

Date _____

CHAPTER 3

THEORIES OF COVALENT BONDS

VSEPR Stand for: - Valence Shell Electron pair
repulsion

PRONUNCIATION: - "Vesper"

NEED FOR THESE THEORIES

Lewis concept did not describe the structure or shape of any molecule so more theories were proposed to remove the defects or limitations.

IMPORTANCE OF VSEPR MODEL

Lewis structure only tells the number and types of bonds between atoms, as they are limited to "two" dimensions. The VSEPR model predicts the 3D-shape of molecules & ions and helps to convert Lewis 2D structure into 3D structure.

INTRODUCTION

This theory was suggested by "Sidgwick" and "Powell (1940)".

STATEMENT OF THEORY

According to VSEPR theory:-

"The shape or geometry of a molecule or ion depends upon the number of shared pairs as well the lone pairs of electrons around the central atom of the molecule or ion."

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ELECTRON PAIRS

↔ Bond pairs. (also called active set of Electrons)
↔ Lone pairs

BOND PAIR

The pair of electron which participate in chemical bond/bonding

LONE PAIR

The pair of electron which do not participate in chemical bond/bonding

BACKGROUND

"Gillespie" and "Nyholm" in 1957 proposed that the arrangement in a molecule determined by the repulsive interactions among all electron pairs in the valence shell of central atom. They named this theory valence shell electron pair theory (VSEPR).

STABILITY

less the repulsion, more the stability (less the energy)
More the repulsion, less the stability (more the energy)

BASIC ASSUMPTION OF VSEPR theory

The electron pairs around the central atom are arranged in space in such a way that they keep themselves as far apart as possible so that there is "minimum repulsion" between them

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MAIN CAUSE

The arrangement of electron pairs in this manner gives minimum energy and maximum **Stability** to the molecules or ions around an atom "A".

POSTULATES OF VSEPR THEORY

The postulates of VSEPR theory are :-

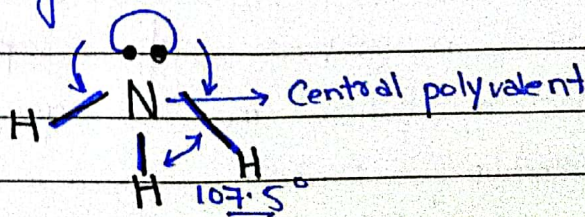
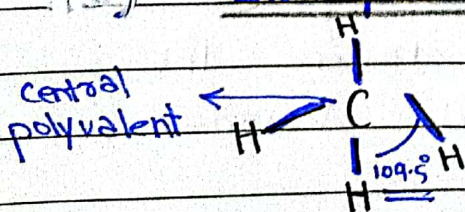
(i) CENTRAL POLYVALENT ATOM OR LEAST REPULSION

The electron pairs present around the central "polyvalent" atom are arranged in space as "far" as possible so that there is minimum repulsion between them.

→ Polyvalent atom :- An atom that can form multiple chemical bonds with other atoms, often due to having multiple valence electrons available for bonding (3 or more mostly)

→ Monovalent atom :- An atom that can form one chemical bond with another atom. Similarly "Divalent" & "trivalent" are those that can form 2 & 3 bonds respectively

→ Examples :- (for polyvalent)



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PKMZ PHUPPO EXAMPLE:- You are always far & distant from your phuppo (Electron pairs) to prevent laxai & fasad (AKA repulsion and energy) to maintain SAKOON & Peace (AKA Stability).

Cii) LONE PAIR OCCUPIES MORE SPACE

A non-bonding pair or lone pair of electron occupies more "Space" on the surface of an atom than a bonding pair.

CKMZ Example:- Just like a fat man occupies more space (lone pair) than a smart man (Bonding pair).

→ Lone pair has more influence, force of repulsion effect & also occupies more space.

Ciii) GEOMETRY OF MOLECULE

Both the lone pairs as well as Bond pairs determine the geometry of the molecule.

CKMZ:- The Shape, structure or geometrical orientation is dependent on both lone & bond pairs not me.

Civ) ORDER OF REPULSION

The magnitude of repulsion between the electron pairs in a given molecule decreases in following order.

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LONE PAIR- > LONE PAIR- > BOND PAIR-
LONE PAIR > BOND PAIR > BOND PAIR ^{which change geometry}

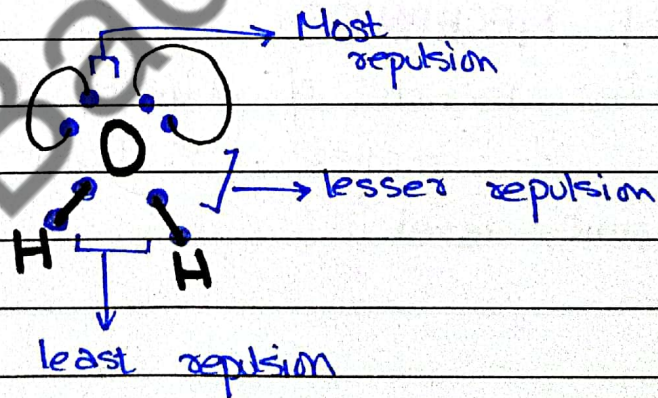
Lone pair causes deviation from ideal bond angles, \uparrow

CKMZ:-

- Maximum / greatest or largest repulsion = **Between 2 lone pairs**
- less than lone pairs but more than Bond pairs (Average) = **Between a lone & bond pair**
- least / smallest or weakest repulsion = **BTW 2 Bond pairs**

(2 fat men will cause most destruction than 1 fat & 1 weak man cause lesser destruction & 2 weak men will cause least destruction.)

