Hybridization :→

"The process of mixing of different atomic orbitals of comparable energies in an isolated atom to give rise to new orbitals of equivalent energy is called as hybridization."

New orbital so formed are known as hybrid orbitals.

Concept of Hybridization

Valence bond theory explain the formation of H_2O, HCl but can not explain the formation of molecule like $BeCl_2$, BCl_3, CH_4 by means of overlap of atomic orbitals.

The electronic configuration of Be, B, C in its ground state is

$Be_4 - 1s^2\ 2s^2$

$B_5 - 1s^2\ 2s^2\ 2p_x^1$

$C_6 - 1s^2\ 2s^2\ 2p_x^1\ 2p_y^1$

∴ Be, B, C has 0, 1, 2 unpaired electron in ground state ∴ Be is zero valent, B is monovalent & C is divalent but actually Be is bivalent, B is trivalent & C is tetravalent as they form $BeCl_2$, BCl_3, CH_4 molecule respectively.

In order to explain above fact concept of promotion of electron from lower energy level to upper vacant higher energy level ~~take~~ introduced.

- concept of hybridization is explain by considering the formation of CH_4 molecule.
- The Ground State of C atom can be represented as

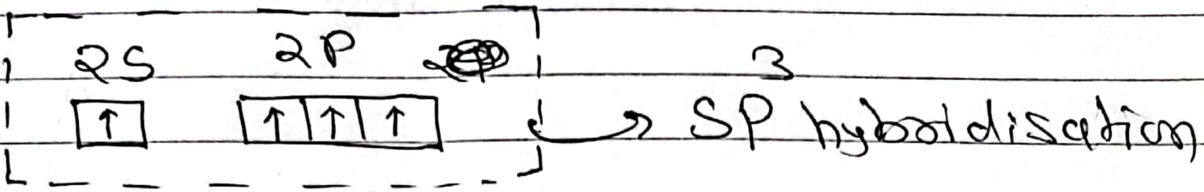
	1S	2S	2P		
G.S. of carbon atom	↑↓	↑↓	↑	↑	

- Ground State carbon has two unpaired electron. ∴
- But 'C' exhibit tetravalency in almost al compound.
- The tetravalency of carbon is explained by assuming one of two 2S electron is excited to vacant $2P_z$ orbital.
- The excited State of carbon atom can be represented as

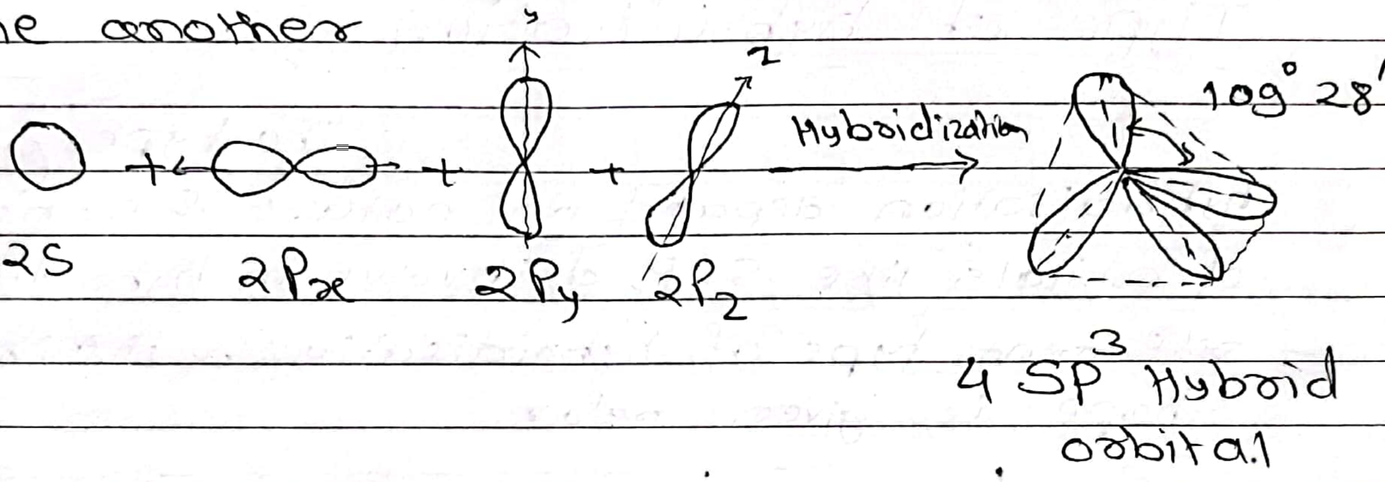
	1S	2S	2P		
E.S. of Carbon atom	↑↓	↑	↑	↑	↑

- In excited state C atom posses four unpaired electron & can Form 4 covalent bonds with four H-atoms.
- out of 4 bonds, 3-bond are of one type (S-P overlap) & Fourth of other type (S-S overlap).
- But actually all four C-H bonds in CH_4 molecule are of one type. & equivalent.

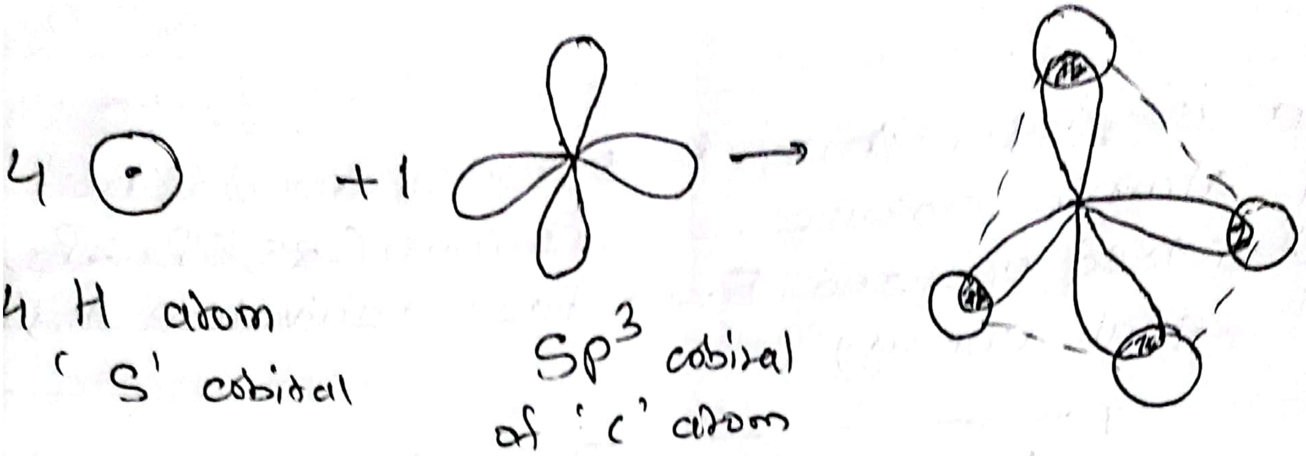
- To explain this, it is assumed that 4 atomic orbitals of carbon (2S, $2P_x$, $2P_y$, $2P_z$) get mixed up and form four equivalent hybrid of equal energy

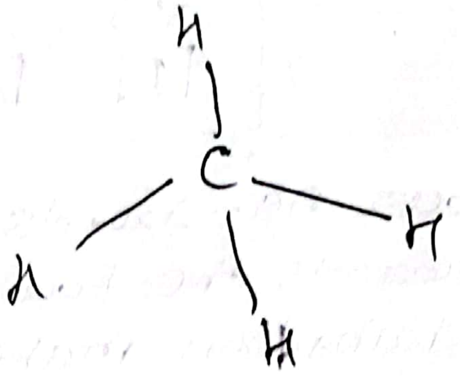


- Four new bonds are formed are directed towards the four corners of regular tetrahydron making bond angle 109° 28' with one another
-



- Hybridization take place by combination of one S and 3 p-orbitals, it is called sp^3 hybridization
- These 4 hybrid orbital overlap with 4 hydrogen atom to form sigma bond.
- carbon lies in center & 4 Hydrogen atom occupy corners of regular tetrahydron
- H–C–H bond angle 109° 28'. It is represented as follows.





Type of hybridisation :->

The type of hybridisation depand on nature & number of orbitals like s, p, d involve in hybridisation.

- Different type of hybridisation & their shape is given below.

No. of A O involved	Hybridization	shape of molecule	Bond angle	Ex:
2	sp	Linear	108°	BeF_2
3	sp^2	Trigonal plane	102°	BF_3
4	sp^3	Tetrahydral	109° 28'	CH_4
4	dsp^2	square planar	90°	$(Ni(CN)_4)$
5	dsp^3	Trigonal bipyramidal	120°, 90°	PCl_5
6	d^2sp^3	octahydral	90°	SF_6
7	d^3sp^3	pentagonal bipyramidal	72° 90°	If_7

Ni_{28} - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^8\ 4s^2$

Date : 3

dsp^2 hybridisation :→

"The combination of one d, one s, two p orbitals to form four hybrid orbitals of equal energy is known as dsp^2 hybridisation."

∴ Example of this hybridisation is $[Ni(CN)_4]^{-2}$

Geometry of $[Ni(CN)_4]^{-2}$:

outer electronic configuration of Ni atom & Ni^{+2} ion can be represented as

	3d					4s	4p		
Ni atom	↑↓	↑↓	↑↓	↑	↑	↑↓			
Ni^{+2} ion	↑↓	↑↓	↑↓	↑	↑				

- The observed geometry of $[Ni(CN)_4]^{-2}$ ion is square planer which indicate Ni^{+2} ion undergo dsp^2 hybridisation and 4 dsp^2 hybrid orbital is should be empty.
- dsp^2 hybridisation is possible only if one of the 3d orbital is empty & can be made available for hybridisation.
- This is possiable only if a strong field ligand like CN^- ion approache towards the metal ion and cause pairing of two unpaired electron in 3d orbital making available one d empty orbital for hybridisation.
- Now one 3d, one 4s, two p orbital undergo dsp^2 hybridisation to form 4 hybrid orbital.
- 4 hybrid orbital are directed towards the

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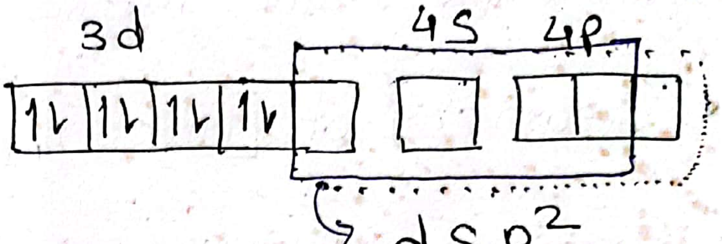
corners of a squar, making bond angle of 90 with one another.

The pairing of 3d unpaired electron & dsp^2 hybridisation is as follows.

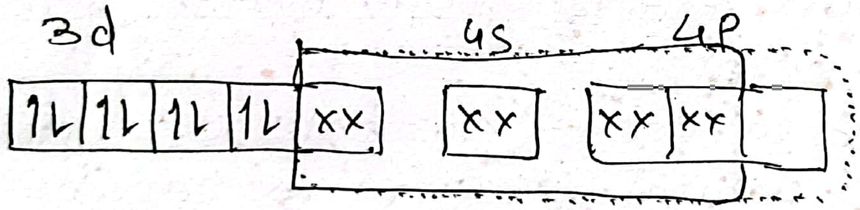
pairing of 3d electron



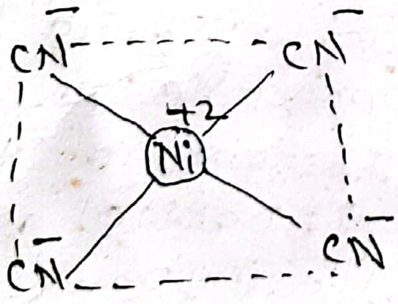
The 4 empty dsp^2 hybrid orbital can occommodate 4 lone pairs of electron donated by 4 $CN^{\ominus}$ ion to form $[Ni(CN)_4]^{-2}$ complex ion.

