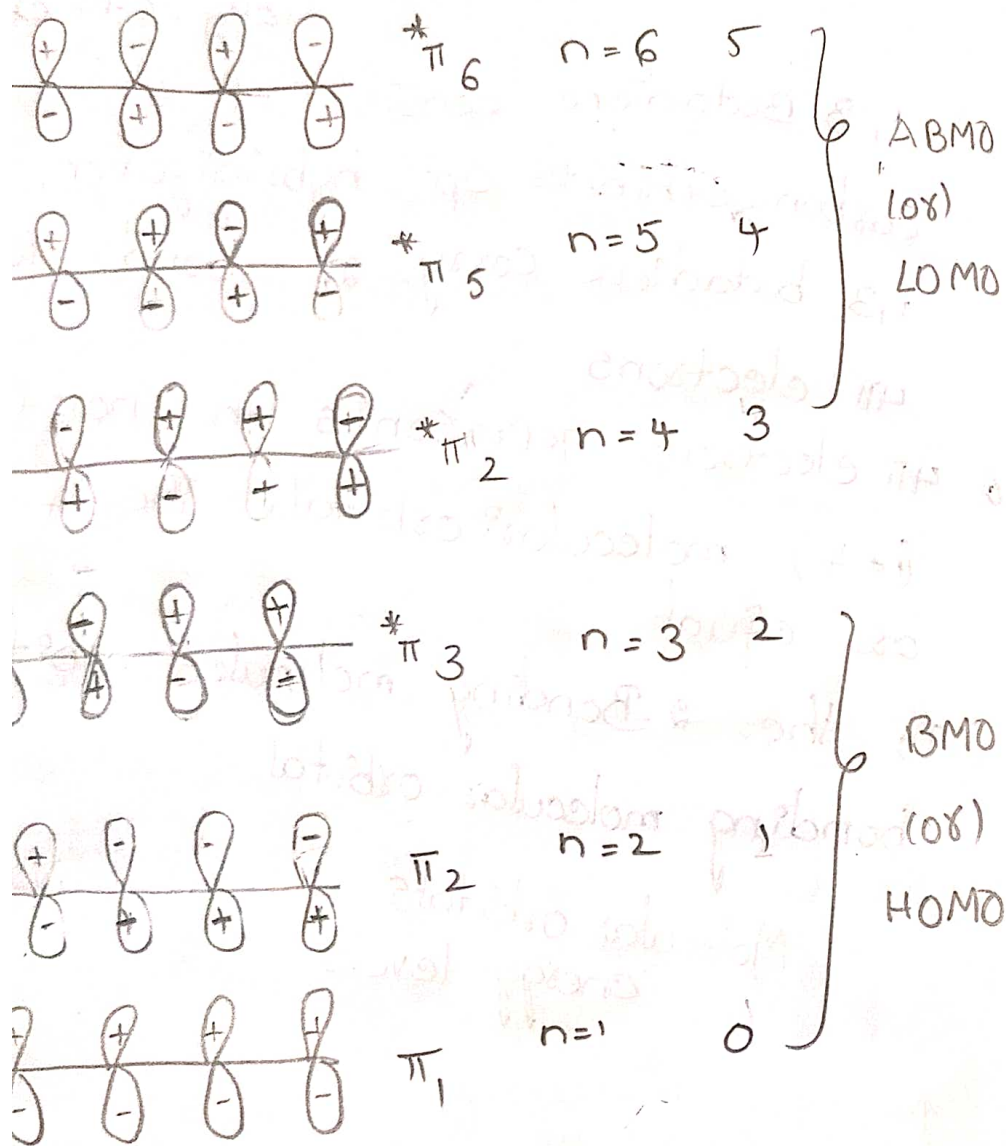
Benzene consists of 6 carbon atoms, each carbon exhibits sp^2 hybridization, all carbon atom exhibits planar structure. Benzene carries 3π bonds which is equal to $6\pi e^-$. $6\pi e^-$ represents 6 MO. The 6 MO are again divided into 3 BMO and 3 ABMO