Example:-



(v) ELECTRON PAIR DENSITY

The two electron pairs of a double & three electron pairs of a triple bond contain higher Electron charge density. Therefore, they occupy more space than one electron pair of a single bond. However, they behave like a

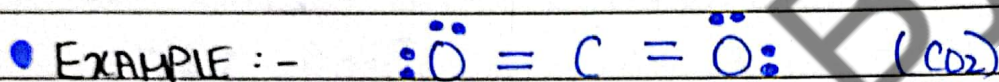
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'Single Electron pair' in determining the geometry of the molecules

VIP TERMS

LEWIS STRUCTURE

It is a simplified representation of the valence shell electrons in a molecule. It is also known as Lewis dot structure or electron dot structure. Lines represent shared pairs or bonds & dot represent electrons.



QUANTAM MECHANICS

It is the branch of physics that deals with the behaviour of matter & light on a 'Subatomic' and 'Atomic level'.

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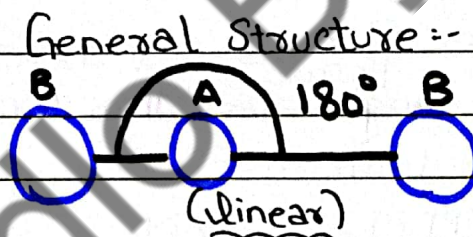
APPLICATIONS OF VSEPR

MAIN TERMINOLOGIES

- A → Central Atom
- B → Surrounded Atom
- E → Lone pair

a) TWO ELECTRON PAIRS AROUND CENTRAL ATOM

- Type :- AB_2 type
- Lone pairs :- None
- Bond pairs :- Two
- Geometry :- Linear
- Angle :- 180°
- Example :- $:\ddot{\text{Cl}}-\text{Be}-\ddot{\text{Cl}}:$ (BeCl_2)
- Explanation :-



The two B atoms have arranged themselves around A in such a way that they have minimum repulsion making 180° angle.

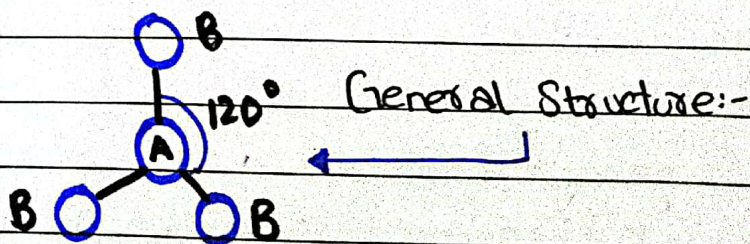
b) THREE ELECTRON PAIRS AROUND CENTRAL ATOM

(i) AB_3

(ii) AB_2E

→ AB_3 TYPE

- Type :- AB_3
- Lone pairs :- None
- Bond pairs :- Three
- Geometry :- Planar triangular geometry

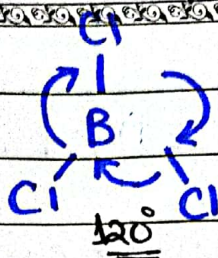


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(trigonal planar shape)

- Angle:- 120°
- Example:- BCl_3
- Explanation:-

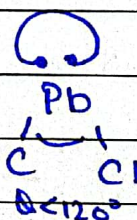
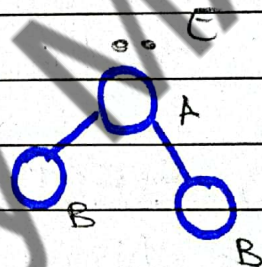
The 3 atoms "B" arrange around A to form a triangular planar structure with 120° .



Other e.g.:- AlH_3
 $AlCl_3, GaH_3$
 InH_3

→ (ii) AB_2E

- Type:- AB_2E type
- Lone pairs:- One
- Bond pairs:- Two
- Geometry:- Angular or V shape or Bent
- Angle:- less than 120°
- Example:- $PbCl_2$ & $SnCl_2$
- Explanation:-

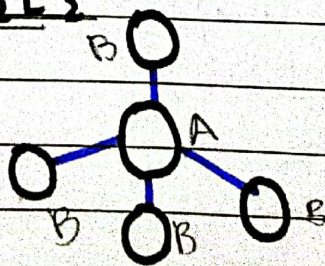


The lone pairs exert a large force of repulsion due to which the angle becomes less than ideal 120° & forms a V shape

(c) FOUR ELECTRON PAIRS AROUND CENTRAL ATOM

(i) AB_4 (ii) AB_3E (iii) AB_2E_2

- (i)
- Type:- AB_4
- Lone pairs:- None
- Bond pairs:- Four
- Geometry:- Regular tetrahedral structure
- Angle:- 109.5°

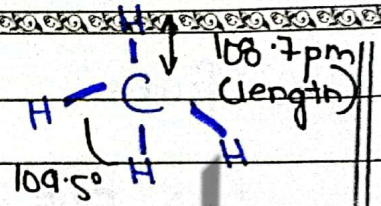


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• Example:- CH_4 (Methane), CCl_4 , SiF_4 , SnCl_4

• Explanation:-

The 4 atoms B surround around A with angle 109.5° forming a tetrahedron or tetrahedral structure



(ii) AB_3E Structure

• Type:- AB_3E

• Lone pairs:- One

• Bond pairs:- Three

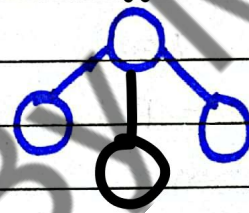
• Geometry:- pyramidal geometry

• Angle:- reduced to 109.5°

• Example:- NH_3

• Explanation:-

Due to strong repulsive force of lone pairs the angle is reduced to 107.5° as the bond pairs come close due to lone pairs.