Ni^{+2} ion lies in center of a square & 4 $CN^{\ominus}$ ion occupy corners of a square making bond angle 90°. shown in fig.

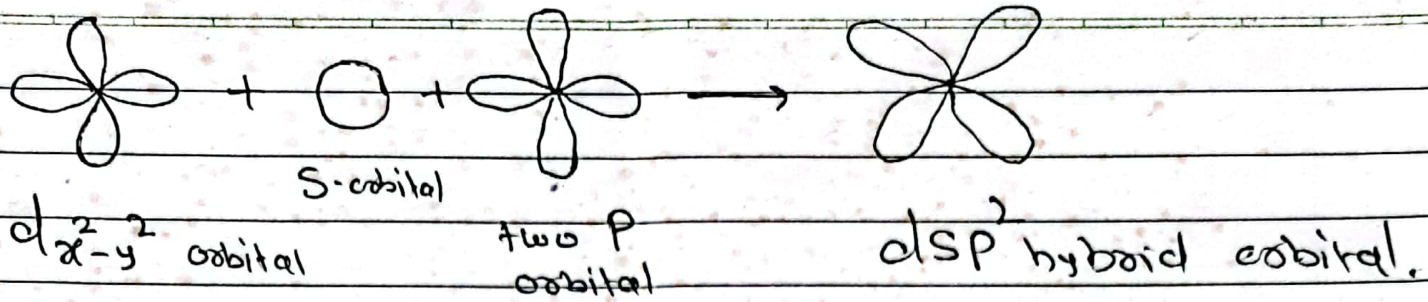
X = electron of $CN^{\ominus}$ ion.



dsp^2 hybridisation.



Formation of $[Ni(CN)_4]^{-2}$ complex ion.



sp^3d hybridisation :→

"The combination of one s, three P and one d orbitals to form five hybrid orbitals of equal energy is known as sp^3d hybridisation."

Geometry of sp^3d hybridisation depend on d orbital involved in —"—.

- Geometry of PCl_5 molecule.

$P_{15} - 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$

sp^3d hybridisation can be illustrated with PCl_5 molecule.

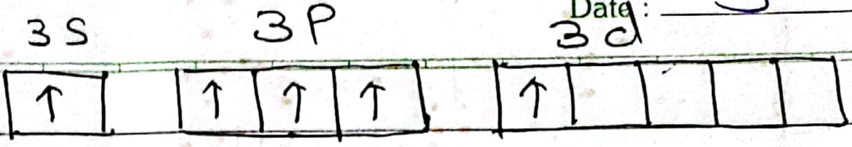
- Outer configuration of P atom in PCl_5 in ground state is

	3S	3P			3d				
G.S. of P atom	↑↓	↑	↑	↑					

- As P atom has 3 unpaired electron ∴ ~~it can not form PCl5 molecule.~~
- The Formation of PCl_5 is possible when one of 3s electron is excited to vaccant 3d orbital. making available 5 unpaired electrons.
- The outer electronic configuration of P atom in excited state can be represented as

- Excitation is always taking place in same shell.

E.S. of P atom

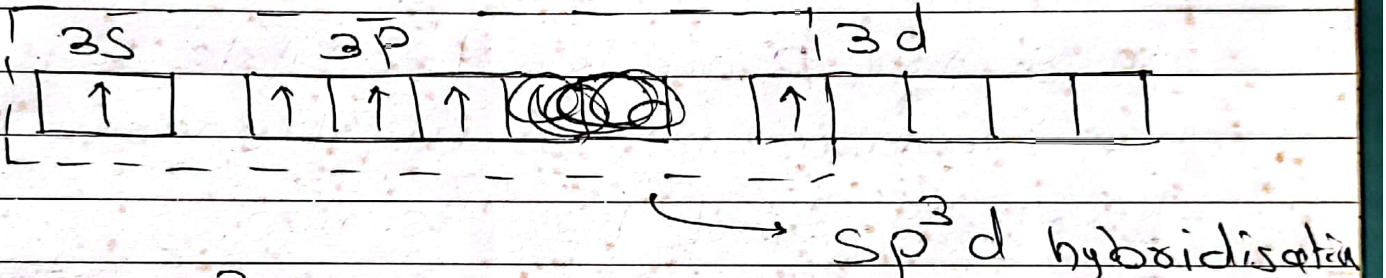


The Five unpaired electron of P atom can form PCl_5 molecule by overlap with P - orbital from Five different Cl atom.

These Five bond so formed are equivalent. Formation of equivalent bonds can be explain by hybridisation.

one 3S orbital, three 3P orbital and one 3d orbital of P atom undergoes hybridisation to give 5 sp^3d hybrid orbital having trigonal bipyramidal shape and bond angle 120° and 90° with one another.

sp^3d hybridisation of P atom is



Now 5 sp^3d hybrid orbitals overlap axially with one P orbital each from Five Cl atom to Form a sigma covalent bond.

P atom lies in center of trigonal bipyramid and 5 Cl atom occupy corners of trigonal bipyramid.

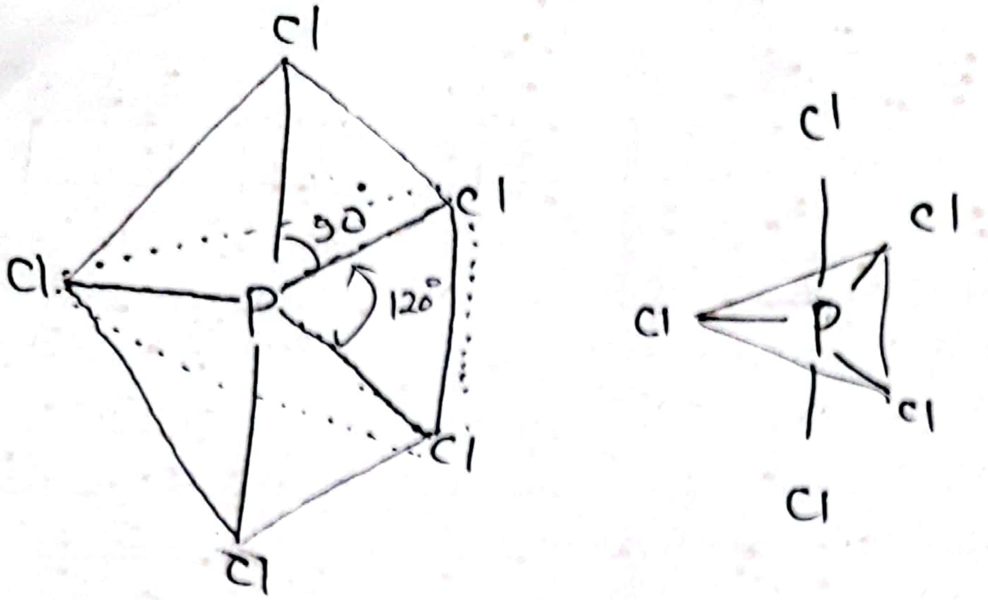


Fig:- Geometry & ~~b~~ Shape of PCl_5
Trigonal - Bipyramid.
St. of PCl_5

3] d^2sp^3 Hybridisation :→

"The combination of one s, three p and two d-orbitals to form six hybrid orbitals of equal energy is known as sp^3d^2 hybridisation."

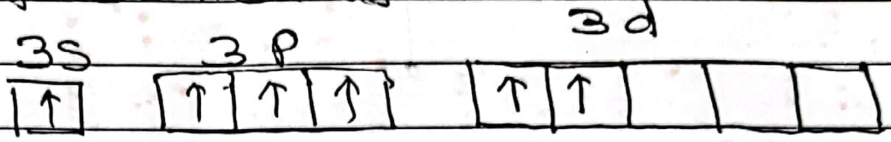
Ex:- SF_6 S_{16} - $1s^2\ 2s^2\ 2p^6\ \underline{3s^2\ 3p^4}$

- Geometry of SF_6 molecule
- Example of sp^3d^2 hybridisation of SF_6 molecule as follows.
- The outer electronic configuration of S atom in SF_6 can be represented as

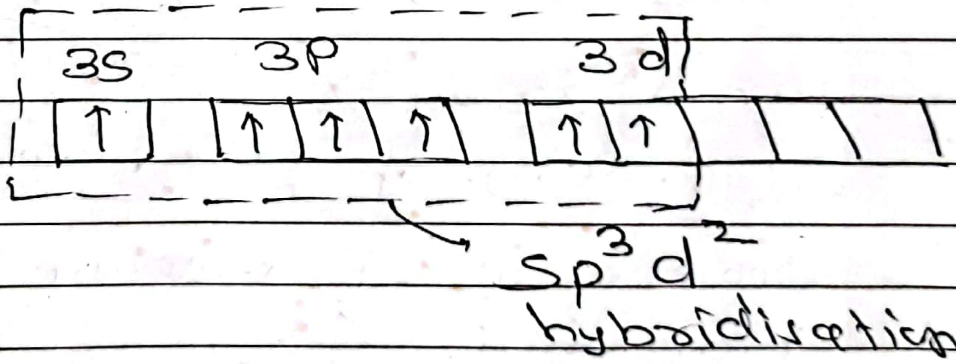
	3s	3p			3d				
G.S. of S atom	↑↓	↑↓	↑	↑					

- As S atom posses two unpaired electrons formation of SF_6 is possible only when one electron each from 3S and $3P_x$ orbital are excited to vacant 3d orbital, making available six unpaired electrons.
- The excited state electronic configuration of S atom is represented as

E.S. of S atom



- Six unpaired electron of 'S' atom can form SF_6 molecule by overlap with P orbital from six different F atoms.
- Six bond formed in SF_6 molecule is equivalent
- Formation of equivalent bond can be explain on the basis of hybridisation.
- one 3S orbital, three 3P orbital and two 3d orbital of S atom undergoes hybridisation to give rise to six sp^3d^2 hybrid orbitals which are directed towards corners of a octahydron & making an angle 90° with one another.
- sp^3d^2 hybridisation of S atom



- Now six sp^3d^2 hybrid orbital overlap axially with one P orbital each from six F atom to form a sigma covalent bond.

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The S atom lies in the center of a octahydron & six F atoms occupy the corners of octahedron.

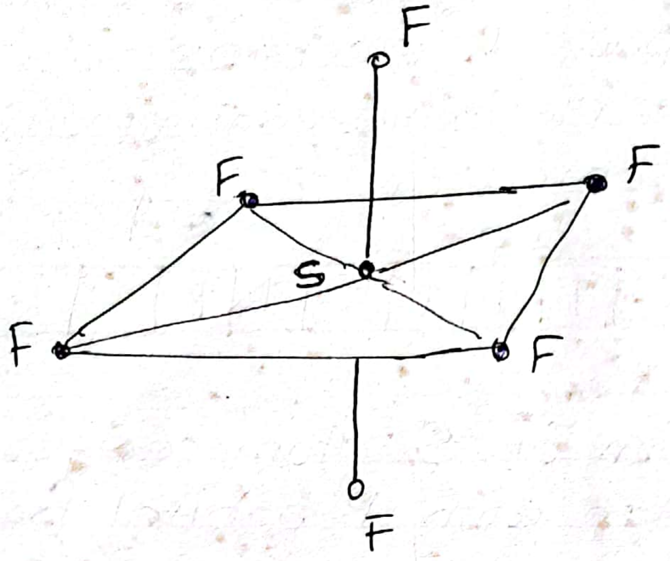

Fig:- structure of SF_6 molecule,

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d^3sp^3 Hybridisation ⇒ Ex:- IF_7

"The combination of one s, three p and three d-orbitals to form seven hybrid orbitals of equal energy is known as sp^3d^3 hybridisation."

Ex:- IF_7

∴ Geometry of IF_7 molecule ⇒

- Geometry of IF_7 molecule is pentagonal bipyramid.
- sp^3d^3 hybridisation of IF_7 molecule is given as follows.