π_6^* node = 3
B.I = 0
ABMO (or) LUMO

1,3,5 hexatriene carries 3 π bonds
 $6\pi e^-$

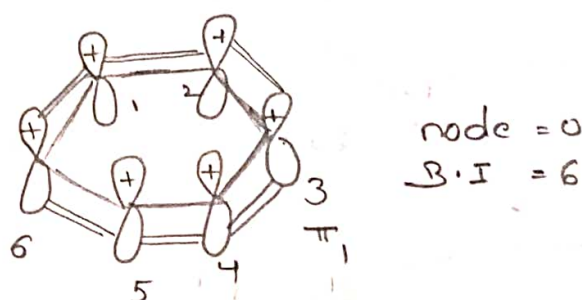
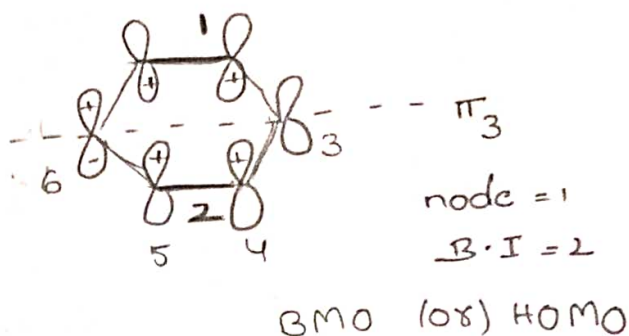
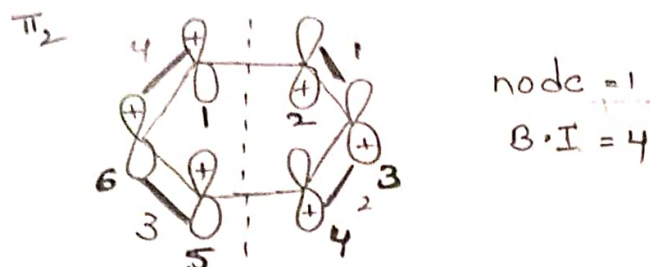
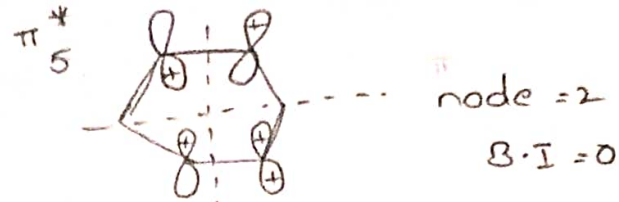
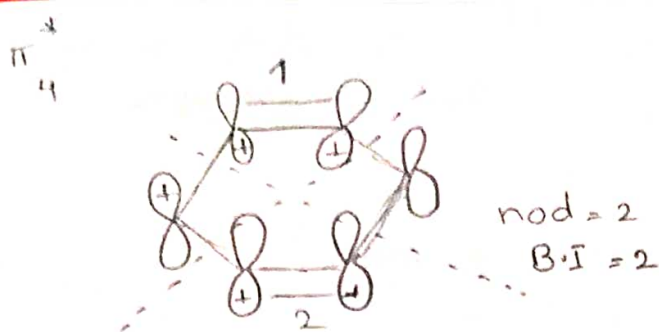
forms 6 molecular orbitals. The 6 MO
 including molecular orbitals and 3 anti
 orbitals.



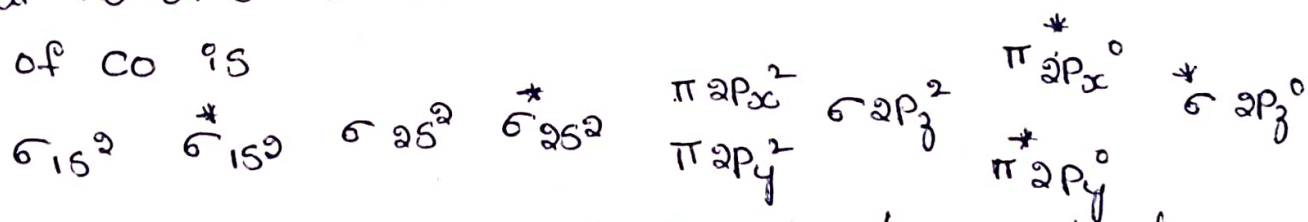
(C_6H_6)

6 carbon atoms, each carbon
 atom, all carbon atom exhibits planar
 3 π bonds which is equal to

6 MO. The 6 MO are equally divided

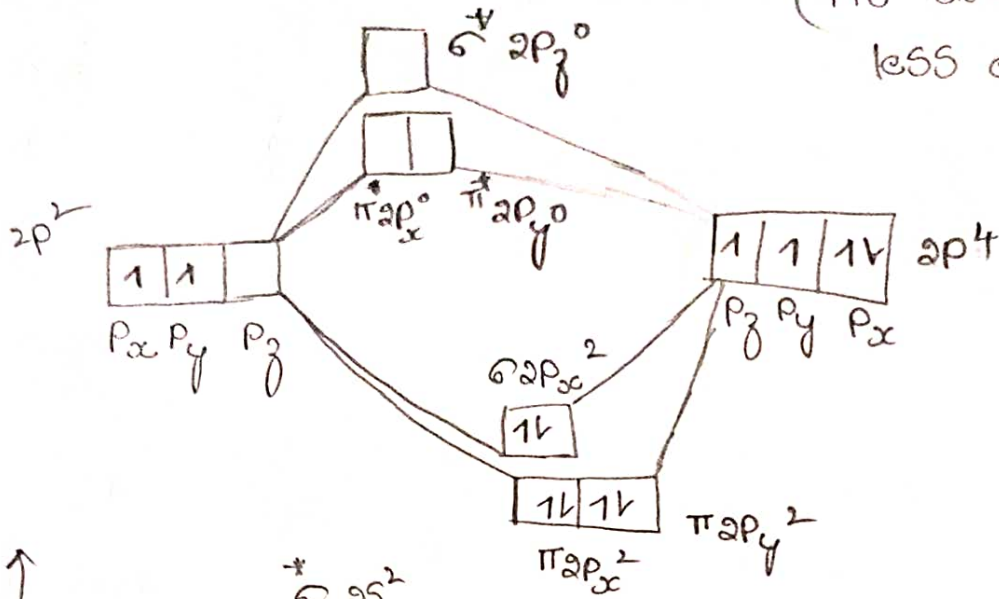


NOT for CO
Consists of carbon and oxygen atoms
The atomic no. of carbon is 6
E.C of C is $1s^2 2s^2 2p^2$
Atomic no. of oxygen is 8
E.C of O is $1s^2 2s^2 2p^4$
Total no. of e^- in CO molecule is $14e^-$
E.C of CO is



(In hetero nuclear diatomic molecules bonding molecular orbitals are closer to high electronegative atom and antibonding (mo) are closer to the less EN element)

(MO are closer to the less EN element)



* diamagnetic and exhibits no properties