Other eg:- PH_3 , AsH_3 , SbH_3

(iii) AB_2E_2

• Type:- AB_2E_2

• Lone pairs:- Two

• Bond pairs:- Two

• Geometry:- V-shaped

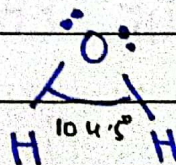
• Angle:- reduced to 104.5°

• Example:- H_2O

• Explanation:-

Due to repulsive force, V shaped structure is

Structure

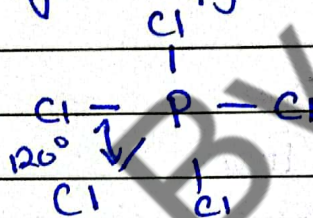


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formed & angle is reduced to 104.5° .

(d) FIVE ELECTRON PAIRS AROUND CENTRAL ATOM

- Type:- AB_5
- Lone pairs:- None
- Bond pairs:- Five
- Geometry:- Trigonal bipyramid
- Angle:- 120°
- Example:- PCl_5
- Explanation:-



(e) SIX ELECTRON PAIRS AROUND CENTRAL ATOM

- Type:- AB_6
- Lone pairs:- None
- Bond pairs:- Six
- Geometry Octahedral
- Angle:- 90°
- Example:- SF_6
- Explanation:-

PREDICTION OF SHAPE OF MOLECULES

- 1) Draw dot diagram
- 2) Identify central atom
- 3) Identify surrounding atoms
- 4) Determine valence electrons of central atom

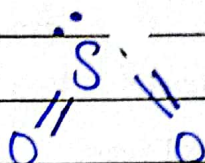
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- 5) Determine bond pairs & lone pairs
- 6) Determine geometrical distribution

HOME ASSIGNMENT EXAMPLES

→ SO₂

• Dot diagram =



- Valence Electrons of S atom = 6
- Electrons contributed by 2 O-atoms = 4 (double bond)
- Total number of electrons around S atom = 10

→ Electron pairs = 3

→ Bond pairs = 2

→ Lone pairs = 1

thus SO₂ is **AB₂E** type molecule. It will possess **V-shaped, Bent or Angular geometry**

→ SnCl₂

• Dot diagram =

Diagram showing the dot diagram for SnCl₂. The central Sn atom is bonded to two Cl atoms via single bonds. The Sn atom has one lone pair.

• Valence shell electrons of Sn atom = 4

• Electrons contributed by 2 Cl-atoms = 2

• Total no of electrons around Sn atom = 6

→ Electron pairs = 3

→ Bond pairs = 2

→ Lone pairs = 1

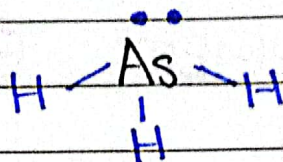
thus SnCl₂ is **AB₂E** type molecule. It will

Date _____

possess Bent, V shaped or Angular geometry

→ AsH₃

• Dot Diagram =



- Valence Electrons of As atom = 5
- Electrons contributed by 3 H-atoms = 3
- Total no of Electrons around As atom = 8

→ Electron pairs = 4

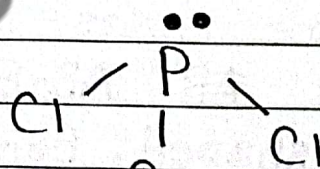
→ Bond pairs = 3

→ lone pairs = 1

thus AsH₃ is AB₃E type molecule. It will possess **pyramidal geometry**.

→ PCl₃

• Dot Diagram =



- Valence shell electrons of P atom = 5
- Electrons contributed by 3 Cl-atoms = 3
- Total no of Electrons around P atom = 8

→ Electron pairs = 4

→ Bond pairs = 3

→ lone pairs = 1

thus PCl₃ is AB₃E type molecule. It will possess **“pyramidal geometry”**

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THEORIES OF COVALENT BOND

CHAP:3

⇒ DEFECTS VSEPR THEORY

VSEPR theory fails to explain shapes of "isoelectronic" species and transition metal compounds. It also explain shapes of simple molecules but does not explain formation of "Chemical bond" that's why we need MOT & VBT.

VALENCE BOND THEORY

⇒ FOUNDERS

The theory was first proposed by W. Heitler and Fritz Londonⁿ (1927) and later developed by "Linus Pauling" and "J.C Slater" in 1931.

⇒ IMPORTANCE

This theory explains Bond formation (sharing of electrons), Bond strength, bond energies, bond lengths & Shapes/geometry of covalent bonds.

⇒ STATEMENT

According to VBT "A covalent bond between 2 atoms is formed where atoms come so close that a partially filled orbital of one atom "overlaps" with partially filled atomic orbital of the other.

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→ POSTULATES (ONLY MAIN HEADINGS)

- RETAINMENT OF OVERLAPPING ORBITALS
- OPPOSITE SPIN OR PAULI EXCLUSION PRINCIPLE BY ELECTRONS OF OVERLAPPING ORBITALS
- UNPAIRED VALENCE ELECTRONS EQUALS NO. OF BONDS
- TWO ORBITALS OVERLAP TO FORM ONE BOND
- SAME SYMMETRY WRT BOND AXIS
- GREATER THE OVERLAP, GREATER THE ENERGY RELEASED
- MULTIPLE BONDS (Double or triple) → By overlap of MORE ORBITALS
- GREATER OVERLAP → STRONGER BOND

TYPES OF OVERLAPPING

On the basis of overlapping of orbitals, covalent bonds can be divided in two i.e. sigma and pi bond.

SIGMA BOND

DEFINITION

Any **first** bond formed between two partially filled atomic orbitals by head on overlap or "head to head" linear overlap is called sigma bond.

ORIGIN

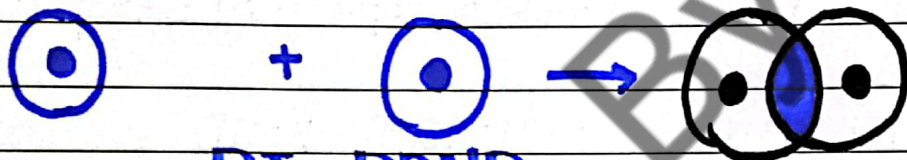
Sigma is the English word for the "greek" letter, which corresponds to English letter σ .

