

Atomic Structure & Bonding Models

Introduction: The classical mechanics are developed by Drude & Lorentz. According to this theory, the metals containing free electrons obey the laws of classical mechanics. In the metal the electrons move freely. Basing on this phenomenon successfully explained by Kinetic Theory of gases, Ohm's law, Electrical & Thermal properties & optical & conductivity properties.

Quantum mechanics is a branch of science that explains the behaviour of matter and its interaction with energy and the scale of atoms & sub atomic particles. This theory was developed by Max Planck, Albert Einstein, Louis de Broglie, Werner Heisenberg & Erwin Schrödinger.

Particle: It contains some shape & quantity. The particle has occupying a certain space and has mass, when its position changes it has velocity. Due to its mass & velocity, the particle has momentum and energy. The characteristic properties of particle are

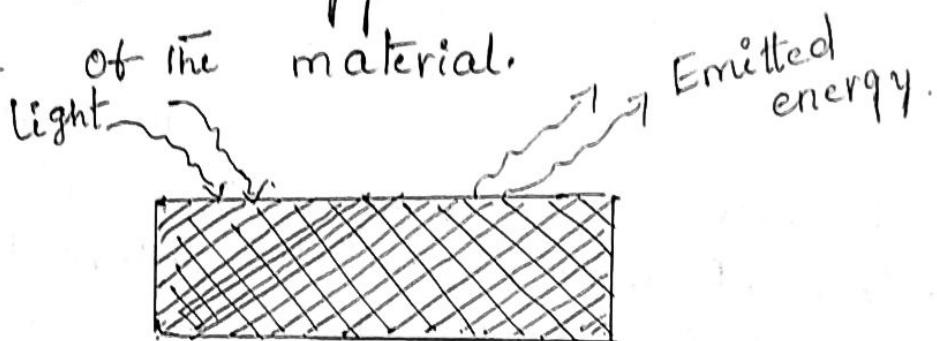
- Mass.
- Velocity
- Momentum
- Energy.

WAVE: A wave is nothing but spreading of disturbance in a medium. The characteristic properties of wave are

→ Amplitude	→ wavelength
→ Time period	→ phase
→ Frequency	→ Intensity.

Photo Electric Effect:

The emission of electrons (or) other free energy carries when light hits the surface of the material.



Dual nature of light:

It means light (or) radiation access both particle & wave. Light being a particle can be given by double slit experiment, when light being a wave can be explained by photo electric effect.

The existing theories failed to explain the photo electric effect which lead Max Planck to propose a new theory on electromagnetic radiation, which now known as Planck's quantum theory.

Black body Radiation: It is an object that absorbs all radiations falling on it, at all wavelength is called black body. Its emission is called black body radiation. Perfect black body does not exist in nature.

Planck's quantum Theory:

(2)

This Theory says that, light contain small packets of energy of photons, which are quantized. The amount of energy associated with a photon of radiation is directly proportional to the frequency of radiation.

$$E \propto \nu$$

$$\boxed{E = h\nu}$$

'h' is the Planck's constant

$$h = 6.624 \times 10^{-34} \text{ Js.}$$

' ν ' is the frequency of radiation

[The no. of waves passed through a particular point at 1 sec]

This theory comes under quantum mechanics which explains many phenomena, where classical mechanics failed.

De-broglie equation (or) De-broglie hypothesis:

In 1925, Louis De-broglie gave a special hypothesis that radiation has dual nature [both particle & wave]. The dual nature of light can be explained by combining the Planck's expression & Einstein mass-energy equation.

According to De-broglie a moving particle is always associated with a wave, this wave is known as De-broglie wave and its wavelength has De-broglie wavelength. This phenomenon was known as De-broglie hypothesis.

consider a photon of mass 'm' moving with a velocity of light 'c' then the energy of photon is given by

$$E = mc^2 \rightarrow ①$$

$$E = h\nu \rightarrow ②$$

where 'h' is the planck's constant.

' ν ' is frequency of radiation. From eq (2) it is clear that the photon is associated with a wave.

from eq ① & ② we get,

$$h\nu = mc^2 \rightarrow ③$$

If ' λ ' is the wave length of the photon,

$$\nu = c/\lambda \rightarrow ④$$

ν value substituted in eq (3) we get

$$h \cdot c/\lambda = mc^2$$

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

$$\therefore \lambda = \frac{h}{mc} \text{ (or)}$$

$$\boxed{\lambda = \frac{h}{P}} \rightarrow ⑤ \quad \text{where } 'P' = mv \text{ (or)} P = mc$$

'P' is the momentum associated with the photon.

If we consider, when a particle of mass 'm' moves with a velocity 'v' associated with the particle is given by

$$\lambda = \frac{h}{P} = \frac{h}{mv} \rightarrow ⑥$$

(3)

From the above eqn. we can conclude that the particles are accelerated to various velocities and can produce waves of various wavelengths.

De-brogli wavelength expressed in terms of kinetic energy.

'E' is the kinetic energy of the moving particle then

$$E = \frac{1}{2}mv^2$$

$$= \frac{1}{2} \frac{m^2v^2}{m} \text{ (multiply 'm' on NR $\approx \cancel{m}$)}]$$

$$E = \frac{1}{2} \frac{p^2}{m}$$

$$p^2 = 2mE$$

$$p = \sqrt{2mE} \rightarrow \textcircled{7}$$

Substitute eq \textcircled{7} in eq \textcircled{6}

$$\text{Then we get, } \lambda = \frac{h}{\sqrt{2mE}} \rightarrow \textcircled{8}$$

The above eqn. gives the de-brogli wave length in terms of kinetic energy.

... De-brogli Principle

CHEMICAL BOND:

A chemical bond is a continuous attraction between molecules and ions gives the formation of chemical compounds.

There are four types of chemical bonds,

- covalent bond - sharing of electrons
- Ionic bond - Transfer of electrons
- polar bond - unequal sharing of electrons.
- Hydrogen bond - weak forces between atoms.

Valency bond Theory:

This theory was established in the year 1927. According to this theory chemical bond is formed between two atoms basing on valency electrons. Bonding is formed by the overlap of half-filled atomic orbitals. Sigma (σ) and Pi bond (π) formation can be explained by using this theory.

This theory can't explain some molecules contain two equivalent bonds with same bond order and magnetic properties.

Molecular orbital Theory:

This theory was developed by scientist "Hunds & Mullikan" in the year "1932". This theory explains,

- Formation of chemical bond
- Bond strength of the molecule
- Magnetic nature of the molecule.

The salient features of MOT are:

- MOT is a method for describing the electronic structure of molecules using quantum mechanics.
- The atomic orbitals of the combining atoms overlap to form new orbitals, is called molecular orbitals, as a result of this the atomic orbital loose their individual identity.
- The no. of molecular orbitals formed equal to the no. of overlapping atomic orbitals.
- Maximum capacity of a molecular orbital is 2 electrons with opposite spins [1l].
- Only those atomic orbitals can combine to form molecular orbitals, which have comparable energies as well as proper orientations. For example,
 - * 1s orbital overlap with 1s,
 - * 2s orbital overlap with 2s & 2p_x
 - * 2p_y orbital overlap with 2p_y,
 - * 2p_z orbital overlap with only 2p_z.
- According to "LCAO" method [linear combination atomic orbitals], the orbitals can takes place either by addition (or) subtraction of the wave functions of atomic orbitals involve.
- Molecular orbitals obtained by addition of wave functions of atoms involve is called "Bonding molecular orbitals" [BMO].
$$\psi_{AB} = \psi_A + \psi_B$$

→ Molecular orbitals obtained by subtraction of wave functions of atoms involved is called "Anti bonding molecular orbitals [ABMO].

$$\psi_{AB}^* = \psi_A - \psi_B.$$

→ The bonding molecular orbitals are represented by σ , π , δ etc, whereas Antibonding molecular orbitals are represented by σ^* , π^* , δ^* etc.

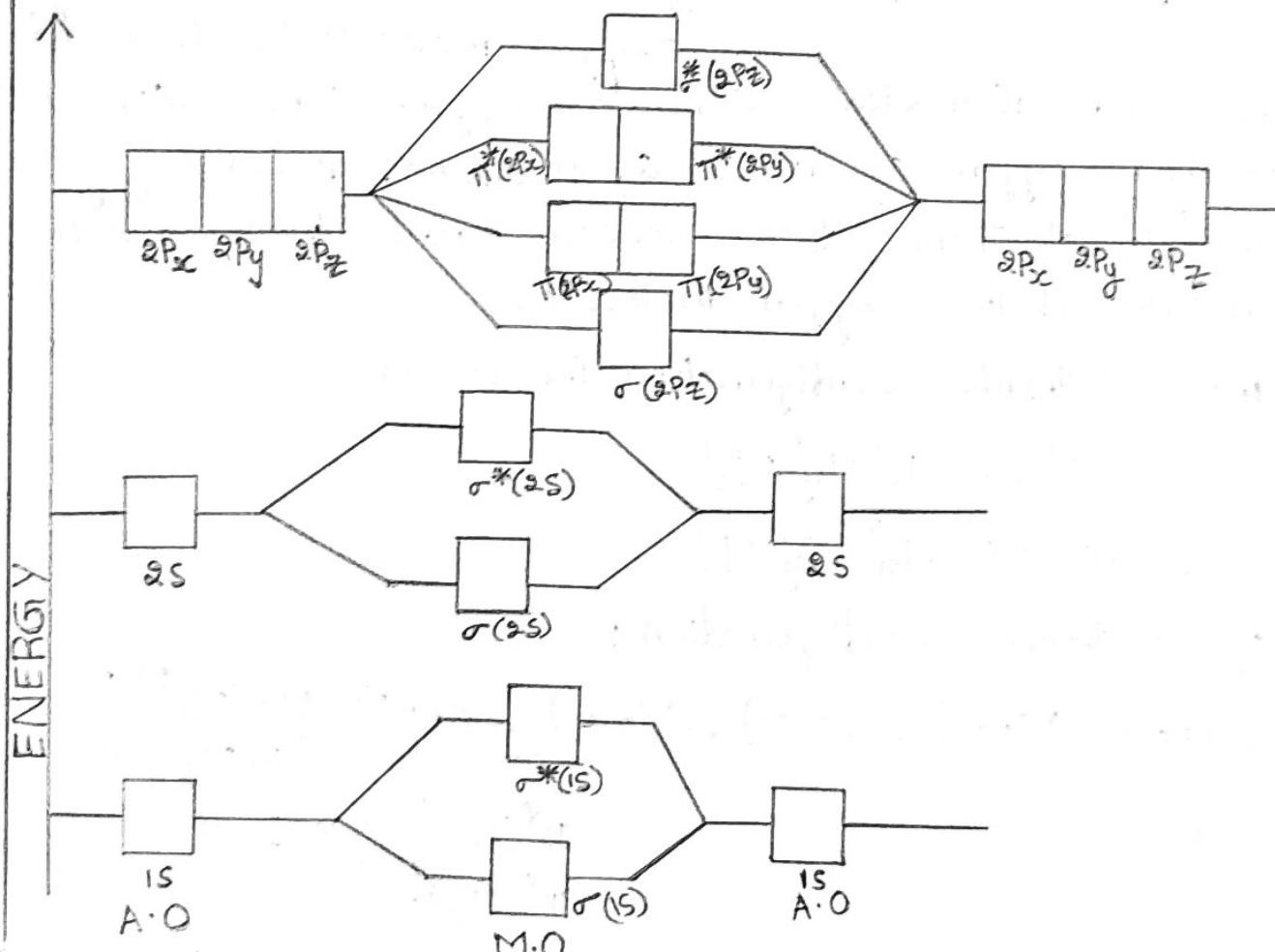
→ Inner molecular orbitals, which do not take part in bond formation are called non-bonding molecular orbitals.