$I_{53} = 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 4d^{10}\ 5s^2\ 5p^5$

$5s^2 \quad 5p^5$

Date : 7

- The outer electronic configuration of ~~IF7 molecule can be re~~ I atom in IF_7 molecule is represented as

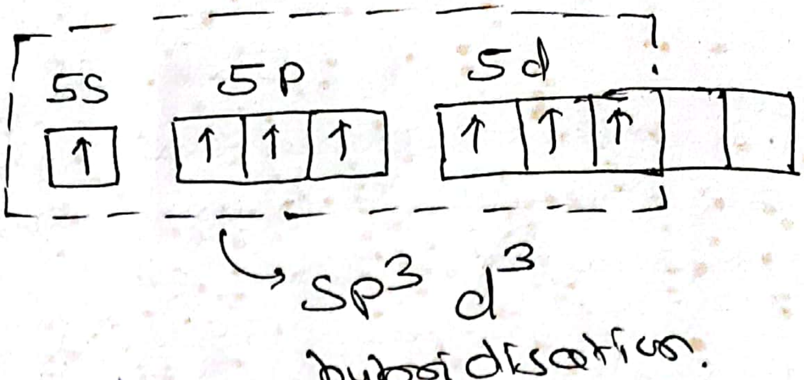
G.S. of I atom 

- I atom posses one unpaired electron.
∴ Formation of IF_7 molecule is possible when one electron each from 5S, $5P_x$ and $5P_y$ orbital is excited to vacant 5d orbital, making available 7 unpaired electron
- The outer configuration of I atom in excited state can be represented as

E.S. of I atom 

- Seven unpaired electron of I atom can form IF_7 molecule by overlap with p-orbital from seven different F atoms.
- Seven bond formed are equivalent.
- Formation of equivalent bond can be explained in term of hybridisation.
- one 5s orbital, three 5P orbital and three 5d orbital of I atom undergo hybridization to give rise to 7 sp^3d^3 hybrid orbitals which are directed toward the corners of a pentagonal bipyramid & make a bond angle 90° with one another.

sp^3d^3 hybridisation of I atom



- Now 7 sp^3d^3 hybrid orbitals overlap axially with one p-orbital each from 7 F atom to form a sigma covalent bond.
- The I atom lies in center of a pentagonal bipyramid and seven F atom occupy the corners of pentagonal bipyramid.
-

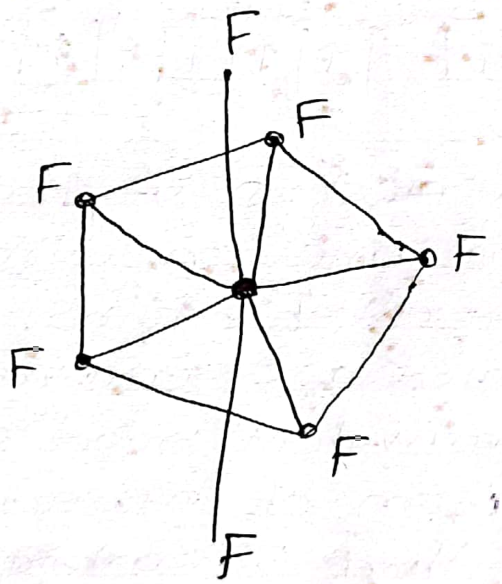


Fig:- Pentagonal Bipyramid Geometry of IF_7 molecule.

Valency Shell electron pair repulsion Theory

Date : 8

VSEPR Theory

- Gillipse and Nyholm proposed this theory in order to explain geometry of a molecule.
- Geommetry of a molecule depend on presence of bonded (shared) & non-bonded electron pairs (lone pair).
- The main point of this theory are

i) Geometry of covalent molecule depand on the number of shared (bonded) and lone pair of electron around central atom of molecule.

ii) These electron pairs are arranged in space as far apart as passiable so that there is a minimum repulsion & maximum stability.

iii) A molecule will have regular geometry only when a central atom is surrounded by bonded electron pairs only. No lone pair is present.

iv) Geometry of a molecule is distorted if one or more hybrid orbital of central atom contein lone pair of electron.

(v) The presence of lone pair decreases bond angle because the repulsion between the two lone pairs is greater than replusion between lone pair and bond pair of electron, which is greater than replusion bet^{n} two bond pair of electrons.

LP-LP > LP-BP > BP-BP

Lone pair-Lone pair repulsion > Lone pair-bond pair repulsion > bond pair-bond pair replusion.

(v) Greater is the number of lone pairs of electron on central atom, greater will be distortion in geometry of molecule.

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(v) Lesser is the electronegativity of central atom, lesser is bond angle.

- Bond angle decreases with increase in electronegativity of bonded atom.

Ex:-

NH_3	PH_3	AsH_3
106° 45'	93° 20'	91° 50'

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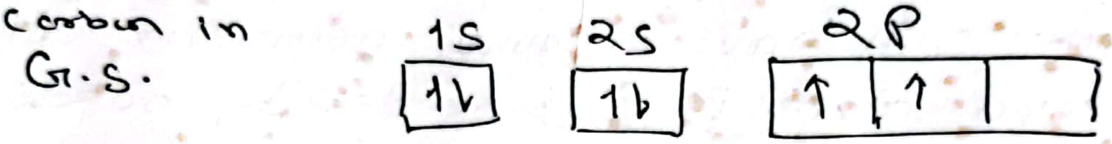
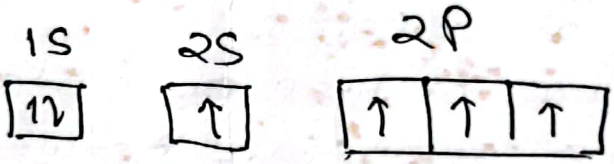
* Explaining geometry and bond angle of CH_4 molecule.

Formation of Methane (CH_4) molecule

- Ground state electronic configuration of carbon is



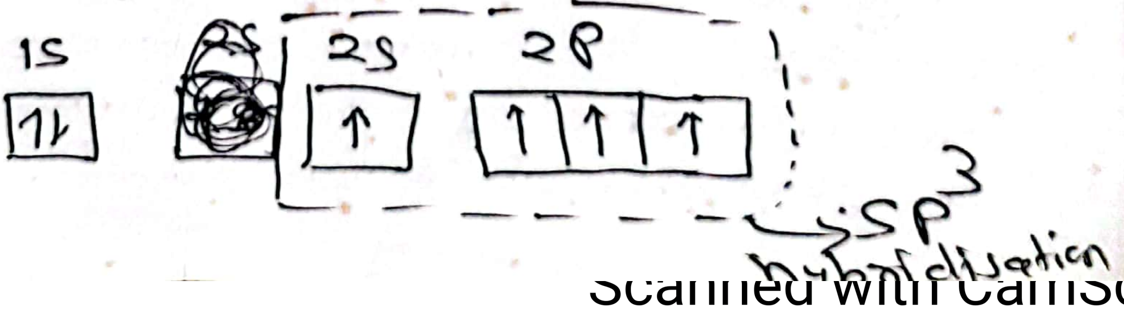
- carbon has two unpaired electron.
- electron pair in 2S orbital is excited to $2P_z$ orbital.
- Carbon in excited state



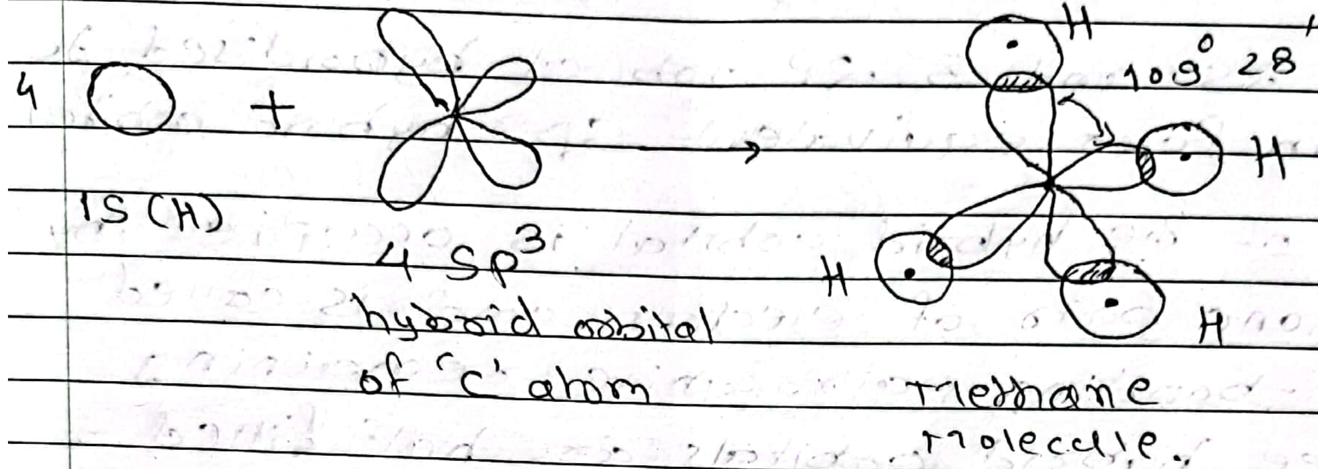
∴ carbon in excited state has 4 unpaired electron.

- These 4 orbital ($2S$, $2P_x$, $2P_y$, $2P_z$) are hybridised to form Four equivalent sp^3 hybrid orbital. Each one contain single electron with ||el (parallel) spin.

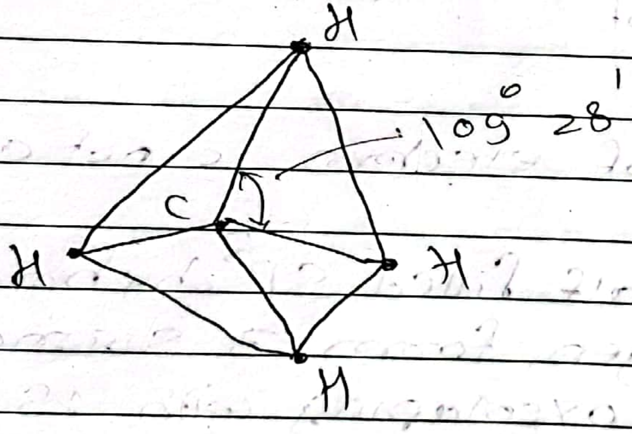
- carbon in Hybridised state

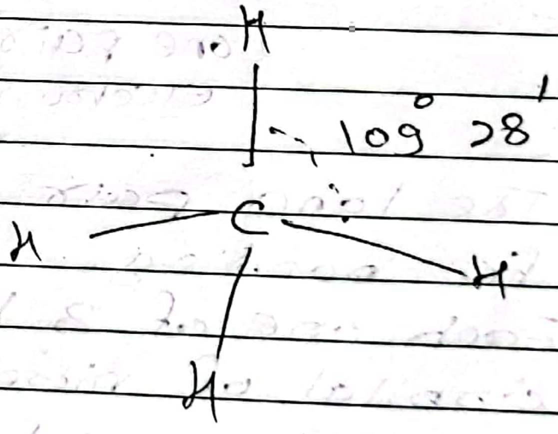


- Each one of SP^3 hybrid orbital overlap axially with half filled 1S atomic orbital of hydrogen atom to form sigma covalent bond (C–H)
- As mode of overlaping is same, all 4 C–H bond in methane are equivalent.



- The methane molecule has tetrahydral geometry with carbon atom in centre & four hydrogen atom at corner of regular tetrahedron.
- Sp^3 hybrid orbital are inclined at $109^\circ 28'$ to have maxium stability & minium replusion.