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PROPERTIES

- Electron density is maximum around the bond axis
- The probability of finding an electron is maximum in the region between 2 "nuclei."
- All single covalents are sigma bonds
- Symbol for sigma is (σ)

DIAGRAM



PI BOND

DEFINITION

A bond formed between two already (σ) bonded atoms by the sidewise or parallel overlap of their 2 half filled p-atomic orbitals is called a Pi (π) bond.

ORIGIN

This bond is named after greek letter " π "

PROPERTIES

- Overlapping orbitals should be coplanar or have same axis
- The electron density is unsymmetrical in around Bond axis & is maximum above and below of Bond axis

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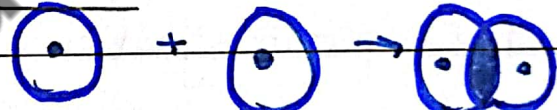
- The side wise overlap is not too efficient and good which results in a weaker bond than sigma bond
- They are often found in molecules with double or triple bond
- Overlapping of hybrid-orbitals always produces a sigma bond
- There can be only "1" sigma bond, rest will be pi bonds.
- "s" orbitals can't form a pi bond coz they lack orientation for sideways overlap

APPLICATIONS OF VBT

SINGLE BOND FORMATION

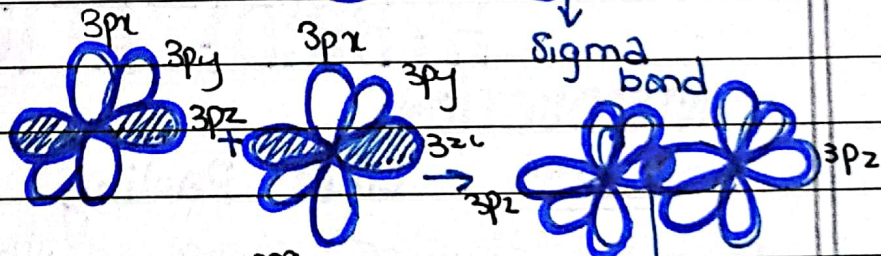
a) H₂ Molecule

(s-s)



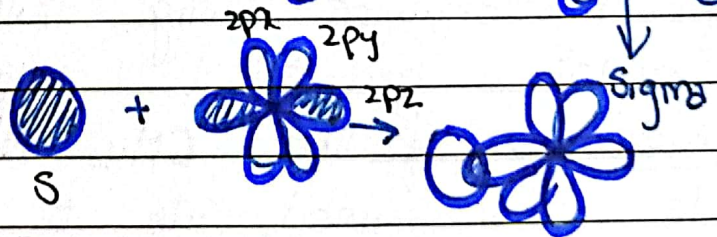
b) Cl₂ Molecule

(3p_z-3p_z)



c) HF Molecule

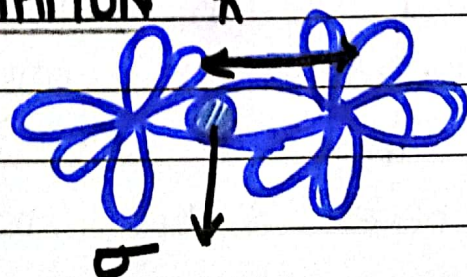
(s-2p_z)



MULTIPLE BOND FORMATION

a) O₂ Molecule

Double bond
1 sigma, 1 pi

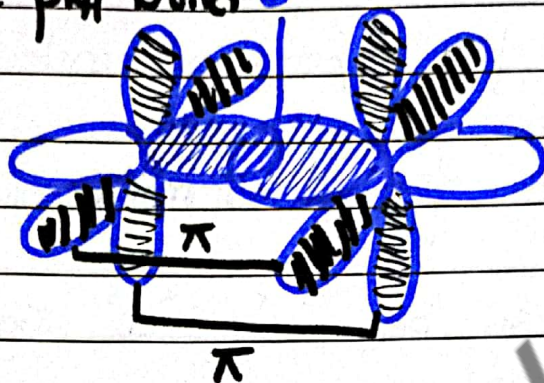


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b) N₂ Molecule

Triple Bond

1 Sigma, 2 pi bond



LIMITATIONS OF VBT

It does not explain

- Bivalency of Be, trivalency of B & tetravalency of C
- The angle between the bonds
- The paramagnetism of O₂ molecule

HYBRIDIZATION

INTRODUCTION

In 1931 Linus Pauling introduced the concept of Hybridization along with Slater to explain geometrical shapes of polyatomic molecules like CH₄, NH₃, AlCl₃ & H₂O etc. He also used it to explain bivalency of Be, trivalency of B & tetravalency of C since at ground state if only unpaired electrons formed bonds then Be will have 2, B will have 3 & C will have 4 but that's not the case while bonding.

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DEFINITION

Atomic orbitals of different energies & shapes combine to form a new set of equivalent orbitals called hybrid orbitals & the phenomenon is known as hybridization."

PROPERTIES / TRAITS

- Hybrid orbitals = No of atomic orbitals combined
- Hybridized orbitals \rightarrow equal in energy & shape
- Hybrid orbital is not a pure atomic orbital
- Shape of hybrid orbital is different from original orbital
- Hybridization takes place before bonding & it is not applied to isolated atoms
- Hybrid orbitals form stable bonds than pure orbitals

TYPES

There are 3 main types of hybridization depending on nature and number of orbitals

sp^3 , sp^2 , sp Hybridization.

sp^3 Hybridization

The process of mixing ~~one~~ ^{one} s & ~~two~~ ^{three} p orbitals to give 4 identical sp^3 orbitals is called sp^3 hybridization.