→ The filling of molecular orbitals takes place according to

(a) Aufbau principle — Filling of molecular orbitals in order of increasing energy.

(b) Pauli exclusion principle — maximum capacity of 'mo' is '2' electrons with opposite spin.

c) Hund's rule — Maximum multiplicity.



Diatomic molecule:

Molecules composed of only two atoms of the same (or) different chemical elements is called diatomic molecule.

Diatomic molecules are two types.

- (a) Homonuclear diatomic molecule
- (b) Hetero nuclear diatomic molecule.

Homonuclear diatomic molecule: Molecules are formed from only one element is known as "Homo nuclear diatomic molecule".

Ex: $N_2, O_2, F_2, Cl_2, I_2, H_2$ etc.

The order of energy levels of homo nuclear diatomic molecular orbitals is

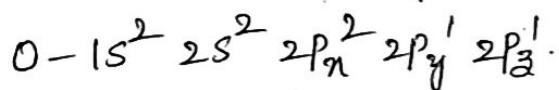
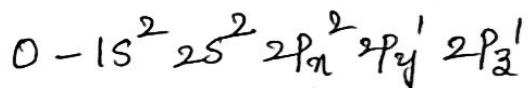
$$\sigma(1s) < \sigma^*(1s) < \sigma(2s) < \sigma^*(2s) < \sigma(2p_z) < \pi(2p_x) < \pi(2p_y)$$

$$\pi^*(2p_x) < \sigma^*(2p_z).$$

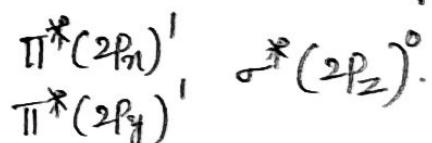
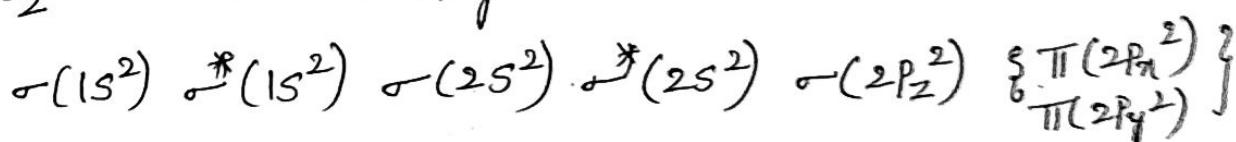
Energy level diagram of O_2 :

Oxygen molecule is formed from the combination of two atomic oxygens. The outer shell of the oxygen contains '6' electrons. Accordingly there are '12' electrons to be accommodated in the molecular orbitals of the oxygen molecule,

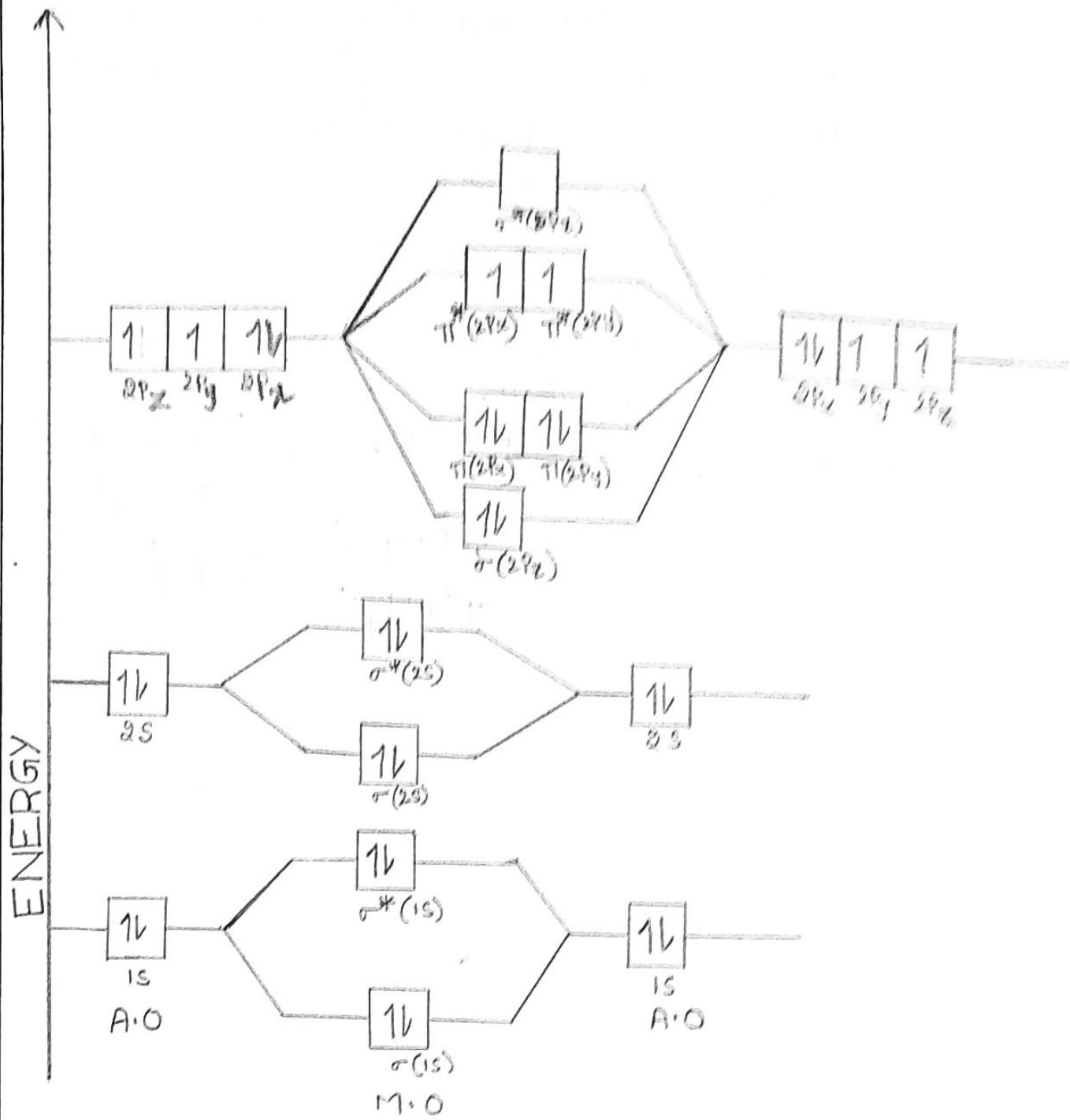
The electronic configuration of O_2 is



O_2 electronic configuration:



(6)



Bond order of molecule:

$$\text{Bond order} = \frac{\text{No. of bonding electrons} - \text{No. of anti-bonding electrons}}{2}$$