Electronic structure of C in CH_4

$$1S\ \boxed{\uparrow\downarrow}\quad \underbrace{2S\ \boxed{\uparrow\downarrow}\quad 2P\ \boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}}_{Sp^3\ \text{hybridisation}}$$

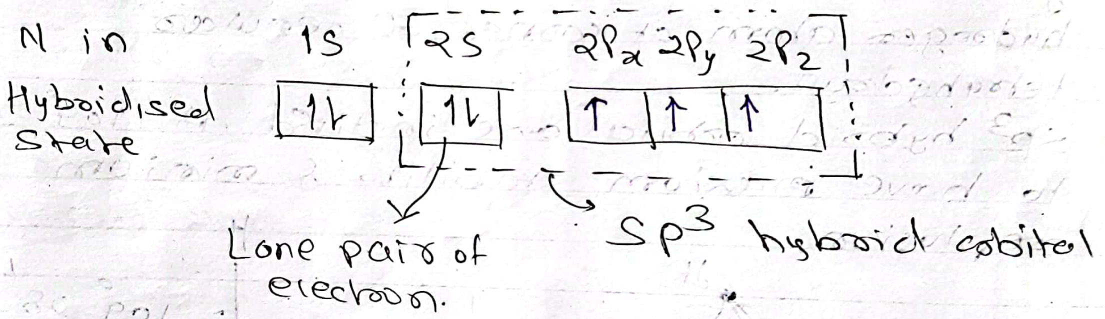
Dotted arrow indicate electron of shared with hydrogen atom

* Formation of NH_3 molecule.

- The electronic configuration of nitrogen in ground state is

$$1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z$$

- one 2s and 3 2p orbital hybridised to form four equivalent sp^3 hybrid orbital.
- one of the hybrid orbital is occupied by a lone pair of electron and is called non-bonding pair. while remaining three hybrid orbitals are half filled i.e. contain single electron with parallel spin.



- The lone pair of electron is not available for bonding.
- Each one of 3 half filled sp^3 hybrid orbital of nitrogen form 3 sigma bond by axial overlaping with 1s orbital of 3 hydrogen atom.

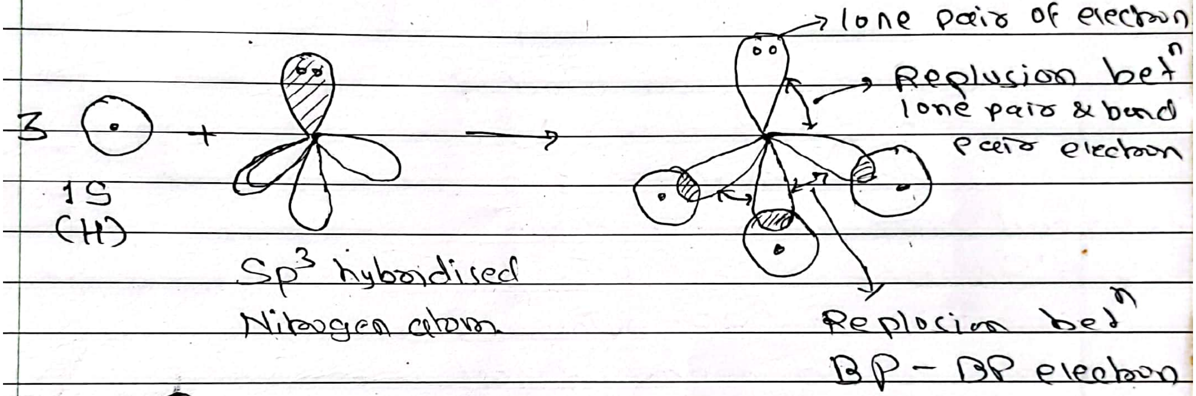
Date :

Electronic structure of N in NH_3 1S [↑↓] 2S [↑↓] 2P [↑⇣][↑⇣][↑⇣]

Dotted ~~electron~~ indicate electron of H atom

→ sp^3 hybridisation.

Force of repulsion betn the lone pair of electron and electron in bonding orbitals is greater than that of bonding - bonding electronic pairs.
∴ H–N–H bond angle is ~~reduced~~ compressed to 107° 28' from 109° 28'
So regular tetrahedral structure get distorted to pyramid.
Three hydrogen atom form the base of pyramid & lone pair of electron form the apex of pyramid while nitrogen remains at the centre.



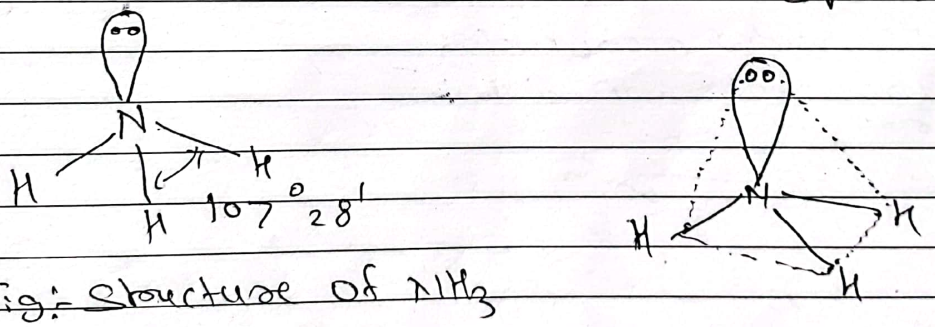
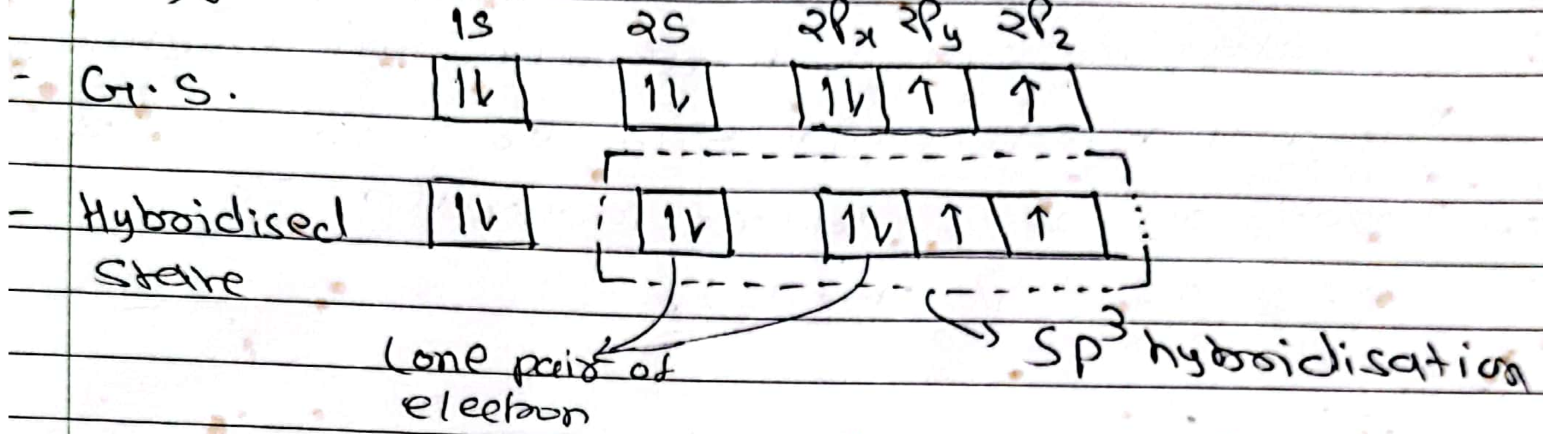


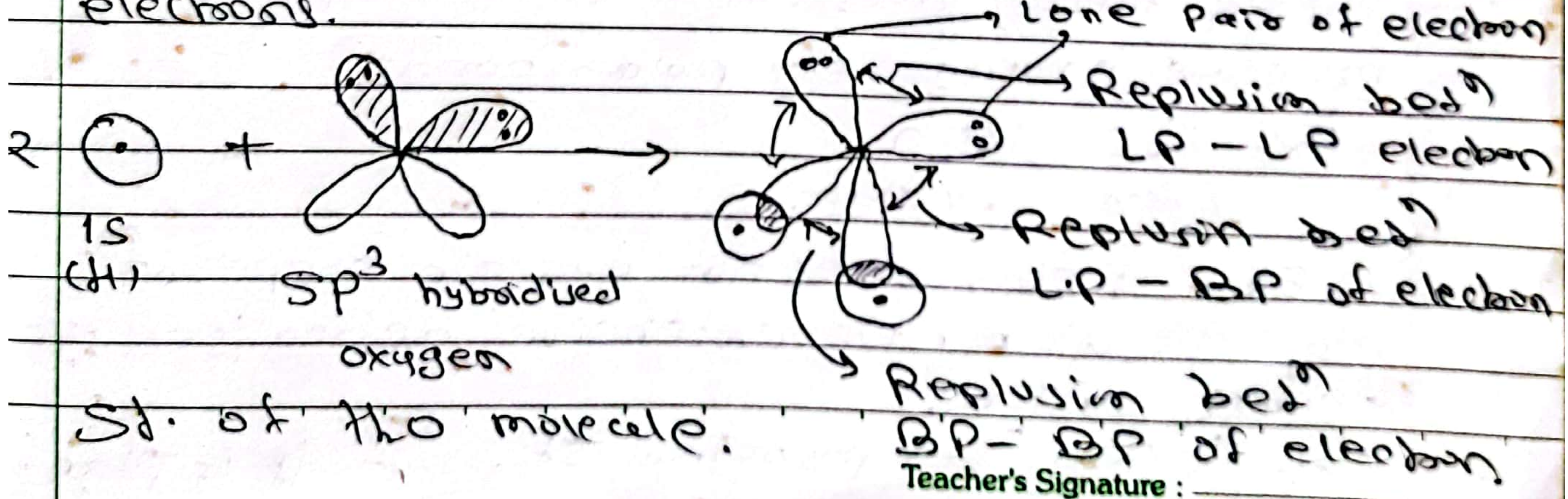
Fig:- Structure of NH_3

* Formation of Water (H_2O) Molecule

- The electronic structure/configuration of oxygen atom in ground state is
- It is assumed that one 2S & three 2P orbitals undergo SP^3 hybridisation producing Four tetrahedrally hybrid orbitals.
- oxygen in

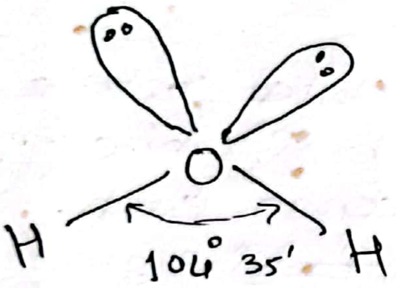


- Two of these SP^3 hybrid orbital contain 2 lone pair (non-bonding) of electron, while remaining 2 orbital contain one electron each.
- These ~~one~~ 2 unpaired electron form sigma bond by axial overlaping with 1S orbital of 'H' atom. Thus O–H bond involve SP^3–S overlap.
- In H_2O molecule, two hydrogen atoms are at two corner of a tetrahydron while other two corner are occupied by two lone pair of electrons.



St. of H_2O molecule.

- Thus, in water molecule the replusion bet^n two lone pairs of electron is greater than the replusion bet^n lone pair and bond pair electron. which is greater than replusion bet^n bond pair and bond pair electrons.
- H–O–H bond angle is compressed to greater distortion in tetrahedral structure.
- H–O–H bond angle in water is 104° 35' & not 109° 28' ∴ water molecule is angular (V shape).



St. of H_2O molecule.

Limitation of VSEPR Theory

- VSEPR theory does not explain shape of molecule having very polar bonds.
  Ex:- Li_2O , H_2O
  Linear V-shape.

VSEPR theory does not explain shape of molecule which have extensive delocalised π electron system.
Ex:- $[C(N_3)]^-$ ⇒ pyramid st. but it is planar

- This theory fails to explain shape of certain compound of transition element.
Ex:- complexes of transition —"— of d^8 configuration are square planar & not tetrahedral as predicted theory.
- It does not make any distinction betⁿ electron which are present in different type of orbitals. (s, p, d, f) of valence shell.
- VSEPR theory fail to predict exact bond angle in molecule such as H_2O, NH_3 having distorted geometry.
- It fails to explain difference in bond angle in a given series of compound (NH_3, PH_3, AsH_3, SbH_3) in which central atom is different.