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Each sp^3 has 25% s character and 75% p character

EXAMPLES

METHANE, WATER, AMMONIA

EXCITED STATE

During hybridization, Atom is excited to increase the unpaired electrons. In the ground state, they cannot be hybridized.

sp^2 Hybridization

- The process of mixing 1 s & 2 p to give 3 identical sp^2 hybrid orbitals is called sp^2 hybridization
- Each sp^2 orbital has 33% s-character and 67% p-character

EXAMPLES

BORON TRI-FLUORIDE, ETHENE

SP HYBRIDIZATION

The process of mixing 1 's' & 1 'p' orbital to give 2 identical sp orbitals is called sp hybridization.

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Each sp has 50% s character & 50% p character

EXAMPLES

BERYLLIUM CHLORIDE, ACETYLENE

DRAWBACKS OF VBT

It fails to explain :-

- The formation of coordinate covalent bond
- The formation of odd electron molecules or ions
- The paramagnetic behaviour of oxygen molecule and diamagnetism of N_2 molecule
- Don't explain Electronic spectra of molecules

MOLECULAR ORBITAL THEORY

INTRODUCTION

In 1932 a German physicist ~~Paul~~ Friedrich Hund and American chemist Robert Sanderson Mullikan gave the concept of MOT

DEF OF MOLECULAR ORBITAL

A wave function whose square gives the probability of finding an electron within a given region of space in a molecule is known as molecular orbital.

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TWO MOLECULAR ORBITALS

2 atomic orbitals after combining linearly form 2 molecular orbitals BMO & ABMO

BONDING MOLECULAR ORBITAL (BMO)

BMO has lower energy

It is symmetrical about the axis joining the nuclei of the bonded atoms (molecular axis)

It is designated as σ (sigma BMO)

ANTI-BONDING MOLECULAR ORBITAL (ABMO)

ABMO has high energy

It is designated as (σ^*) the asterisk read as star, tells us about ABMO

MAIN POSTULATES

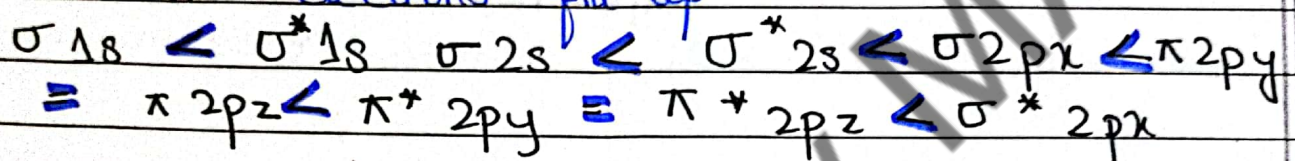
- Number of molecular orbitals = Number of atomic orbitals combining
- Overlapped atomic orbitals do not maintain their identity
- BMO has greater stability than ABMO because it has low energy
- $\text{energy} \propto \frac{1}{\text{Stability}}$
- The filling of electrons take place acc to
- Auf Bau, Pauli exclusion & Hund's rule
- BMO will have electrons but ABMO will remain empty or have electrons.

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Larger the overlap, stronger the bond,
lower the energy of BMO & higher the
energy of ABMO

SEQUENCE OF ENERGY LEVELS

in which electrons fill up:-



TYPES OF OVERLAPPING IN MOT

Head on Approach (linear overlapping) or
Linear combination.

Sideways approach (parallel overlapping)

Linear overlapping

It can take place btw s-s, s-p, & p-p
orbitals

This is basically sigma bond and results
in BMO & ABMO.

Parallel overlapping

this is basically pi (π) bond
p_x mostly forms sigma bond and p_y & p_z
form pi bond

Electron density is max at low & higher
points

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BOND ORDER

DEFINITION

The number of bonds between 2 atoms after atomic orbitals overlap is called Bond order. It is taken as difference between number of Bonding & anti-bonding electrons & dividing by 2.

FORMULA

$$\text{Bond order} = \frac{\text{No of electrons in BMO} - \text{No of electrons in ABMO}}{2}$$

EXAMPLES

For hydrogen, Electrons in BMO = 2
Electrons in ABMO = 0

$$\text{So no of Bond is } \frac{2-0}{2} = 1$$

in Hydrogen molecule

MAIN POINTS

- ▶ Only valence orbitals are considered in bond order calculations commonly. BMO electrons should be greater than ABMO electrons or Auf Bau principle is validated.
- ▶ If Bond order = 0, it doesn't exist in molecular form.
- ▶ He has zero bond order so doesn't exist in molecular form but in Atomic form.

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RELATIVE ENERGIES

Heavier Molecules

- They include O_2, F_2 , or any molecule whose sum of atomic orbitals give more than 14
- Order:- $\sigma(1s) < \sigma^*(1s) < \sigma(2s) < \sigma^*(2s) < \sigma(2p_x) < \pi(2p_y) = \pi(2p_z) < \pi^*(2p_y) = \pi^*(2p_z) < \sigma^*(2p_x)$
- Lower energy of $\sigma(2p_x)$:- The lower the energy, the more the stability and this because of High Energy difference between 2s & 2p

Lighter Molecules

- They include H_2, He_2, B_2, C_2 & N_2 or whose sum is less than 14
- Order:- $\sigma(1s) < \sigma^*(1s) < \sigma(2s) < \sigma^*(2s) < \pi(2p_y) = \pi(2p_z) < \sigma(2p_x) < \pi^*(2p_y) = \pi^*(2p_z) < \sigma^*(2p_x)$
- High energy of $\sigma(2p_x)$:-
 - This is because of mixing of 2s & 2p due to less energy difference thus σ_{2p_x} & $\sigma^*_{2p_x}$ don't retain pure p-character. All 4 MOs acquire sp character. σ_{2p_x} & $\sigma^*_{2p_x}$ become unstable and their energy increases.