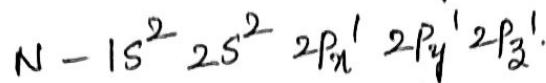
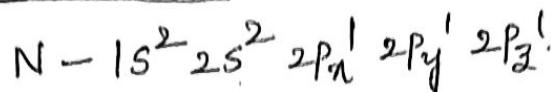
$$= \frac{10 - 6}{2} = 4/2$$

$$= 2.$$

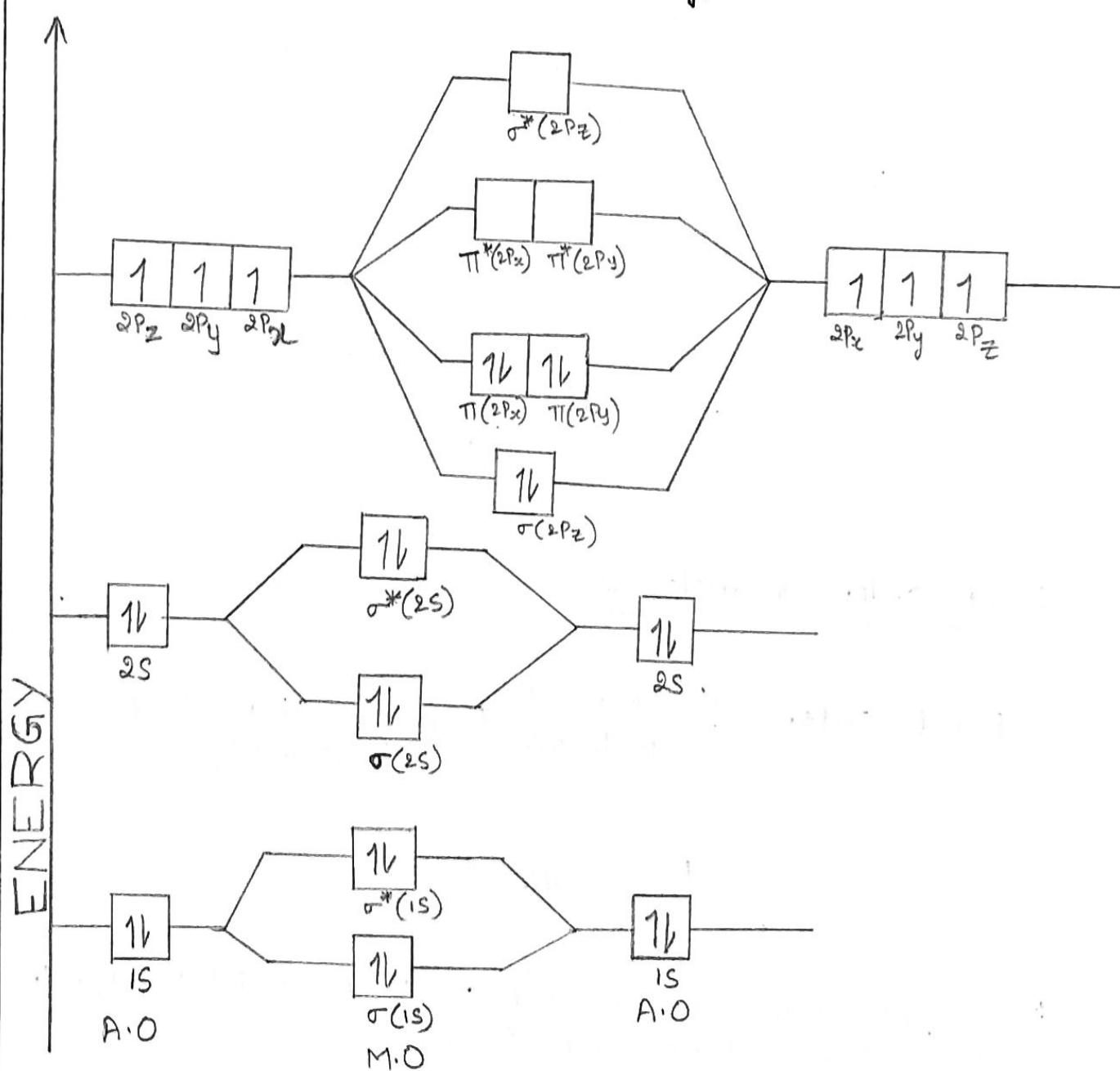
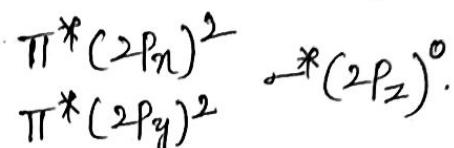
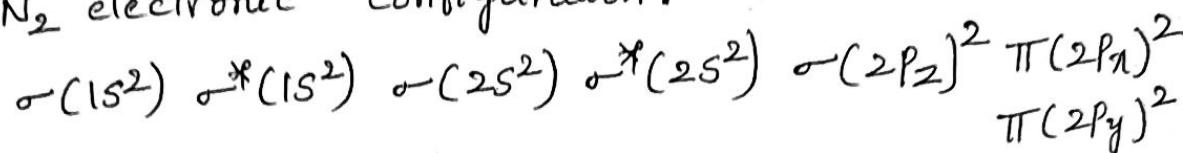
The oxygen atoms are bonded 2 [1 σ bond, 1 π bond]. The molecule is stable and exist.

According to Hund's rule, the last 2 electrons in $\pi^*(2p_x)$ and $\pi^*(2p_y)$ orbitals remain unpaired. Therefore the molecule oxygen is paramagnetic due to the presence of '2' unpaired electrons.

Energy level of N_2 :



N_2 electronic configuration:



Bond order of N_2 molecule:

$$B.O = \frac{10 - 1}{2} = 6/2$$

= 3.

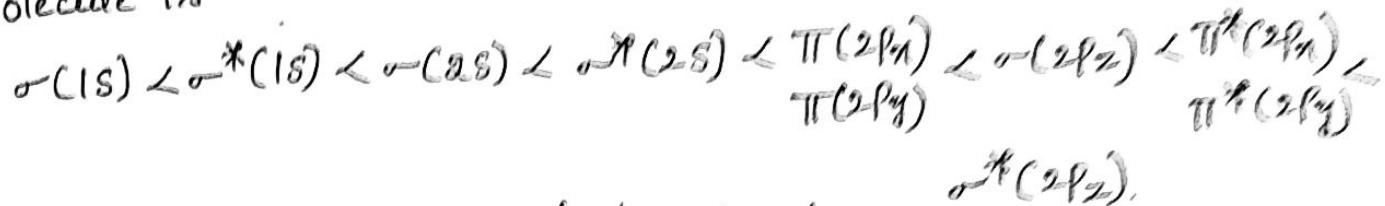
N_2 molecule is diamagnetic, due to no lone pair of electrons.

Heteronuclear diatomic molecule:

molecules are formed from one element is known as heteronuclear diatomic molecule.

e.g.: CO, NO, HF, CN, HeI etc.

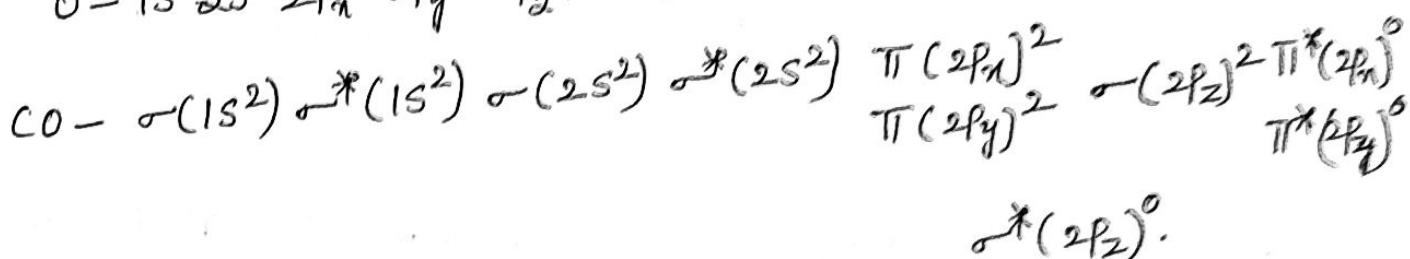
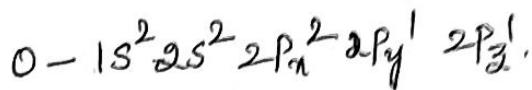
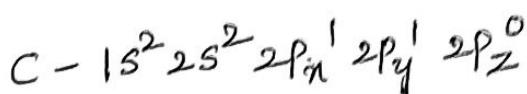
The order of energy levels of heteronuclear diatomic molecule is

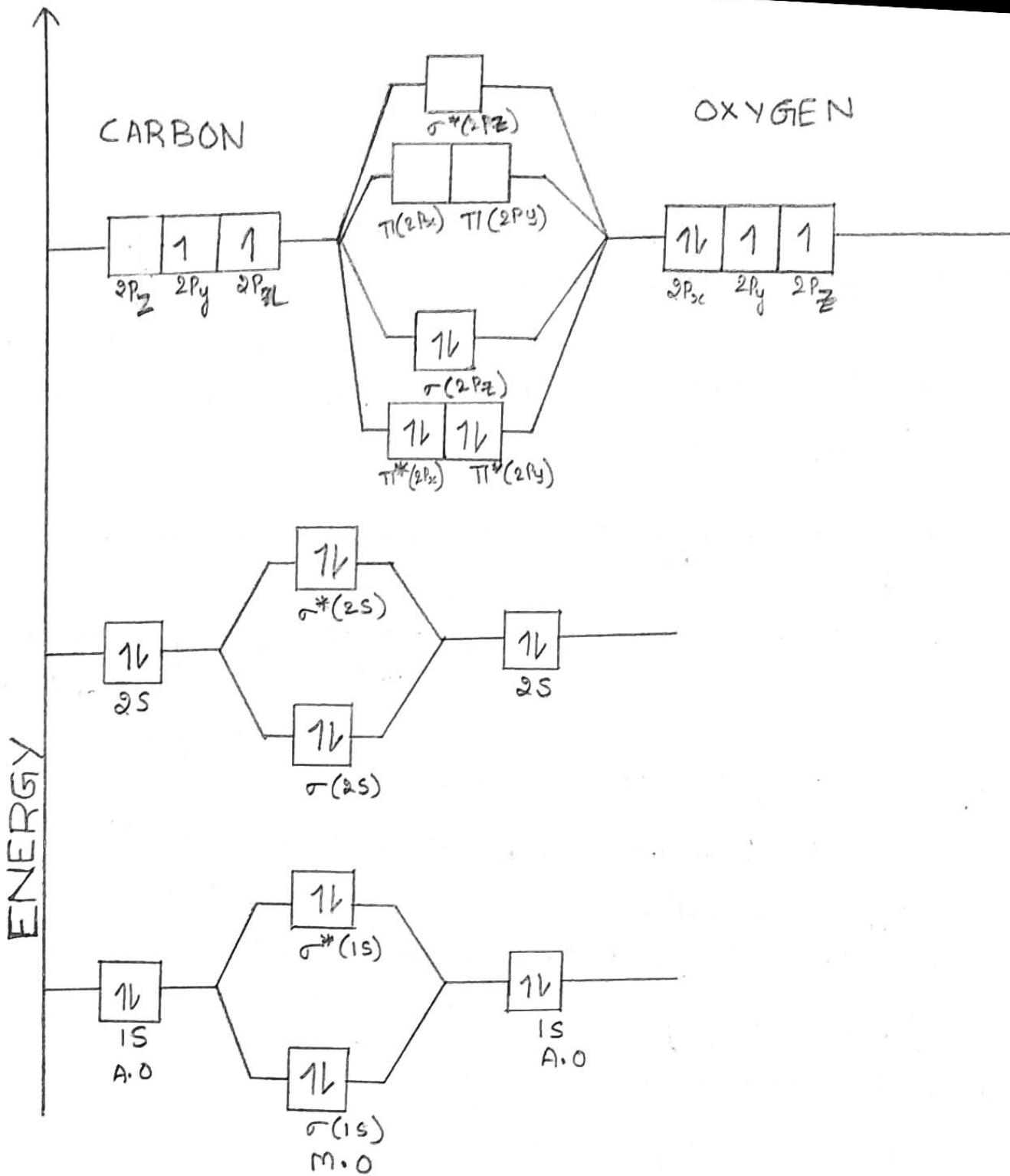


Energy level diagram of 'CO' molecule:

'CO' is formed from the combination of one 'C' atom & one 'O' atom. The outer shell of the carbon atom contains '4' electrons $[2s^2 2p^2]$, and oxygen atom contains '6' electrons '4' electrons $[2s^2 2p^4]$. Accordingly there are '10' electrons to be accommodated in the molecular orbitals of 'CO'.

The electronic configuration of 'CO' molecule is,





Bond order of 'CO' molecule:

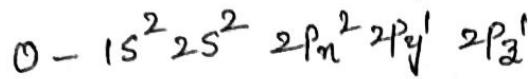
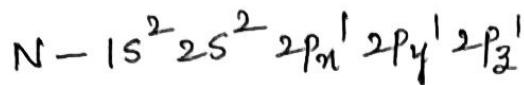
$$\text{Bond order} = \frac{\text{No. of bonding electrons} - \text{No. of non-bonding electrons}}{2}$$

$$= \frac{10 - 4}{2} = \frac{6}{2} = 3.$$

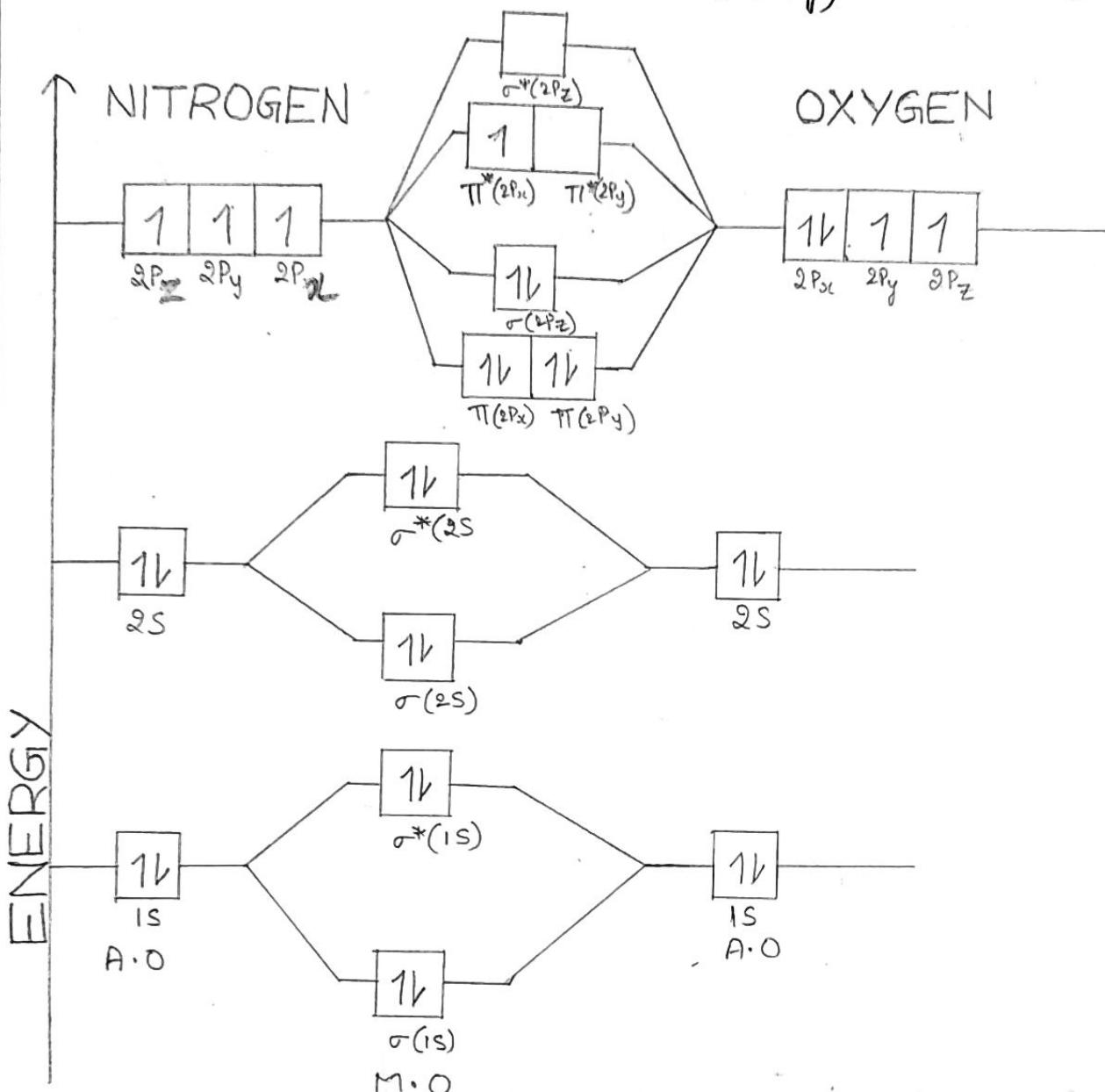
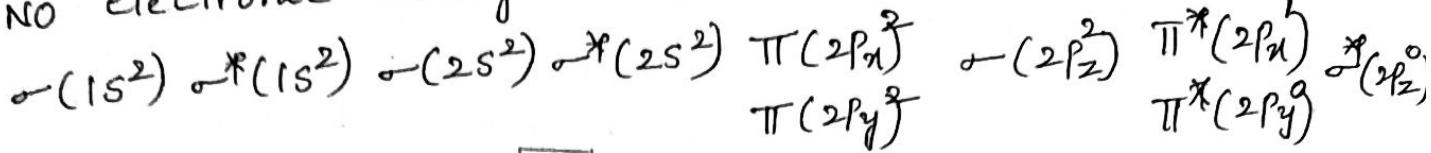
'CO' molecule contains one ' σ ' bonds \approx 2 ' π ' bonds.
The 'CO' molecule is diamagnetic due to no lone pair of electrons.

Energy diagram of 'NO' molecule:

(8)



'NO' electronic configuration,



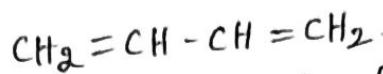
Bond order of NO:

$$BO = \frac{10-5}{2} = 2.5$$

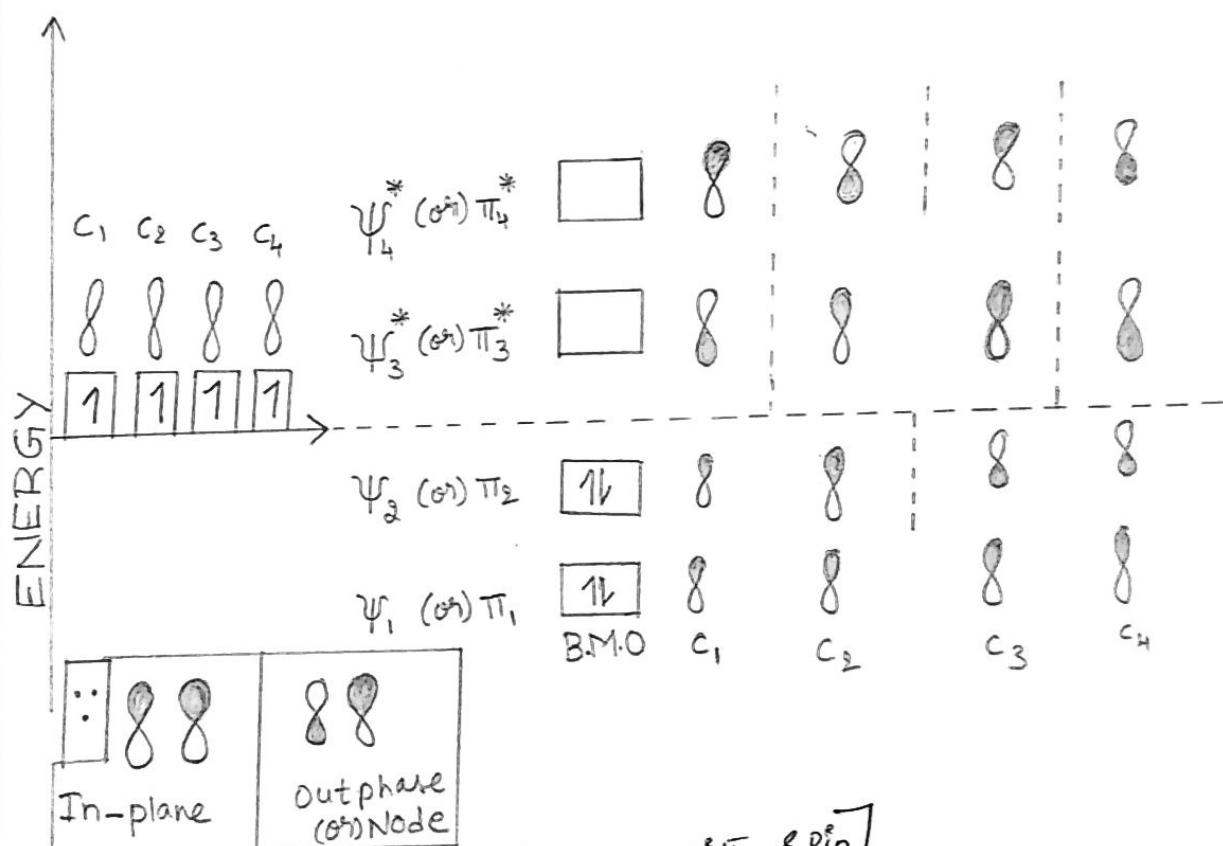
'NO' is paramagnetic in nature, due to one lone pair of electron.