Molecular orbital Theory(M.O.T.)

Basic principle of M.O.T.

) When two atoms come close to each other their atomic orbitals interact leading to the formation of molecular orbitals. The atomic orbital of atom in a molecule completely lose their identity.

) Each molecular orbital is described by a wave Function ψ, known as molecular orbital wave Function.

3) ψ is such that ψ^2 represent probality density or electron density

) Each M.O. wave Function ψ, is associated with a set of quantum number which determine shape & energy of M.O.

) Electron is Filled in M. orbital by the same rule as filled in Atomic orbital Following aufbau principle, pauling exclusion principle, Hund's rule of maxium multiplicity.

) Each electron in a M.O. belong to all nuclei present in the molecule.

) Each electron in a M.O. has a spin of $+1/2$ or $-1/2$.

LCAO (Linear Combination Atomic Orbital)

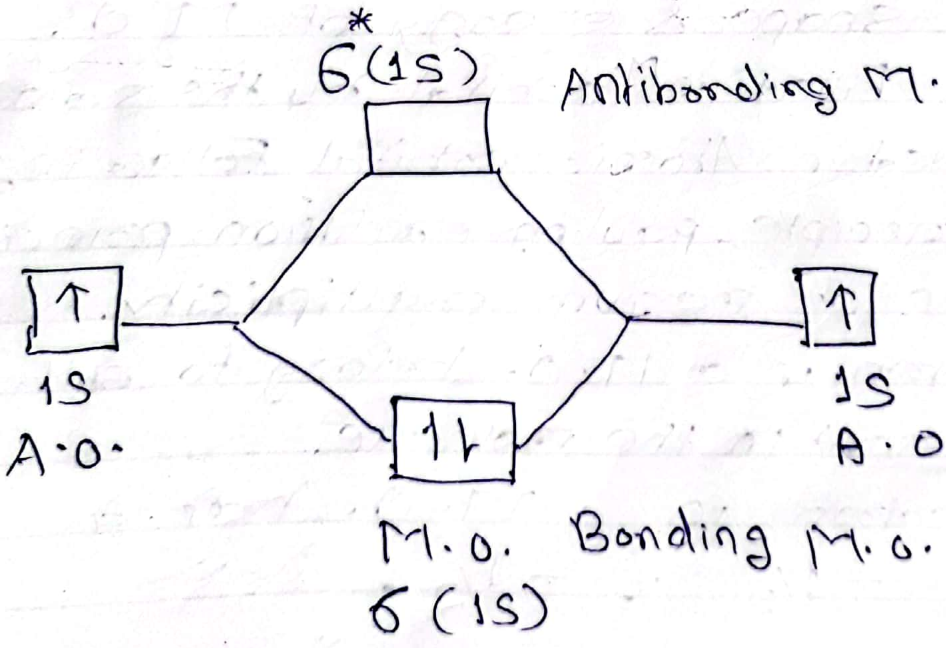
Method for formation of M.O.

In LCAO method, two atoms approach one another along a line. when they come close to one another, two atomic orbitals, overlap interact with each other to form two molecular orbital.

One of the molecular orbital will have lower energy than combining atomic orbitals gives rise to an attractive state known as bonding molecular orbitals (BMO).

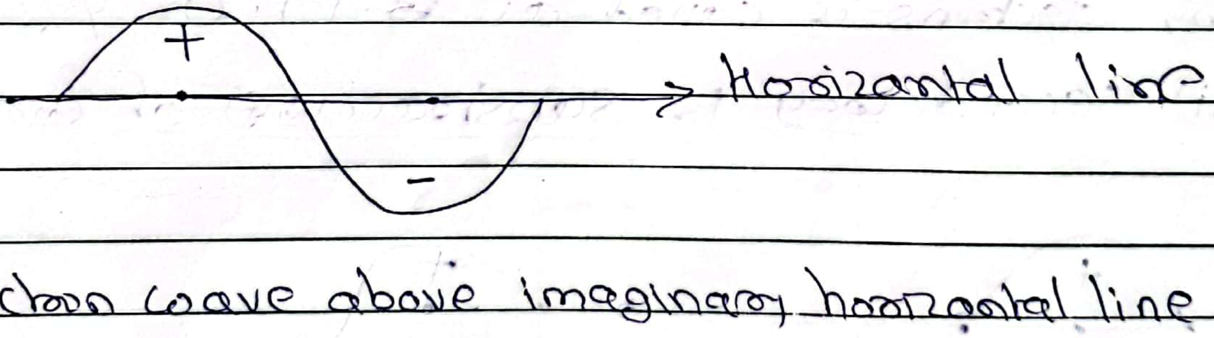
The second molecular orbitals has higher energy than the combining atomic orbitals gives rise to replusive state is called antibonding molecular orbitals (AMO)

Formation of bonding & antibonding M.O. with energy difference shown in fig.



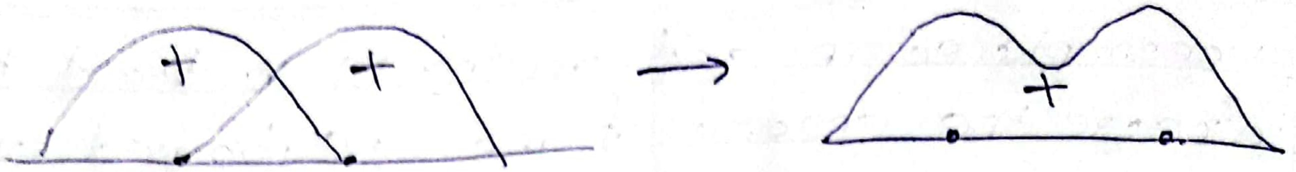
- Electron placed in antibonding M.O. tend to increase the energy of molecule formed and ~~and~~ decrease stability.
- Electron placed in B.M.O. tend to decrease the energy of molecule & increase stability.
- Bonding & Antibonding distinguished by putting an asterisk (*) on antibonding M.O.

- Formation of Bonding & Antibonding M.O. is illustrated by considering the formation of H_2 molecule.
- In H_2 molecule 1S orbital of one hydrogen atom overlap with 1S orbital of another hydrogen atom to form two M.O.
- Before we discus this method, it is necessary to explain meaning of electron wave ψ. Electron wave can be represented as



- Electron wave above imaginary horizontal line is give +ve sign while below the line -ve.
- There are two ways of combining atomic orbital i.e. electron waves.

(i) one way is Addition of wave :-

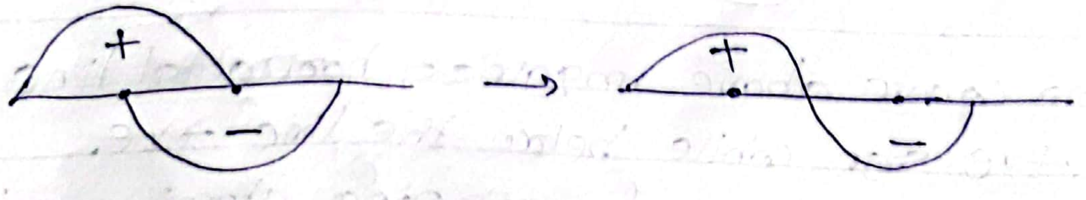


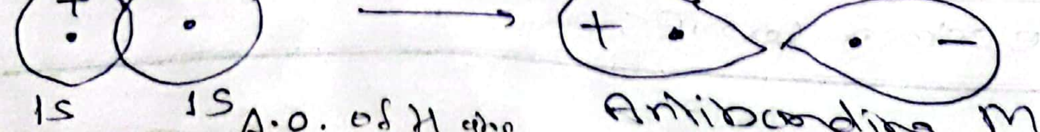
1s A.O. 1s A.O. in H-atom

σ (1s) B.M.O. in H_2 molecule.

- Two dot represent two nuclei.
- Both the electron wave are on same side (+ve) & on adding result in formation of of M.O. called B.M.O. shown in fig. & designated as σ (1s) orbital.
- combination of two 1s orbital to form M.O.
- Bonding M.O ⇒ The M.O. produced by additive overlap of atomic orbitals and having lower energy than combing atomic orbital, which lead to bonding state occupied by electrons is called as B.M.O ψ.

(ii) Second way is substraction of wave :-





1s A O 1s A.O. of H atom

Antibonding M.O. in H_2 molecule

Here two electron wave are oriented in two opposite direction $\therefore$ they cancel out each others and probability of finding electron in this region of overlap is practically nil.

- As there is no electron in this region $\therefore$ nuclei repelled each others as shown in figer. such a M.O. is called antibonding M.O. designated as $\sigma^*(1s)$
- Antibonding M.O. :-> M.O. produced by substractive overlaping of atomic orbital & having higher energy than combining atomic orbitals, which leads to the antibonding state of molecule occupied by electron is called A.M.O. ψ^2

* Difference bet^n Bonding & Antibonding M.O.

Bonding M.O.	Antibonding M.O.
1. It is Foormed by additive overlaping of atomic oobital.	1 It is Foormed by subsroactive overlaping of atomic oobital.
2. It has lowes energy than combining A.O.	2. It has highes energy than combing A.O.
3 Electoon charge density in bet^n nuclei is high	3. Electoon charge density in bet^n nuclei is very low.
4. Replusion bet^n nuclei is very low	4. Replusion bet^n nuclei is very high.
5. Electoon in B.M.O. i Favours Stable bond Foomcation.	5. Electoon in A.B.M.O. / oppose Favours unstable bond Foormation.
6 Difference in energy bet^n B.M.O. & combining A.O. is called stabilization energy.	6. Difference in energy bet^n antibonding M.O. & combining A.O. is called destabilization energy.

* Energy Level Diagram For Molecular orbit

- In the same way that 1s atomic orbital of 2 atoms form two M.O's designated as $\sigma(1s)$ & $\sigma^*(1s)$. The 2s, 2P atomic orbitals given rise to eight M.O.
- Bonding M.O.'s $\sigma(2s)$, $\sigma(2P_z)$, $\pi(2P_x)$ $\pi(2P_y)$
- Atomic ↑ M.O's : $\sigma^*(2s)$ $\sigma^*(2P_z)$ $\pi^*(2P_x)$ $\pi^*(2P_y)$
Antibonding

- The energy level's of these M.O. have been determined experimentally from spectroscopic data.
- The energy increase as we move from left to right in following list.

$$\sigma(1s),\ \sigma^*(1s),\ \sigma(2s),\ \sigma^*(2s),\ \sigma(2P_z),\ \pi(2P_x) = \pi(2P_y)$$
$$\pi^*(2P_x) = \pi^*(2P_y),\ \sigma^*(2P_z).$$

- The energy level of different M.O. are shown diagramatically in fig.
- In this digram M.O. are in centre & Atomic orbital are on two extreme.

Atomic orbital of same energy are shown at the same level while B.M.O are shown lower & A.B.M.O shown at higher than corresponding atomic orbitals.

This indicate B.M.O are more stable & A.B.M.O are less stable than A.O. from which they formed.