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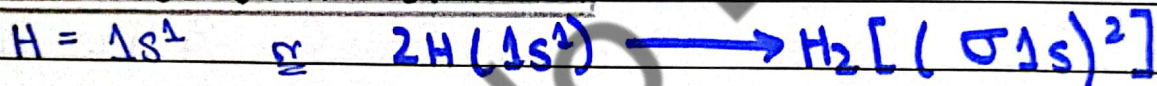
APPLICATIONS

MAIN HEADINGS:-

- 1) ELECTRONIC CONFIGURATION
- 2) EXPLANATION
- 3) BOND ORDER
- 4) BOND DISSOCIATION ENERGY (Optional)
- 5) MAGNETIC CHARACTER
- 6) DIAGRAM

HYDROGEN MOLECULE

ELECTRONIC CONFIGURATION



EXPLANATION

Hydrogen molecule is formed from overlap of 1s atomic orbitals of 2 hydrogen atoms.

They give rise to 2 molecular orbitals $\sigma 1s$ & $\sigma^* 1s$

The molecule has 2 electrons which occupy $\sigma 1s$.
It has one bond and is stable.

BOND ORDER

$$\text{Bond order} = \frac{2-0}{2} = 1 \rightarrow [\text{Shows 1 bond}]$$

BOND DISSOCIATION ENERGY

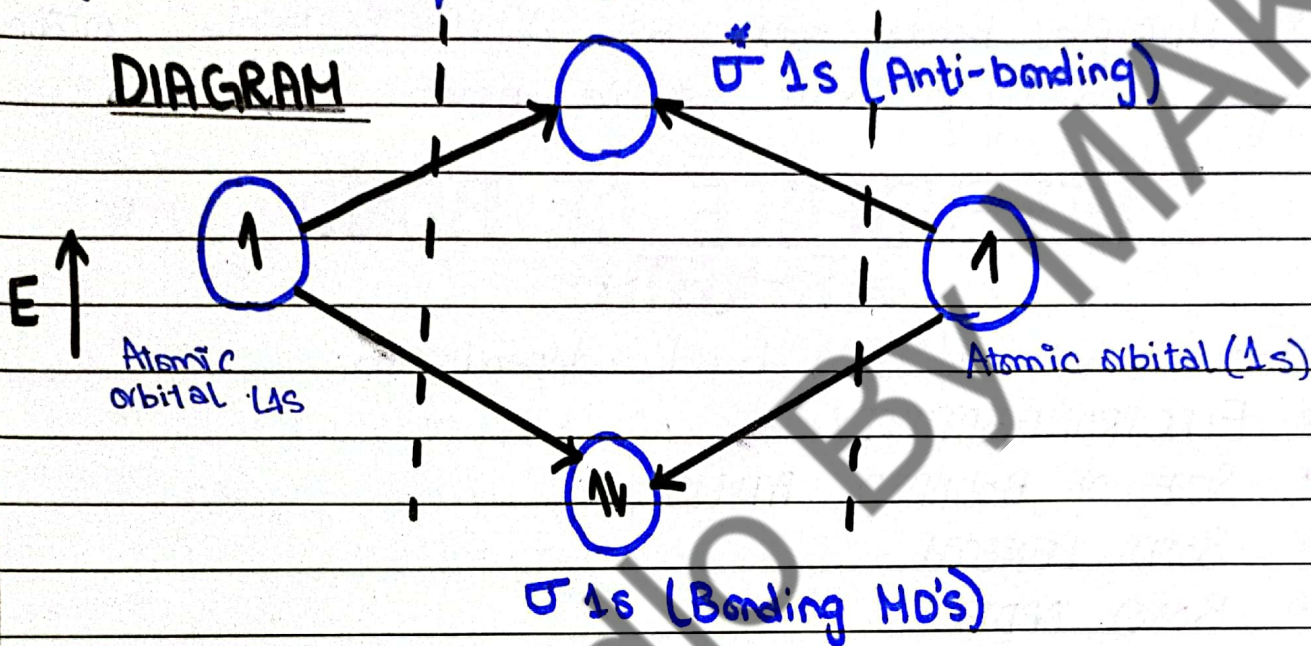
It has bond dissociation energy of 436 kJ mol^{-1}

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MAGNETIC CHARACTER

It is Diamagnetic in nature and repelled by both poles of magnet

DIAGRAM



BOND ENTHALPY

Endothermic process:- When energy is absorbed during breaking of a bond

Exothermic process:- When energy is released during formation of a bond

Definition:- Amount of energy required to break all bonds of particular type in one mole of substance

Enthalpy of Atomization:- The enthalpy change in splitting molecule into its component atoms. It

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- **Units:-** It is expressed in kilojoules per mole (kJ mol^{-1})
- **VIP Points:-**
 - More the energy, stronger the bond
 - Multiple bonds such as double & triple contain larger energy than single bond

DEPENDENCE OF BOND STRENGTH

→ The strength of a bond depends on

- ELECTRONEGATIVITY
- SIZE OF BOUNDED ATOMS
- BOND LENGTH
- BOND ORDER

ELECTRONEGATIVITY

- Electronegativity difference \propto Bond strength
 - Due to greater electronegative distance, partial \oplus & partial \ominus charge is formed, which increases the ionic character, bond energy & bond strength & decreases bond length or size of atoms.

• E.g HF \rightarrow It has energy of 567 kJ mol^{-1}

SIZE

The more the attraction is, the more close they are & size becomes smaller with increasing strength.

Date _____

Size of Bonded atoms $\propto \frac{1}{\text{Bond strength}}$

BOND LENGTH

“Distance between nuclei of atoms joined by covalent bond”

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

- It is never constant (coz molecules are vibrating)
- It is measured in picometer or Angstrom (Å)
- Half of Bond length is in similar bonded atoms gives radius of that atom called covalent radius

BOND ORDER

• The more the bonds, the more the energy & strength

• Bond order \propto Bond strength

DIPOLE MOMENT

- Degree of polarity
- Product of magnitude of charge & distance between them

• Relation = $\mu = q \times r$

↳ Dipole moment = charge \times distance

• Its unit is Coulomb's meter (Cm) or Debye (D)

Date _____

EFFECT OF BONDING

IONIC COMPOUNDS

COVALENT COMPOUNDS

SOLUBILITY

- Hydration energy should be equal or greater than lattice energy so that \oplus & \ominus ions can detach & dissolve in water.