π -molecular orbital diagram of 1,3-butadiene:

The structure of 1,3-butadiene is



Butadiene is composed of '4' carbons with two adjacent pie-bonds. These ' π ' bonds are conjugated [conjugated means one single bond is separated by 2 double bonds]. All the p-orbitals are aligned with each other and built up into a large π -system, but butadiene is consist of '4' individual p-orbitals. The π -system of butadiene will contain 4 π -molecular electrons. During filling the lowest orbital get filled first.



Node - [Wave function changes with spin]

BMO: The molecular orbitals present below the horizontal line is known as "BMO".

ABMO: The molecular orbitals present above the horizontal line is known as "ABMO".

(9)

BMO is more stable than ABMO, overlapping of molecular orbitals is maximum, that structure contain greater stability.

π_1 (or) ψ_1 : This structure contain bonding molecular orbitals, no. of nodes '0',
no. of bonding interactions - 3 [$c_1-c_2, c_2-c_3, c_3-c_4$]
no. of Antibonding interactions - 0.

All the orbitals are aligned "In Phase", orbitals having greatest overlapping being lower energy. This structure is highly stable.

π_2 (or) ψ_2 : ' π_2 ' is HOMO [Highly occupied molecular orbital]. It is the valency electrons of the " π " system. They will be less electrons readily. If butadiene participates in a reaction, it gives electrons [Nucleophile].

No. of Nodes - 1
No. of bonding Interactions - 2 [c_1-c_2, c_3-c_4]
No. of Antibonding Interactions - 1 [c_2-c_3].

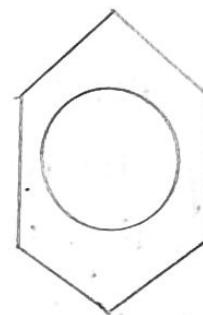
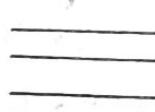
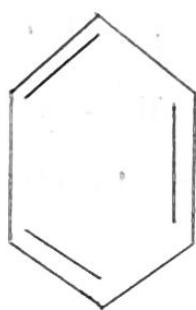
π_3^* (or) ψ_3^* : It is 'LUMO' [lowest unoccupied molecular orbitals]. It is the lowest energy and contain unoccupied orbitals. If butadiene participates in a reaction it accepts electrons. [Electrophile].

No. of Nodes - 2
No. of bonding Interactions - 1 [c_2-c_3]
No. of Antibonding Interactions - 2 [c_1-c_2, c_3-c_4].

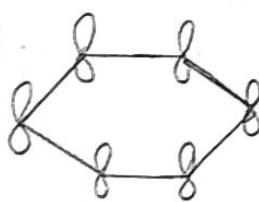
π_4^* (or) ψ_4^* : It is 'ABMO'
No. of Nodes - 3.
No. of bonding interactions - 0
No. of Antibonding Interactions - 3 [$c_1-c_2, c_2-c_3, c_3-c_4$].

π -molecular orbitals of Benzene:

Benzene is a planar molecule containing a ring of '6' carbon atoms, each with a hydrogen atom attached, all c-c bonds have the same bond length having single & double bonds. There is a delocalised electrons above & below plane of ring. There are '6' p-orbitals of electrons that form the stabilizing electron cloud above and below the aromatic ring. In benzene ring '6' carbon atoms are ' sp^2 ' hybridized. The overlapping of 6-p orbitals form 3 bonding and 3 anti-bonding molecular orbitals.



Node "3"



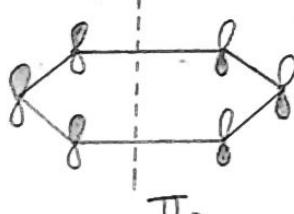
π_4^*

Node "2"

π_5^*

ENERGY

1 1 1 1 1 1

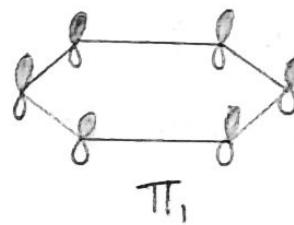


π_2

Node "1"

π_3

B.M.O



π_1

CRYSTAL FIELD THEORY:

(10)

Valency bond theory failed to explain the stability of coordination compounds [metal complex] and the difference between weak and strong ligand.

Crystal field theory explain the metal-ligand bond as an ionic bond arising purely from the electrostatic interactions between metal ions & ligands.

Ligand: The ions (or) group of atoms that surround the metal ion in a co-ordination complex are called Ligands. The ligand is a donor of electrons, metal ion is an electron acceptor.

Salient features of CFT:

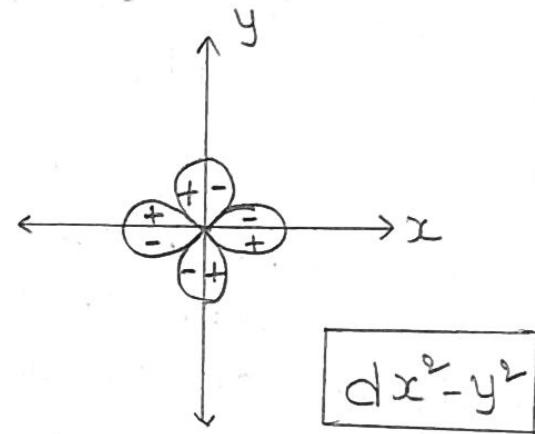
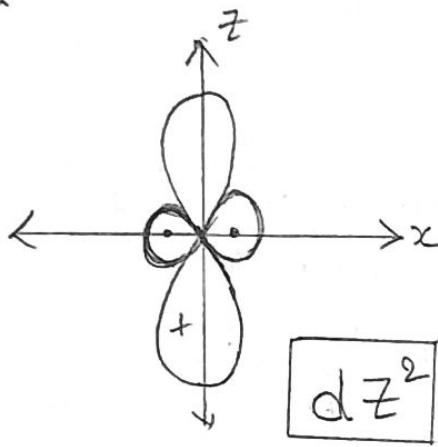
- The central metal cation is surrounded by ligands, which contain one (or) more lone pair of electrons.
- Ligands are treated as point charges.
- The ionic ligands [CN^- , Br^- , OH^-] are treated as negative point charges, while neutral ligands [H_2O , NH_3] are treated as dipoles. In a metal complex the negative end of the neutral ligand is oriented towards the central metal cation.
- There is no interaction between metal orbitals & ligand orbitals.
- The bonding between the metal cation and ligand is purely electrostatic (or) coulombic attraction.
- All the d-orbitals in the metal have the same energy in the free atom. When a complex is formed, the ligands destroy these orbitals, at that time orbitals have different energies.

→ Grouping of d-orbital into 2 sets - Based on the orientation of the lobes with respect to axis, 5-d-orbitals split into two types.

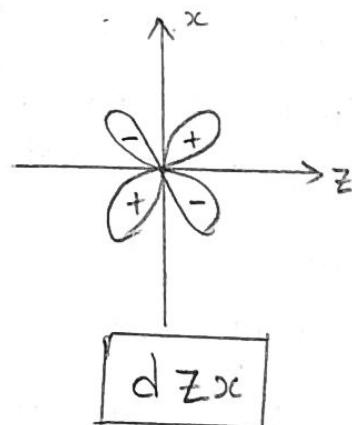
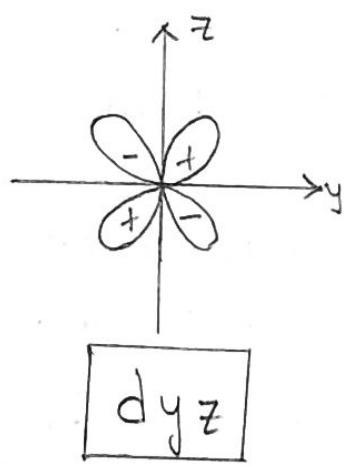
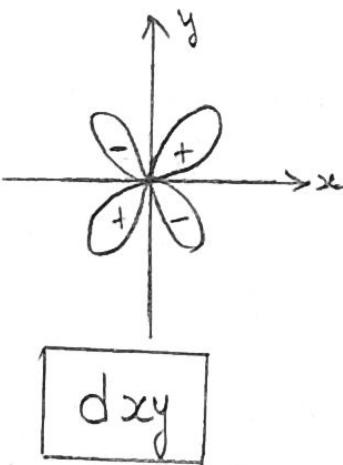
(a) eq set of orbitals $[d_z^2, d_{x^2-y^2}]$: These orbitals contain their lobes along the axis. These are also called "axial orbitals". The letter 'e' in eq represents double degenerate set.

(b) t_{2g} set of orbitals $[d_{xy}, d_{yz}, d_{zx}]$: These orbitals lying in between the axis. They are also called non-axial orbitals. The letter 't' represents in t_{2g} triply degenerate set.