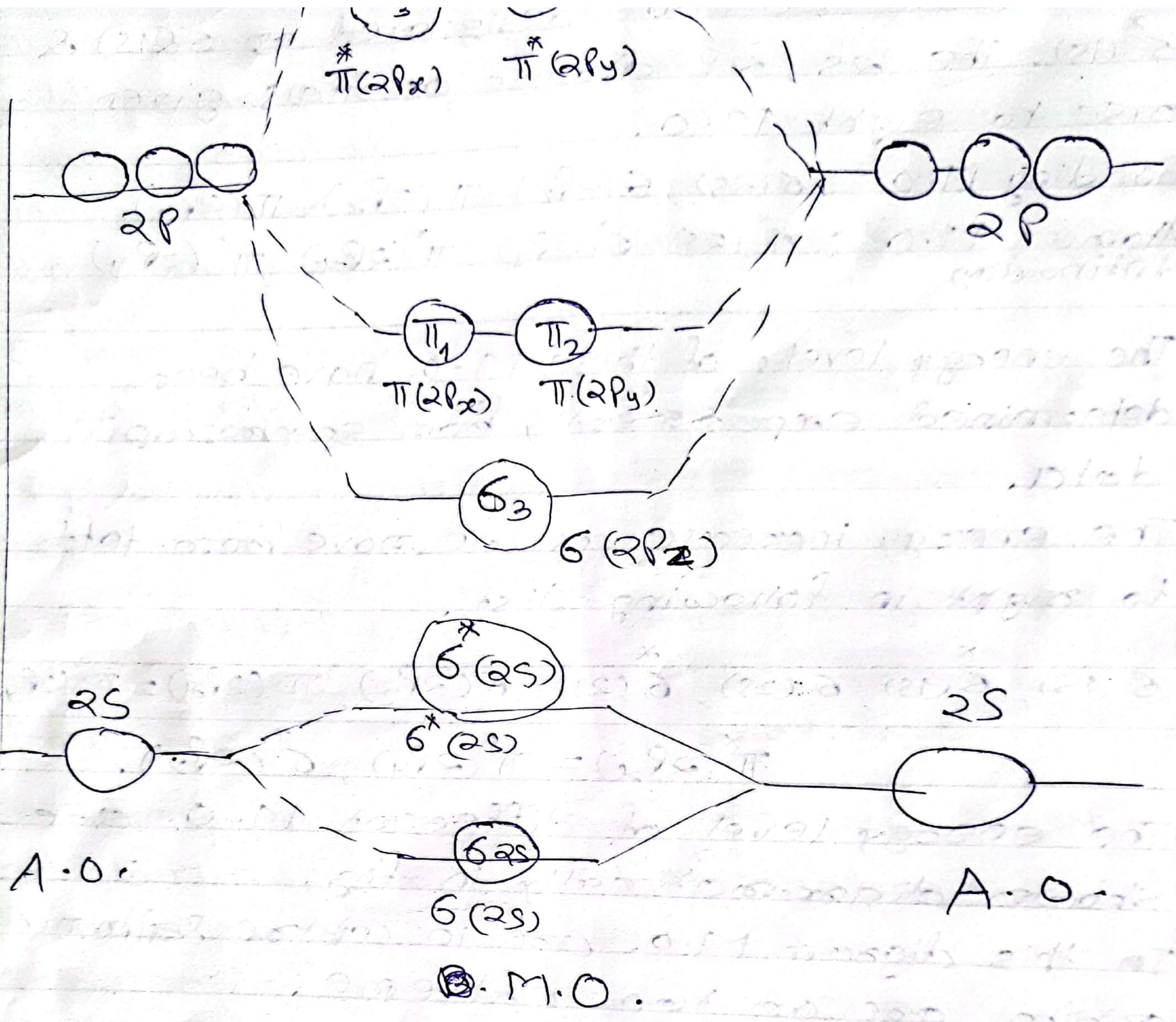


Fig: Energy level of different M.O.

- Spectroscopic studies show that above sequence of energy level of M.O. is not correct for all molecule.

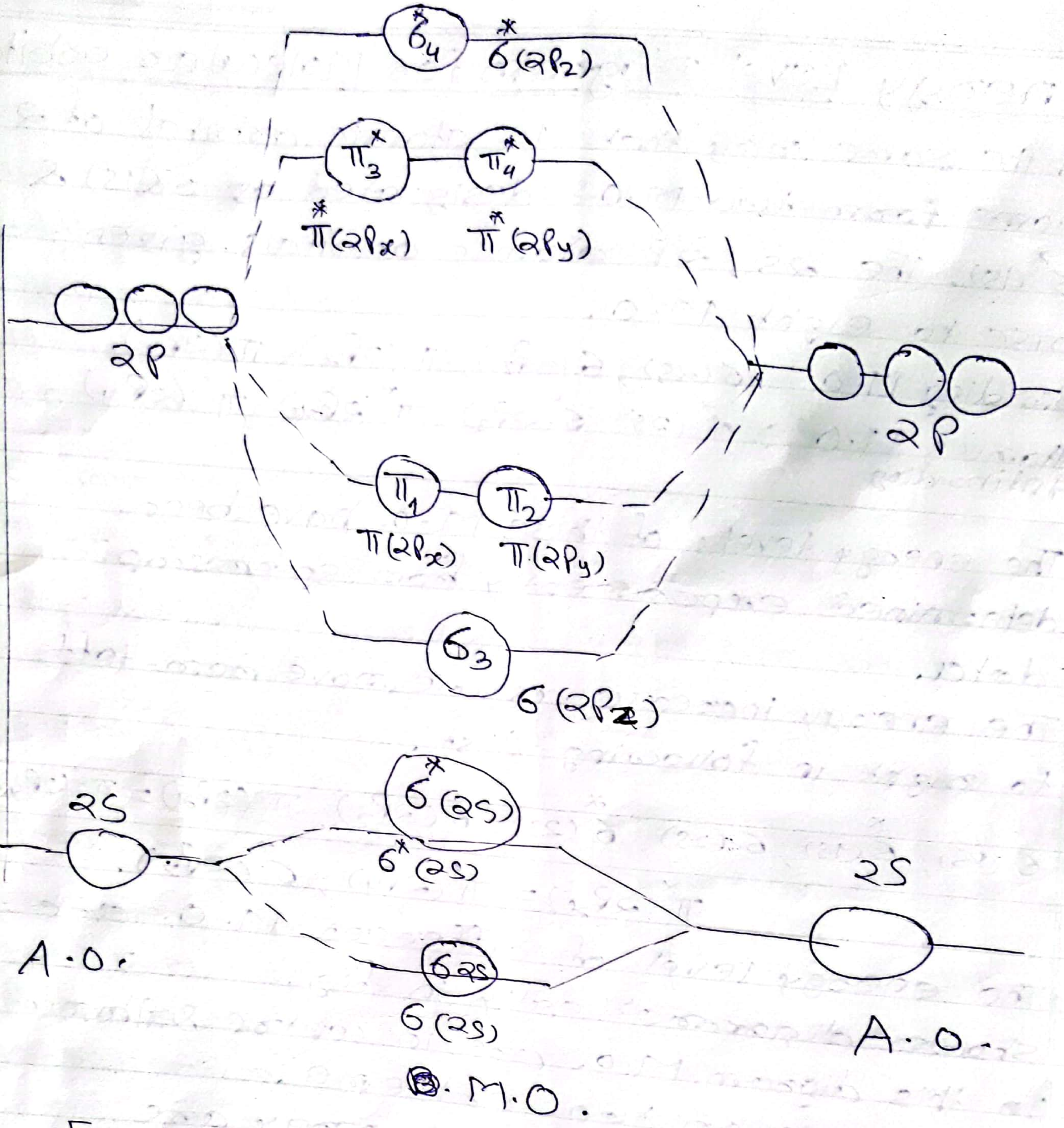


Fig: Energy level of different M.O.

- Spectroscopic studies show that above sequence of energy level of M.O. is not correct for all molecule.

Rules For adding Electron to M.O.:

M.O. with lowest energy is filled 1st. Maxium number of electron in M.O. cannot exceed two and two electrons must be opposite spin.

If there are two or more M.O. at the same energy level, pairing of electrons will occur only after each orbital of same energy has one electron.

Bond order:

Bond order refers to number of bonds formed bet^{n} the two atoms in a molecule.

It is calculated from number of electron in bonding and antibonding M.O. as follows

$$\text{Bond order} = \frac{1}{2}\left[\text{No. of electron in B.M.O} - \text{No. of electron in A.B.M.O.}\right]$$

Bond order is 0, 1, 2, 3 corresponding to zero, single, double, triple bond in bet^{n} ~~molecule~~ atom.

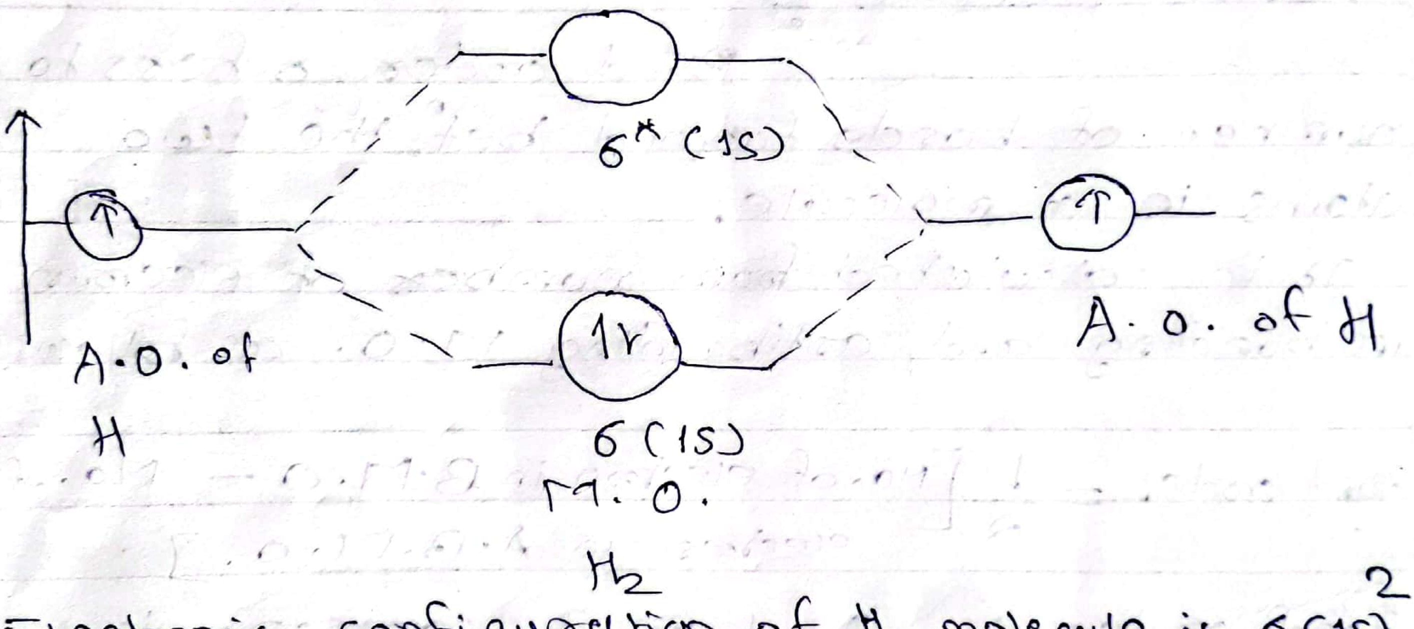
Bond order $\propto$ to bond dissociation energy,

$$\propto \frac{1}{\text{Bond length}}$$

* Molecular orbital digoram For H_2 molecule :-

✓

- H_2 molecule is Formed by combination of two Hydrogen atoms.
- Each hydrogen atom has one electron in 1S orbitals & ∴ there are two electron to be occomodated in M.O.S.
- Both electron occumodate in $\sigma(1S)$ B.M.O.
- According to pauli's exclusion principle these two electron have opposite spins.
- M.O. energy level digoram of H_2 molecule is give below.
- Two 1S A.O. of two atom of -H form two M.O. namely $\sigma(1S)$ and $\sigma^*(1S)$.



- Electronic configuration of H_2 molecule is $\sigma(1S)^2$.
- Bond order = $\frac{1}{2}$ (No. of e^- in B.M.O − No. of e^- in A.B.M.O.)

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

∴ Two Hydrogen atom are bonded together by a single bond.