- Polar molecules dissolve easily in polar solvents like water.
- Non-polar molecules only dissolve in polar molecules under certain conditions but mostly dissolve in non-polar solvents.

DIRECTION

- Non-directional & Rigid

- Non-rigid & directional

REACTION KINETICS

- They dissolve or have higher speed of reaction coz no bond is to be broken

- They take longer time to react coz they involve both breaking & making of bonds

DENSITY

- More density, due to strong forces of attractions btw cations & anions.

- Low density as compared to ionic compounds

CHAPTER 3

HYBRIDISATION

STRUCTURES

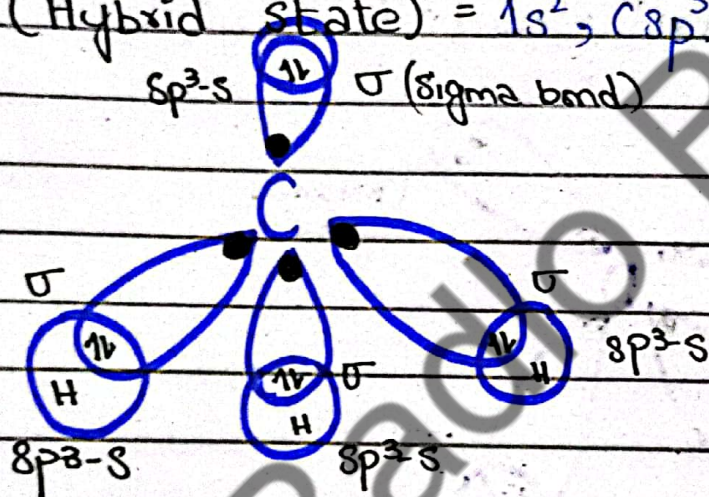
SP³ HYBRIDISATION

(a) Structure of Methane (CH₄)

6C [Ground state] = $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^0$

6C* [Excited state] = $1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^1$

6C (Hybrid state) = $1s^2, (sp^3)^1, (sp^3)^1, (sp^3)^1, (sp^3)^1$



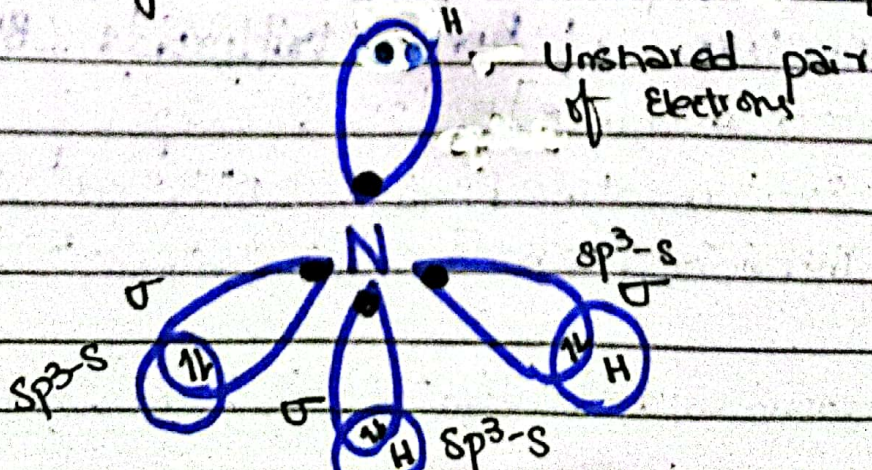
Tetrahedral structure

25% s & 75% p character

(b) Structure of Ammonia (NH₃)

7N [Ground state] = $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1$

7N [Hybridised state] = $1s^2, (sp^3)^2, (sp^3)^1, (sp^3)^1, (sp^3)^1$



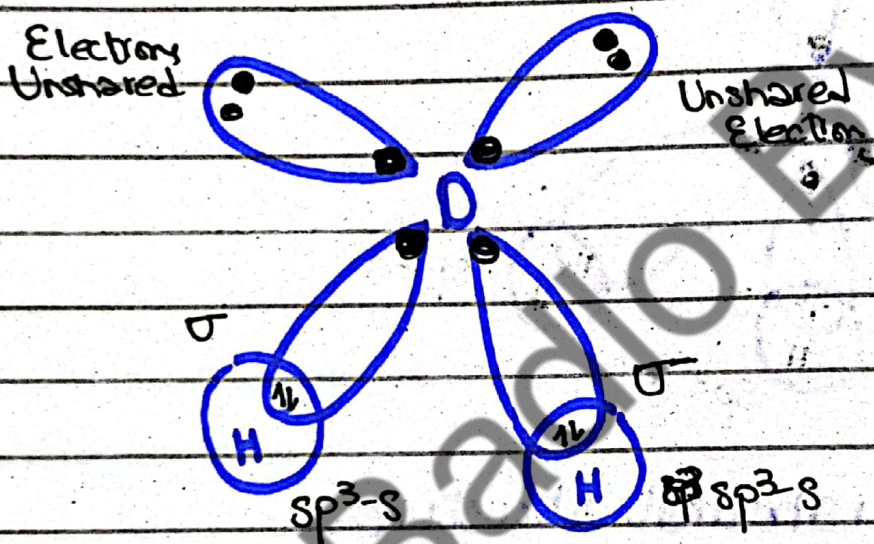
Pyramidal structure
 sp^3 hybridisation
 25% s & 75% p character