Eg →

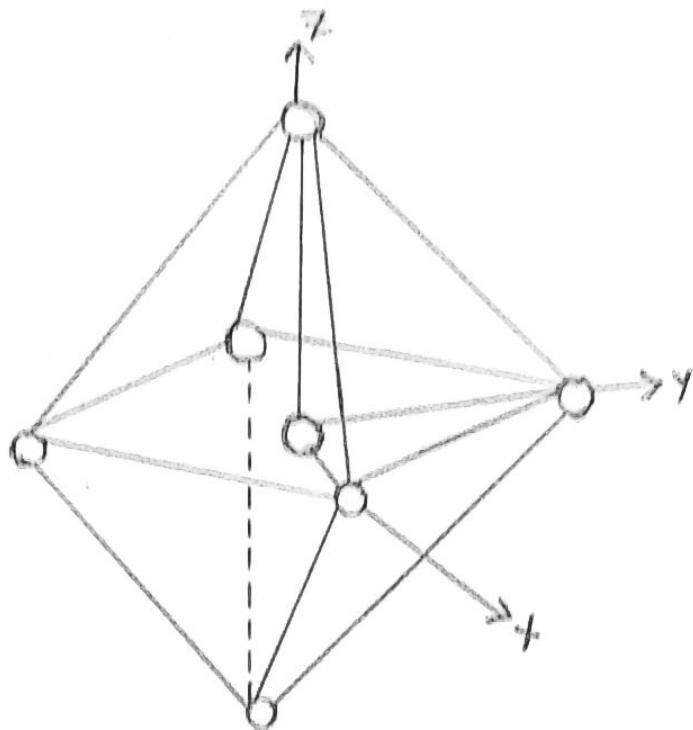


t_{2g} →



Crystal field splitting of d-orbitals in octahedral complex: (11)

In an octahedral complex, the central metal ion surrounded by '6' ligands. In this complex 2 types of electrostatic interactions plays an important role.

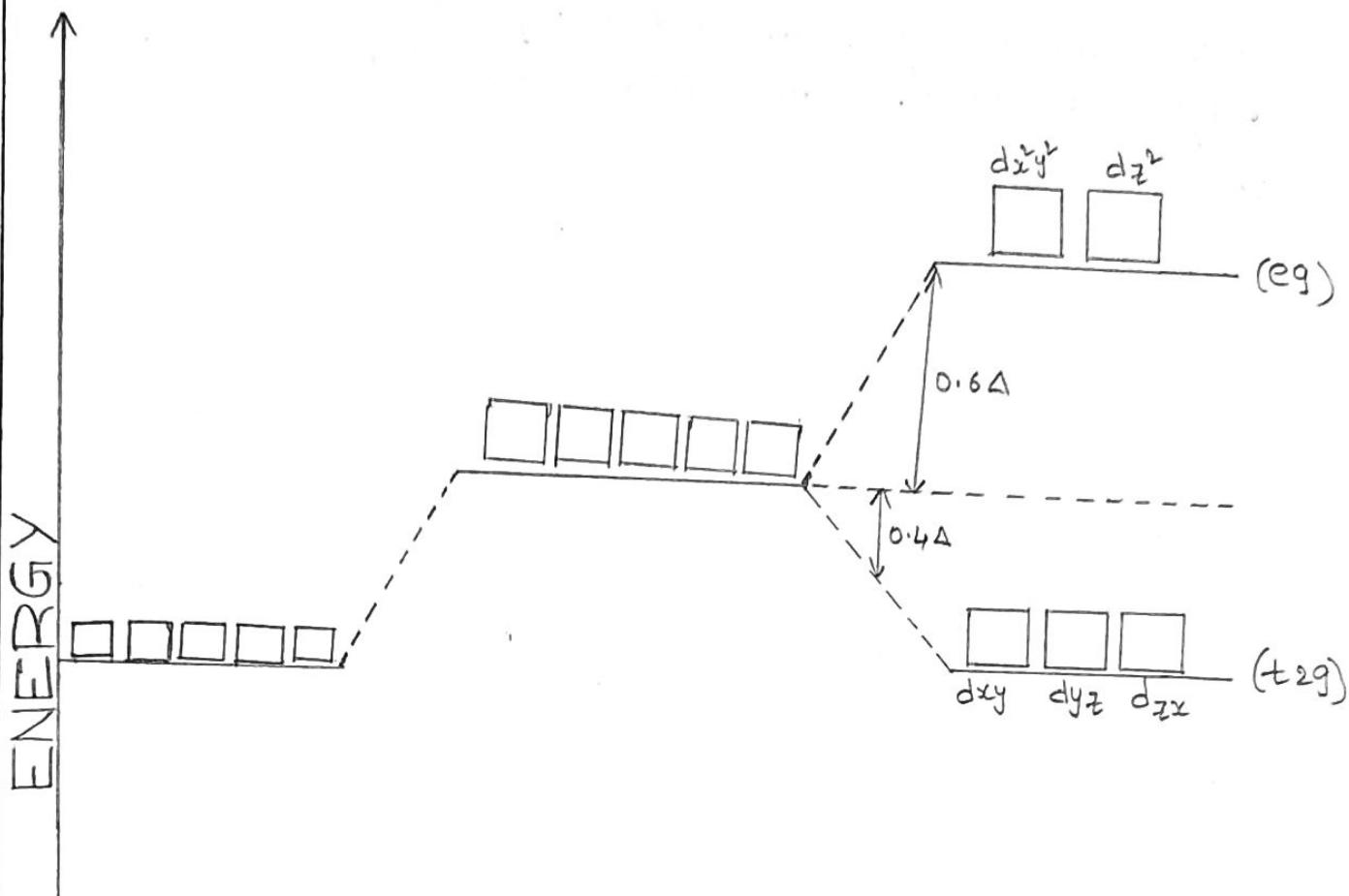


Attraction: There is an attraction between the positive metal ion and the negative end of a ligand.

Repulsion: There is an electrostatic repulsion between the lone pair of electrons in the ligands and the electrons in the d-orbitals of the metal. The magnitude of this repulsion depends on the particular d-orbitals involved.

The orbitals " $d_{x^2-y^2}$ " & d_{z^2} are along the axis $x, y \& z$. and pair of electrons approach the axis. The electrons filling in these orbitals have higher repulsion. So, the energy of $d_{x^2-y^2}$ & d_{z^2} orbitals are increased.

But the orbitals of d_{xy} , d_{yz} & d_{zx} are lies in between the axis will have lower repulsion, so the energy of d_{xy} , d_{yz} & d_{zx} are decreased.



→ The energy difference between these 2 sets of d-orbitals is called the crystal field splitting (Δ).

The ' Δ ' value depends on the metal and nature of the ligand.

Filling up of electrons in the d-orbitals:

The octahedral complex contain more than one electron in d-orbital, First the electrons fill in the lower energy t_{2g} orbitals accordance with Hund's rule of maximum multiplicity.

If the metal ion contains more than '3' electrons, it has 2 options to follow.

- (a) It may pair up with the electrons in the t_{2g} orbitals
(or)

(b) It may enter the higher 'eg' orbitals in accordance with hund's rule of maximum multiplicity. (12)

The chosen path is depend upon the strength of the ligand.

Strong Ligand [Low spin]: In a strong ligand field, the electrons pairs up, since ' Δ ' is very large in the presence of strong ligand field, the complex will be low spin.

Weak Ligand [High spin]:

In a weak ligand field, ' Δ ' is small, it cannot force the electrons to pair up in the presence of weak ligand field, the complex will be high spin.

d-orbital splitting in strong ligand field (low spin):

d^x ions	Distribution of d-electrons		n
	t_{2g} set	eg set	
d^1	1 - -	- -	1
d^2	1 1 -	- -	2
d^3	1 1 1	- -	3
d^4	1 1 1	- -	2
d^5	1 1 1	- -	1
d^6	1 1 1	- -	0
d^7	1 1 1	1 -	1
d^8	1 1 1	1 1	2
d^9	1 1 1	1 1	1
d^{10}	1 1 1	1 1	0

d-orbital splitting in weak ligand [High spin]:

d ⁿ ions	Distribution of d-electrons		n
	t _{2g} set	eg set	
d ¹	1 - -	- -	1
d ²	1 1 -	- -	2
d ³	1 1 1	- -	3
d ⁴	1 1 1	1 -	4
d ⁵	1 1 1	1 1	5
d ⁶	1v 1v 1	1 1	4
d ⁷	1v 1v 1	1 1	3
d ⁸	1v 1v 1v	1 1	2
d ⁹	1v 1v 1v	1v 1	1
d ¹⁰	1v 1v 1v	1v 1v	0

Eg: crystal field splitting of $[\text{Fe}(\text{CN})_6]^{3-}$:

The octahedral complex of $[\text{Fe}(\text{CN})_6]^{3-}$, the central metal Fe^{3+} has electronic configuration $3d^5$. The cyanide ion (CN^-) has a strong ligand field. So pairing of electrons takes place in lower d-orbitals [t_{2g}]. So a low spin complex is formed.