Nitrogen

Molecular orbitals diagram For N_2 Molecule

Electronic configuration of nitrogen atom is
$N - 1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1$

When atomic orbital from two nitrogen atom combine there will be 14 electron in N_2 molecule & these are distributed in various M.O. as

$$\sigma(1s)^2, \sigma^*(1s)^2, \sigma(2s)^2, \sigma^*(2s)^2, \begin{cases}\pi(2p_y)^2 \\ \pi(2p_z)^2\end{cases} . \sigma(2p_x)^2$$

Three A.B.M.O are $\sigma^*(2p_x)$ & $\pi^*(2p_y)$ $\pi^*(2p_z)$ will remain vacant.

$\sigma(1s)$ and $\sigma^*(1s)$ orbitals lie below valency shell & do not take part in bond formation & are known as non-bonding M.O.

Hence nitrogen molecule is stable with bond order given by

$$\text{Bond orders} = \left[\frac{\text{No. of electrons in B.M.O} - \text{No. of electron in A.B.M.O}}{2}\right]$$

$$= \frac{8-2}{2} = 3$$

There are 3 bond in betn N_2 molecule.

As there is no unpaired electron in M.O.
$\therefore$ N_2 is diamagnetic.

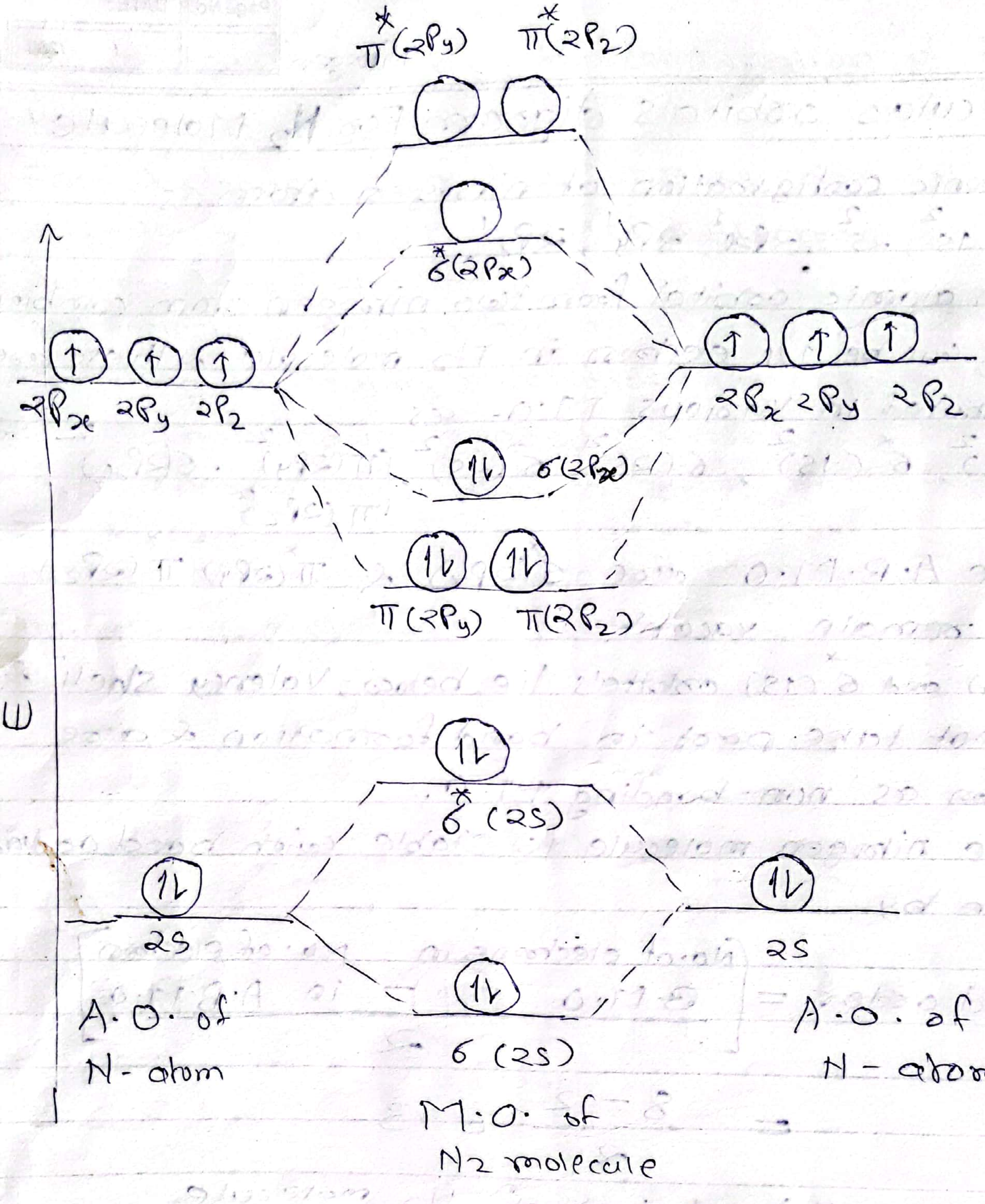


Fig:- M.O. Energy level diagram of N_2 molecule.

Molecular orbital Energy level digram For O_2 molecule :->

- Electronic configuration of oxygen atom in O_8.
$1S^2, 2S^2, 2P_x^2, 2P_y^1, 2P_z^1$.
- Atomic orbital of two oxygen atom combine, there will be 16 electron in O_2 molecule & these are distributed in various M.O. as follows.

$$\sigma(1S)^2, \sigma^*(1S)^2, \sigma(2S)^2, \sigma^*(2S)^2, \sigma(2P_x)^2, \left\{\begin{matrix}\pi(2P_y)^2 \\ \pi(2P_z)^2\end{matrix}\right., \left\{\begin{matrix}\pi^*(2P_y)^1 \\ \pi^*(2P_z)^1\end{matrix}\right.$$

A.B.M.O $\pi^*(2P_y)$ & $\pi^*(2P_z)$ orbital are singly occupied in accordance with Hund's rule.

- $\sigma(1S)$, $\sigma^*(1S)$ orbital lie below the valency shell & not take part in bond formation, called as non-bonding M.O.
- In valency shell, there are 4 bonding M.O. filled with 2 electron are $\sigma(2S)$, $\sigma(2P_x)$, $\pi(2P_y)$, $\pi(2P_z)$ giving total no. of 8 electrons in B.M.O.
- Also 3 A.B.M.O. with 2 electrons.
$\pi^*(2P_y)$ & $\pi^*(2P_z)$ filled with one electron
∴ there are total 4 antibonding electrons.

$$\text{Bond order} = \frac{1}{2}\left[\text{No. of electron in B.M.O} - \text{No. of electron in A.B.M.O}\right]$$

$$= \frac{1}{2}[8-4] = 2$$

Double bond is present in O_2 molecule.

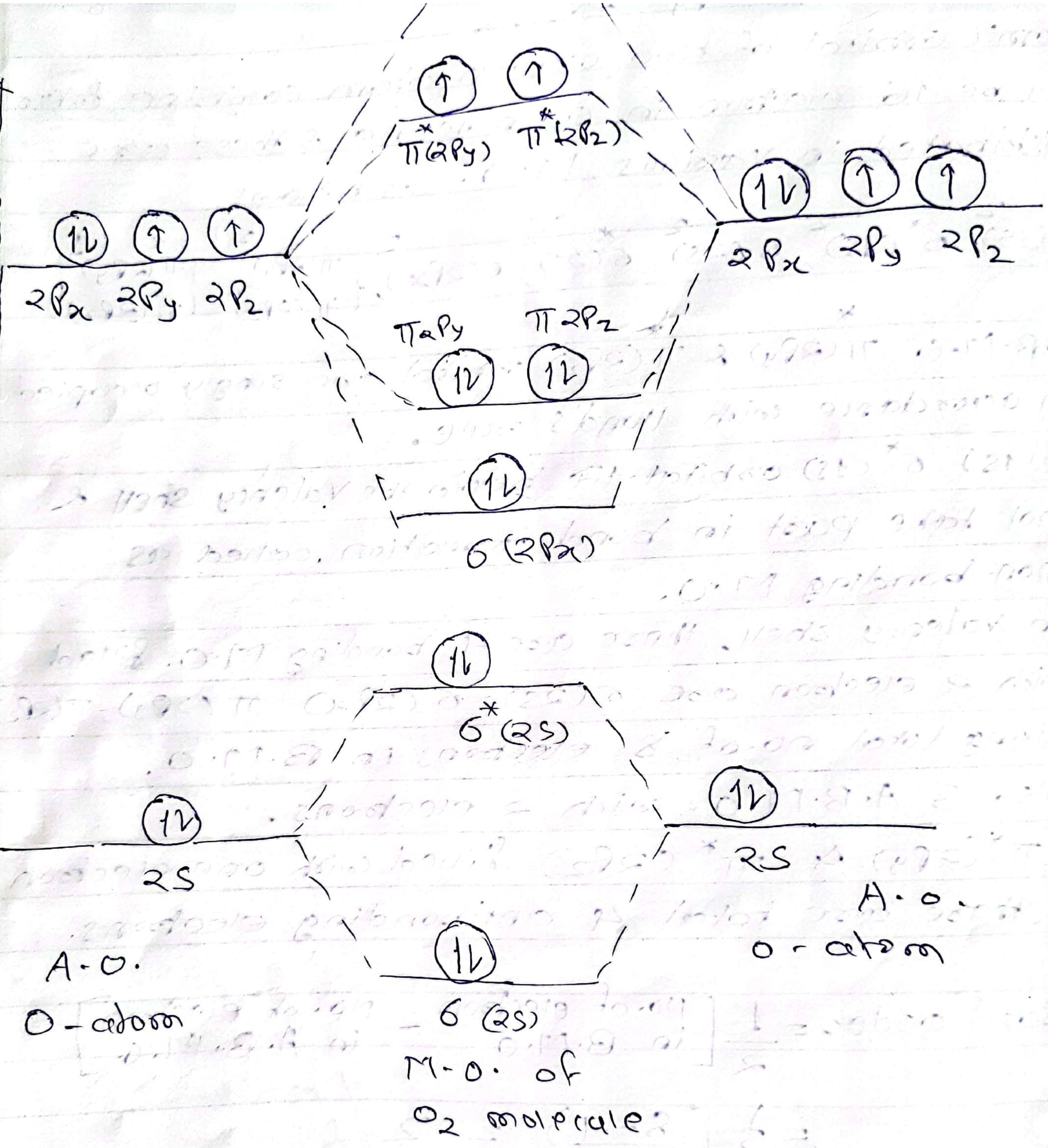


Fig:- M.O. energy level digram of O_2 molecule.