Fe - atomic number - 26

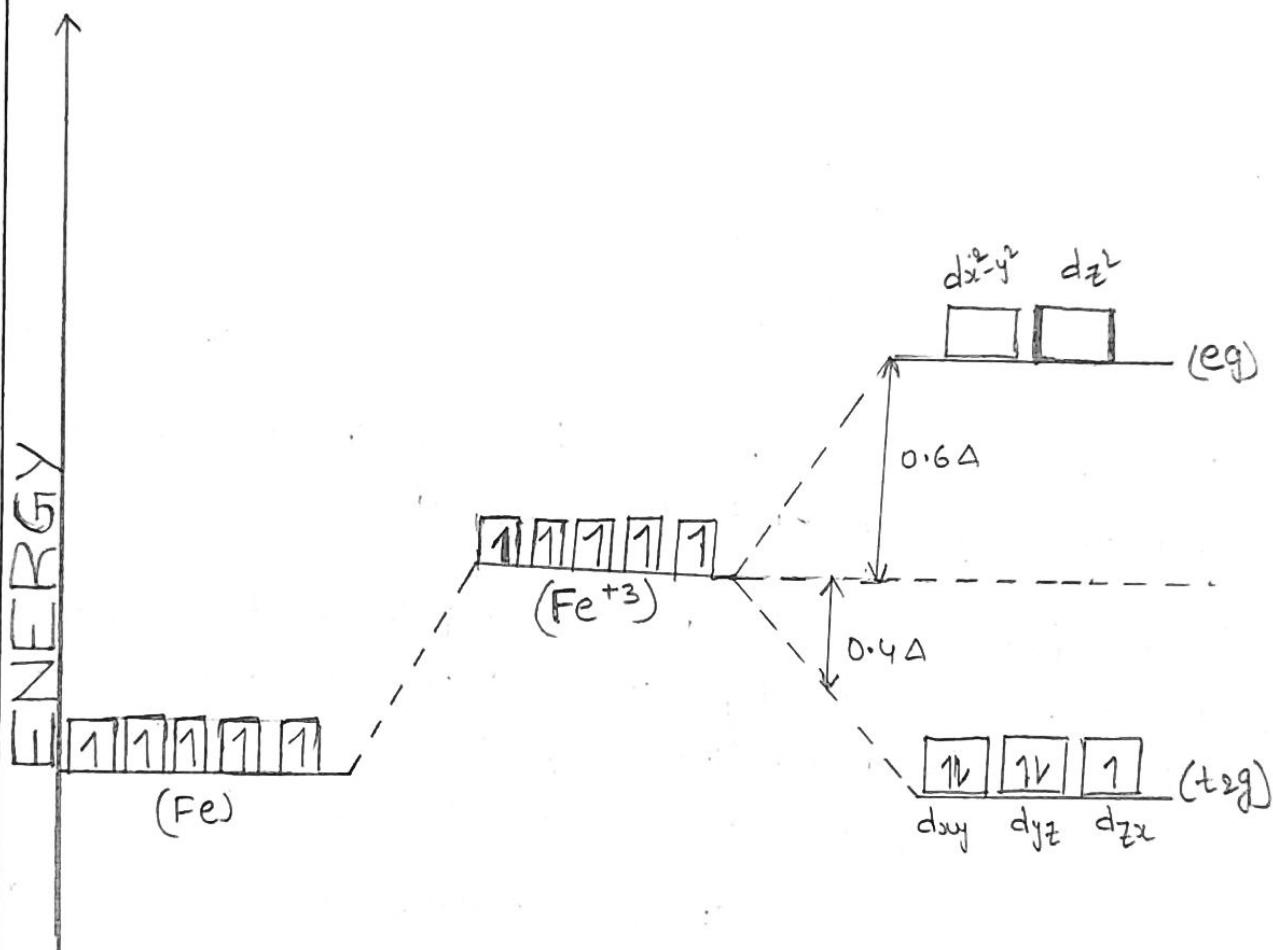
Fe - electronic configuration - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$ H.P.O.

Fe - Atomic Number \rightarrow 26

(13)

Electronic configuration of Fe is $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6 4p^0$.

Fe	-	<table border="1"> <tr><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td></tr> <tr><td></td><td></td><td></td><td></td><td>$3d^6$</td></tr> </table>	1	1	1	1	1					$3d^6$	<table border="1"> <tr><td>1</td><td>1</td></tr> <tr><td></td><td>$4s^2$</td></tr> <tr><td></td><td></td></tr> </table>	1	1		$4s^2$			<table border="1"> <tr><td></td><td></td><td></td></tr> <tr><td></td><td>$4p^0$</td><td></td></tr> <tr><td></td><td></td><td></td></tr> </table>					$4p^0$				
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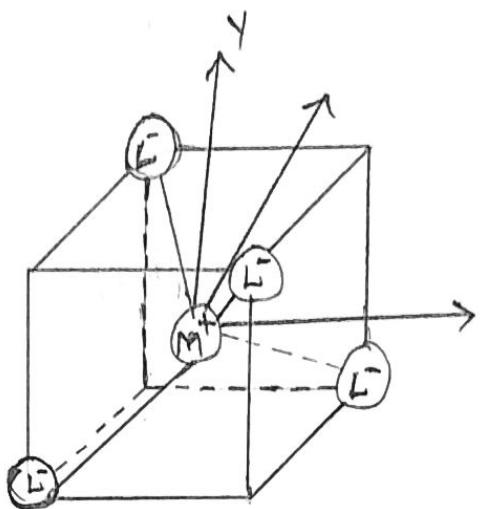


spectrochemical series: When different ligands are arranged in increasing order of crystal field splitting (Δ) then we get spectrochemical series.

(weak ligand) $I^- < Br^- < Cl^- < NO_3^- < F^- < OH^- < EtOH < (COO)_2^- < H_2 < EDTA < NH_3 < NH_2-CH_2-CH_2-NH_2 < NO_2^- < CN^- < CO^-$ (strong ligand).

Crystal field splitting of d-orbital in tetrahedral complex

In tetrahedral complex the central metal cation surrounded by four ligands. In this complex two types of electrostatic interactions plays an important role.

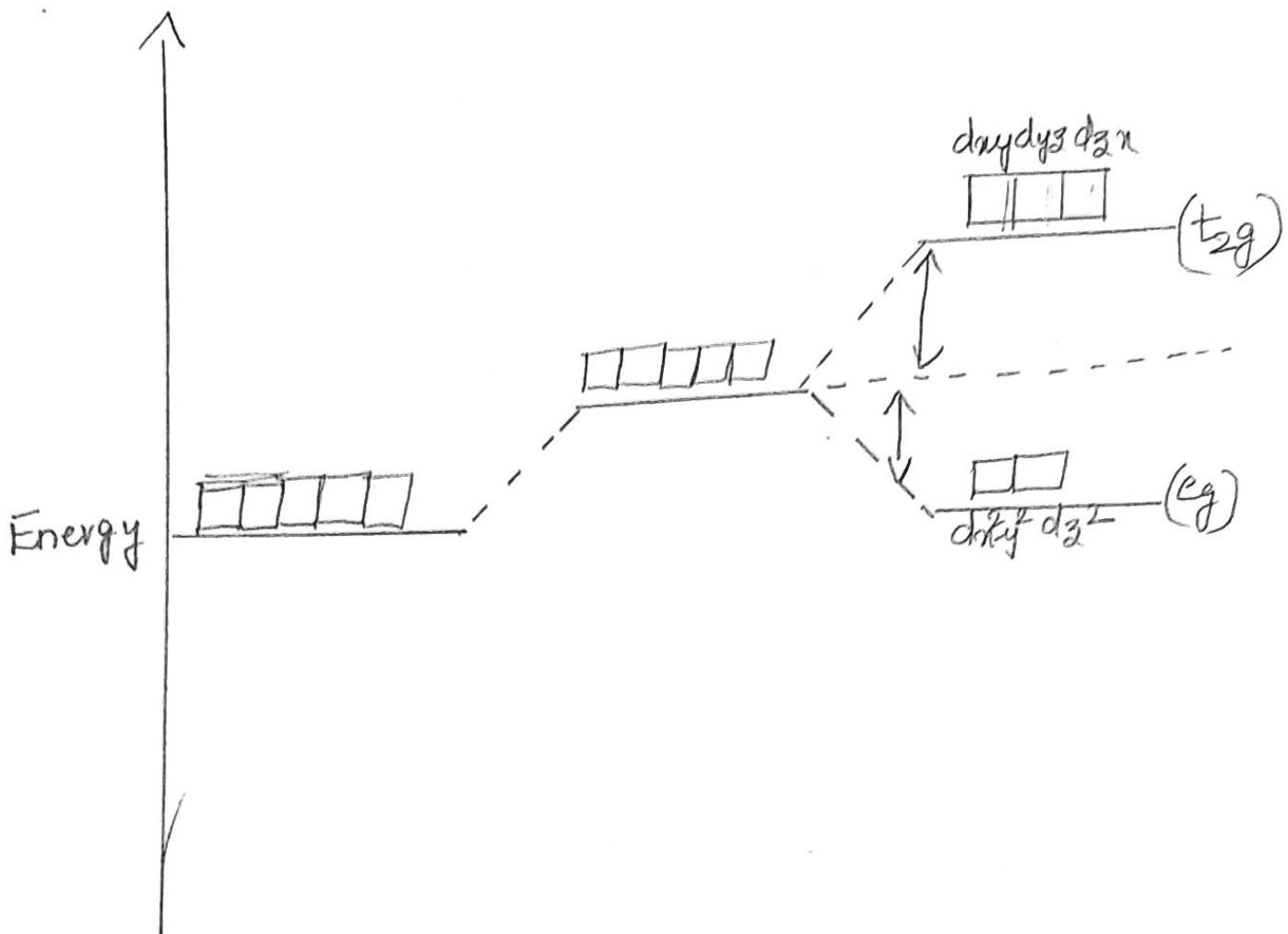


Attraction: There is an attraction between the positive metal ion and the negative end of a ligand.

Repulsion: There is an electrostatic repulsion between the lone pair of electrons in the ligands and the electrons in the d-orbitals of the metal. The magnitude of this repulsion depends upon the particular d-orbitals involved.

In this complex the metal ion does not present in the centre of the cube and the 4 ligands are attached alternate corners of the cube.

The direction of ligands does not coincide with 'eg' and 't_{2g}' orbitals. Any how, the t_{2g} orbitals nearer to the ligands so, the energy of 't_{2g}' orbitals increase maximum, then 'eg' orbitals. consequently the crystal field splitting opposite to octahedral complex.



crystal field splitting of $[\text{CoCl}_4]^{2-}$:

Atomic number of 'Co' - 27
Electronic configuration - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7 4p^0$.

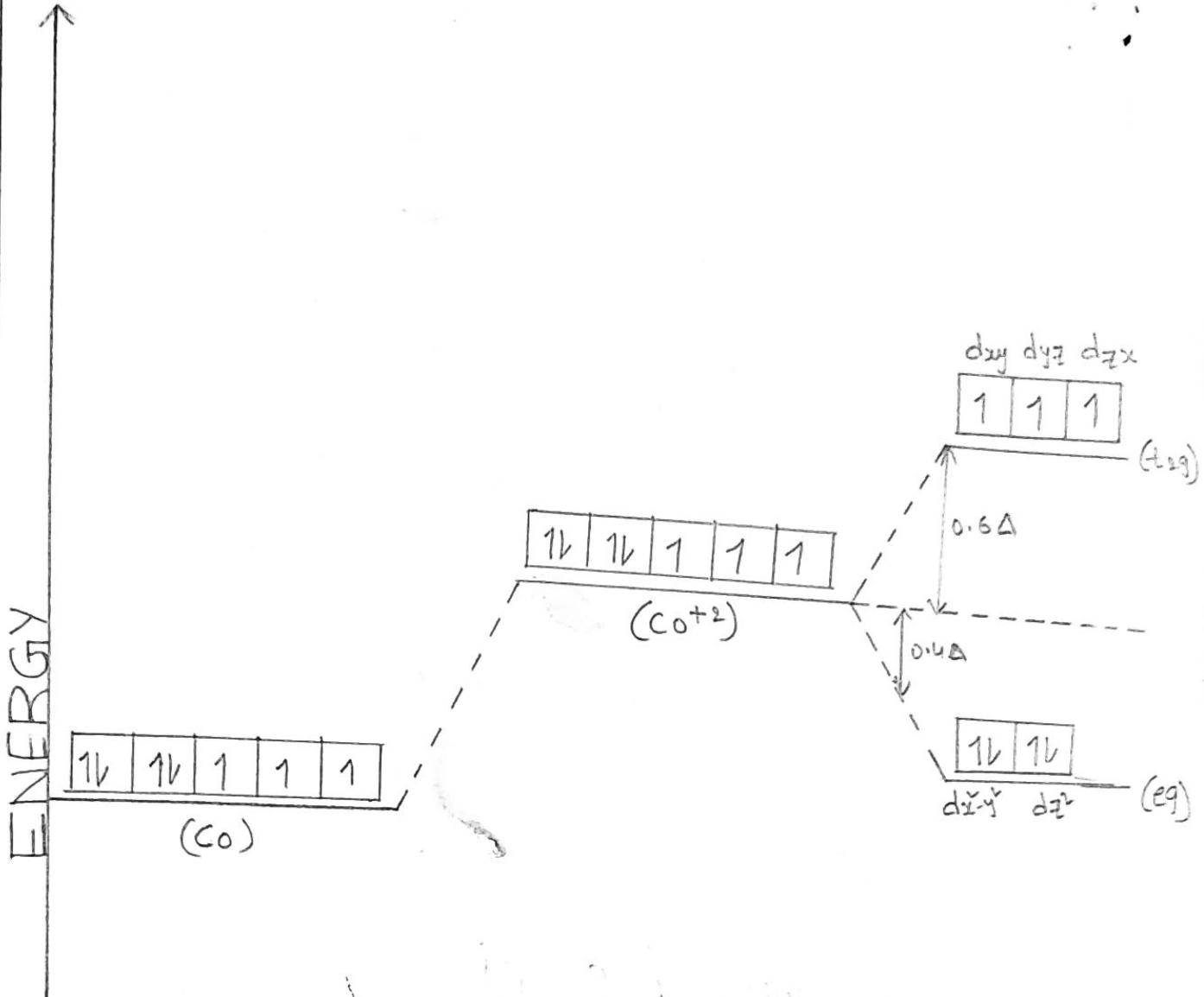
CO	-	<table border="1"><tr><td>1↑</td><td>1↑</td><td>1</td><td>1</td><td>1</td></tr></table>	1↑	1↑	1	1	1	<table border="1"><tr><td>1↑</td></tr></table>	1↑	<table border="1"><tr><td></td><td></td><td></td></tr></table>			
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$[\text{CoCl}_4]^{2-}$	-	<table border="1"><tr><td>1↑</td><td>1↑</td><td>1</td><td>1</td><td>1</td></tr></table>	1↑	1↑	1	1	1	<table border="1"><tr><td></td></tr></table>		<table border="1"><tr><td></td><td></td><td></td></tr></table>			
1↑	1↑	1	1	1									

$3d^7$ $4s^2$ $4p^0$

$3d^7$ $4s^0$ $4p^0$

(eg) (t_{2g}) $4p^0$

Energy diagram continued back side



magnetic property:

The above complex has '3' unpaired electrons, in t_{2g} orbitals, that's why complex is "paramagnetic in nature".

Schrodinger Equation:

According to de Broglie hypothesis, the particle in motion is always associated with a wave. To explain the dual nature of matter Schrodinger in the year 1926 gave a mathematical theory known as wave mechanics.

He derive a wave equation for a single moving particle by incorporating de Broglie wave length equation.

There are two wave equations.

- Schrodinger Time independent wave equation
- Schrodinger Time dependent wave equation.

Schrodinger Time Independent wave equation:

Consider a particle of mass 'm' moving with velocity 'v' along in the 'x' direction and particle is associated with a wave called de-Broglie wave, whose wave length is given by

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

For one dimensional wave motion the displacement of the stationary wave is given by the wave function (ψ) along in the x -direction.

The wave function depends upon the x -coordinate of the moving particle and time 't', it is given by the complex form

$$\psi(x,t) = A e^{i(Kx - \omega t)} \quad \text{--- (1)}$$

where 'A' is amplitude.

Differentiating equation (1) w.r.t 'x', we get

$$\frac{\partial \psi}{\partial x} = A i K e^{i(Kx - \omega t)}$$

Again differentiating above eqn w.r.t 'x', we get

$$\frac{\partial^2 \psi}{\partial x^2} = A i^2 K^2 e^{i(Kx - \omega t)} \\ = i^2 K^2 \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = -K^2 \psi \quad [i^2 = -1] \rightarrow \textcircled{2}$$

We know that wave vector

$$K = \frac{2\pi}{\lambda}$$

$$K^2 = \frac{4\pi^2}{\lambda^2} \rightarrow \textcircled{3}$$

eq(3) is substituted in eq(2), we get

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} \psi \rightarrow \textcircled{4}$$

We know that De-broglie wave length associated with the particle is given by,

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

$$\Rightarrow \frac{1}{\lambda^2} = \frac{m^2 v^2}{h^2} \\ = \frac{2m(\frac{1}{2}mv^2)}{h^2} \rightarrow \textcircled{5}$$

'E' is the total energy of the particle, and 'v' is the potential energy of the particle, then

$$TE = KE + PE$$

$$E = \frac{1}{2}mv^2 + V$$

$$\therefore \frac{1}{2}mv^2 = E - V \rightarrow \textcircled{6}$$

eq(6) is substituted in eq(5), we get

$$\frac{1}{\lambda^2} = \frac{2m(E-V)}{h^2} \rightarrow \textcircled{7}$$

eq(7) is substituted in eq(4), we get

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2 \cdot 2m(E-V)}{h^2} \psi.$$

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

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{2m 4\pi^2 (E-V)\psi}{h^2} = 0$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} + \frac{2m (E-V)\psi}{h^2} = 0 \quad \left[h = \frac{\hbar}{2\pi} \right] \rightarrow ⑧$$

The above eq. is schrodinger time independent wave equation in x -direction.

For 3-dimensional motion of the particle the above equation becomes

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m (E-V)\psi}{h^2} = 0 \rightarrow ⑨$$

$$\boxed{\nabla^2 \psi + \frac{2m (E-V)\psi}{h^2} = 0}$$

$$\text{where } \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

Schrodinger Time dependent wave equation:

For deriving time dependent Schrodinger's wave equation, the wave function is given by

$$\psi(x,t) = A e^{i(Kx - \omega t)} \rightarrow ①$$

where 'A' is Amplitude.

Differentiating above eq. w.r.t 't', we get

$$\frac{\partial \psi}{\partial t} = A i(-\omega) e^{i(Kx - \omega t)}$$

We know that $\omega = 2\pi\nu$

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= -A i(2\pi\nu) e^{i(Kx - \omega t)} \\ &= -i 2\pi\nu A e^{i(Kx - \omega t)} \end{aligned}$$

$$\frac{\partial \psi}{\partial t} = i 2\pi\nu \psi$$

According to Planck's quantum theory,

$$E = h\nu$$

$$\Rightarrow \nu = E/h.$$

' ν ' value substituted in above eq becomes

$$\begin{aligned}\frac{\partial \psi}{\partial t} &= -\frac{i 2\pi E \psi}{h} \\ &= -\frac{i^2 2\pi E \psi}{ih} \\ &= \frac{2\pi E \psi}{ih} \\ \frac{\partial \psi}{\partial t} &\cancel{\times} \frac{2\pi E \psi}{ih} \quad \left[h = \frac{h}{2\pi} \right] \rightarrow ②\end{aligned}$$

$$E\psi \cdot \partial t = ih \partial \psi$$

$$\therefore E\psi = ih \frac{\partial \psi}{\partial t} \rightarrow ③$$

Substituting above eq. in the Schrödinger's time independent wave equation, we get

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0.$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2} [(E - V)\psi]$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2} \left[i\hbar \frac{\partial \psi}{\partial t} - V\psi \right]$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = -\frac{2m}{\hbar^2} \cdot -\frac{\hbar^2}{2m} \left[i\hbar \frac{\partial \psi}{\partial t} - V\psi \right]$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = i\hbar \frac{\partial \psi}{\partial t} - V\psi \rightarrow ④$$

The above equation represents Schrödinger's Time dependent wave equation in x -direction.

for 3-dimensional the above eq. becomes.

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] \psi = i\hbar \frac{\partial \psi}{\partial t} - V\psi.$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi = i\hbar \frac{\partial \psi}{\partial t} - V\psi. \rightarrow ⑤$$