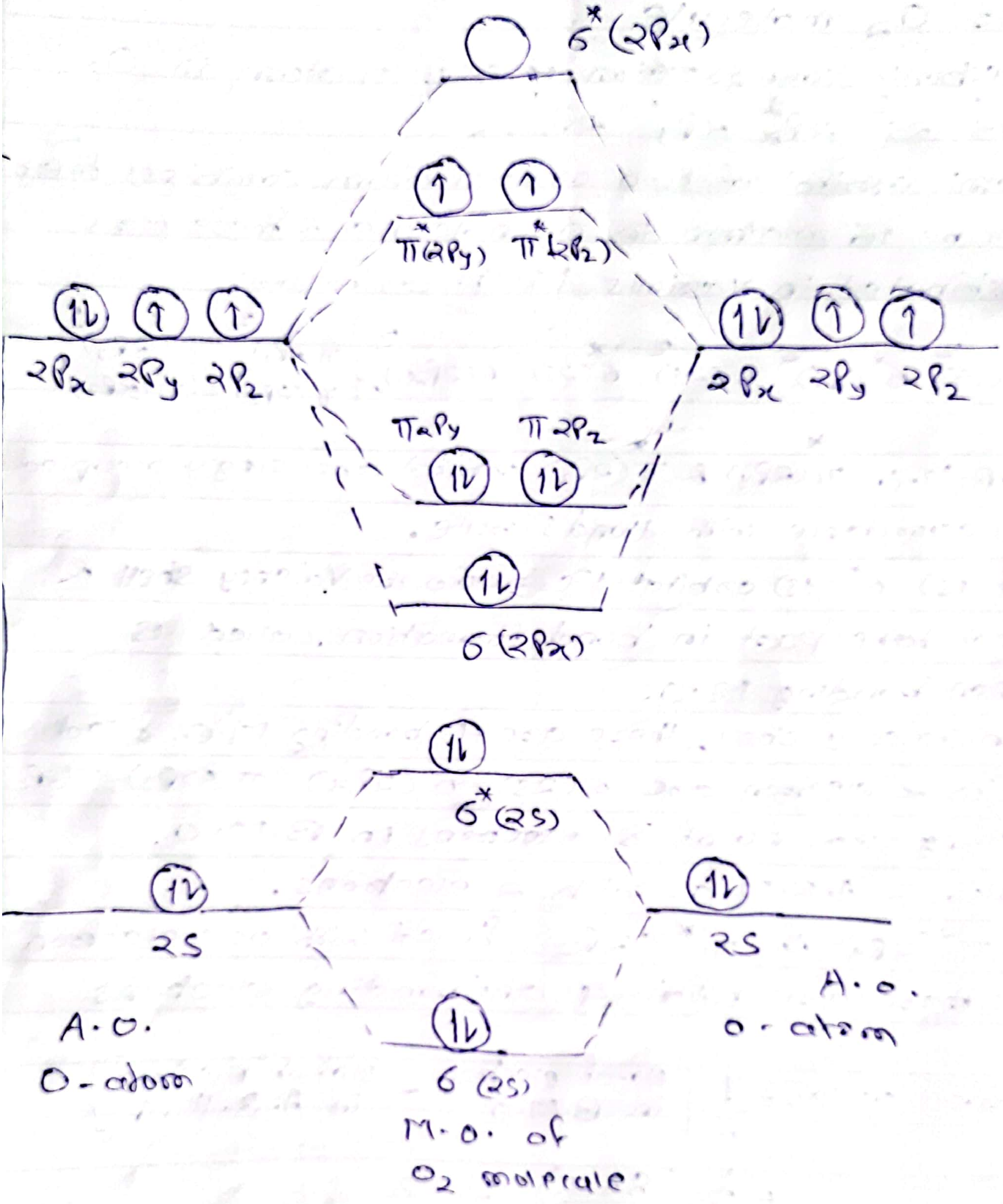


Fig:- M·O· energy level digraam of O_2 molecule.

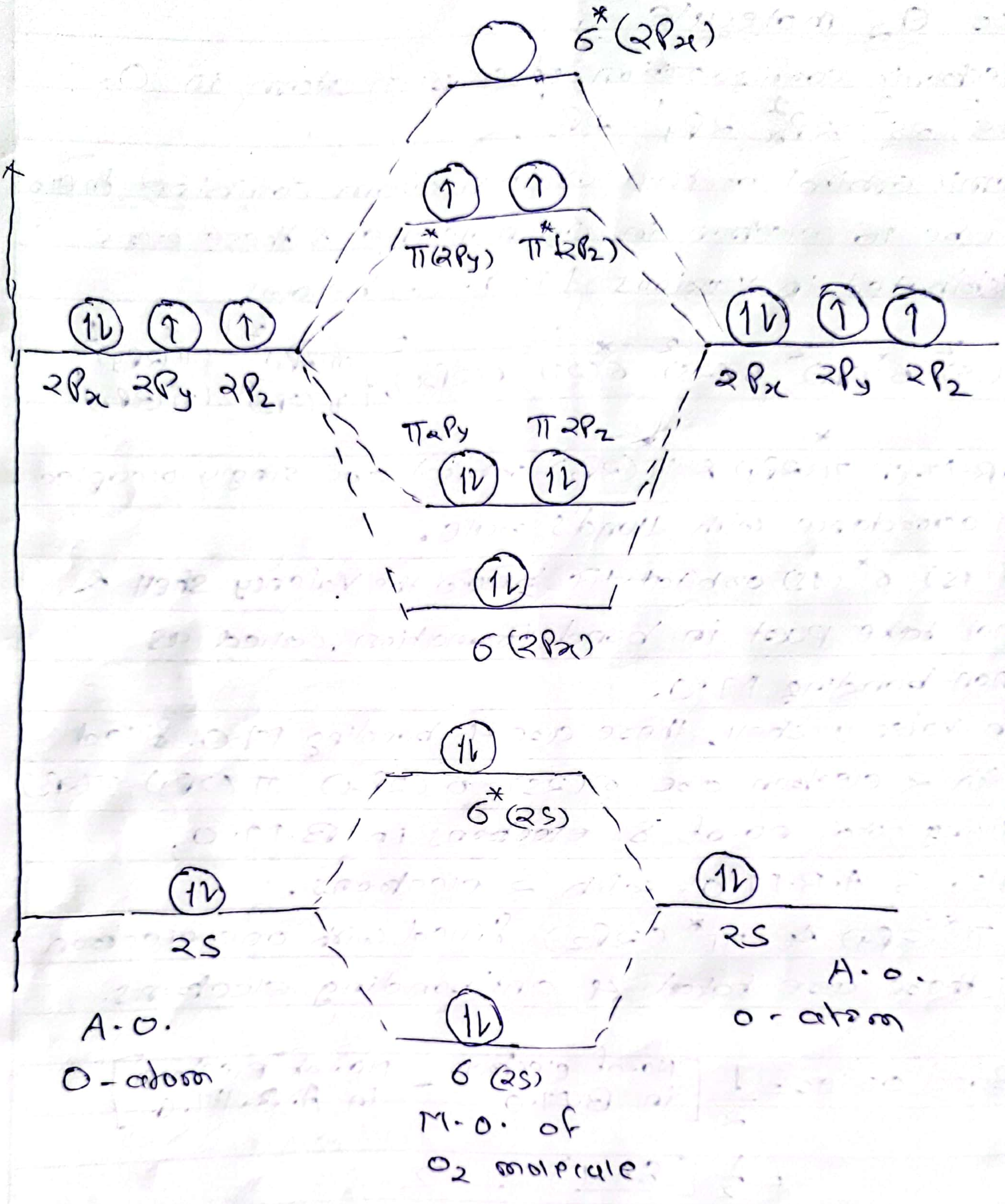


Fig:- M.O. energy level digoram of O_2 molecule.

Molecular Orbital Diagram of Ne_2 molecule :→

Valence shell electronic configuration of Ne atom is Ne_{10} – $2S^2, 2Px^2, 2Py^2, 2Pz^2$.
There are 8 electron in Ne_2 molecule have 16 electron in valence shell.
Distribution of electron in various M.O. is

$\sigma(2S)^2, \overset{*}{\sigma}(2S)^2, \sigma(2Px)^2, \left[\begin{matrix}\pi(2Py)^2 & \pi^*(2Py)^2 \\ \pi(2Pz)^2, & \pi^*(2Pz)^2\end{matrix}\right., \overset{*}{\sigma}(2Px)^2$

There are 4 B.M.O namely $\sigma(2S)$, $\sigma(2Px)$ $\pi(2Py)$, $\pi(2Pz)$ containg 2 electron in each ∴ total 8 electron.
Similarly A.B.M.O. namely $\overset{*}{\sigma}(2S)$, $\overset{*}{\pi}(2Py)$ $\overset{*}{\pi}(2Pz)$ $\overset{*}{\sigma}(2Px)$ containing 2 electron each ∴ total 8 electron.

$$\therefore \text{Bond order} = \frac{\left(\begin{matrix}\text{No. of electron} \\ \text{in B.M.O.}\end{matrix} - \begin{matrix}\text{No. of electron} \\ \text{in A.B.M.O.}\end{matrix}\right)}{2}$$

$$= \frac{8-8}{2} = 0$$

There will be no bond formation betn Ne atoms. This molecule do not exist.
Hypothetical energy level diagram for Ne_2 molecule will be given as follows.

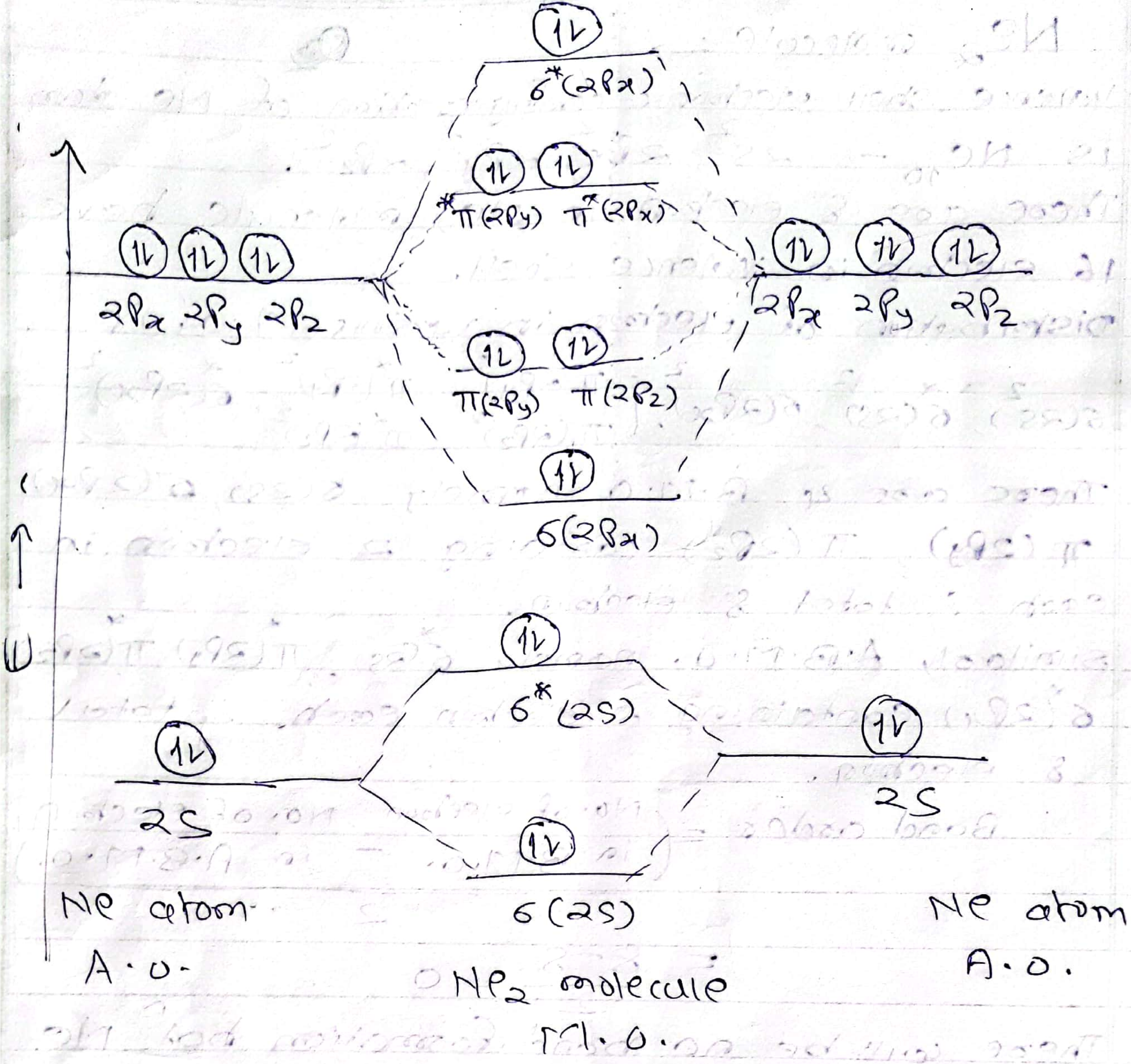


Fig :- Molecular orbital & energy level diagram of Ne₂ molecule.