(c) Structure of Water (H_2O)

8 O [Ground state] = $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1$

8 O [Excited state] = $1s^2, 2s^2, 2p_x^2, 2p_y^1, 2p_z^1$

8 O [Hybridised state] = $1s^2, (sp^3)^2, (sp^3)^2, (sp^3)^1, (sp^3)^1$



Bent, V or angular structure
 sp^2 hybridisation

sp^2 HYBRIDISATION

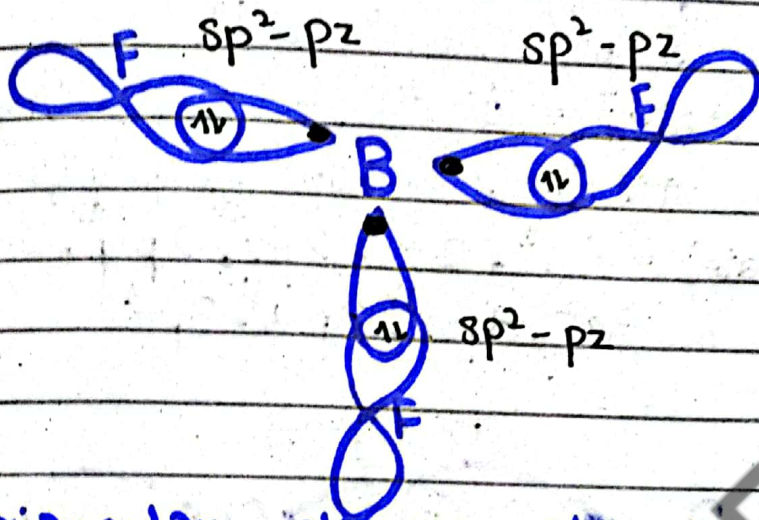
(a) Structure of Boron trifluoride (BF_3)

s B [Ground state] = $1s^2, 2s^2, 2p_x^1, 2p_y^0, 2p_z^0$

s B [Excited state] = $1s^2, 2s^1, 2p_x^1, 2p_y^1, 2p_z^0$

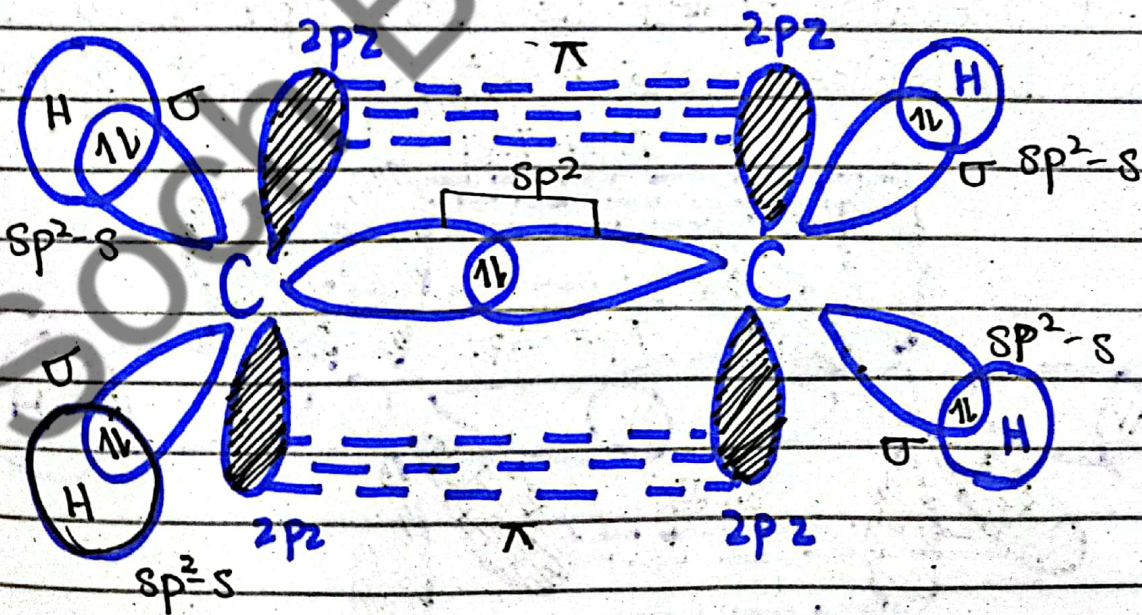
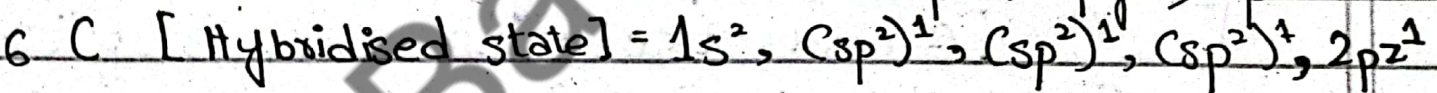
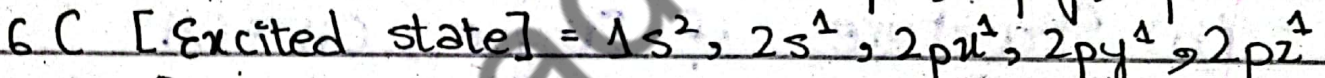
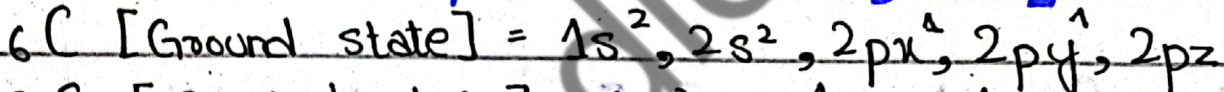
s B [Hybridised state] = $1s^2, 2s^1, (sp^2)^1, (sp^2)^1, (sp^2)^0$

F [Ground state] = $1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^1$



Triangular planar structure

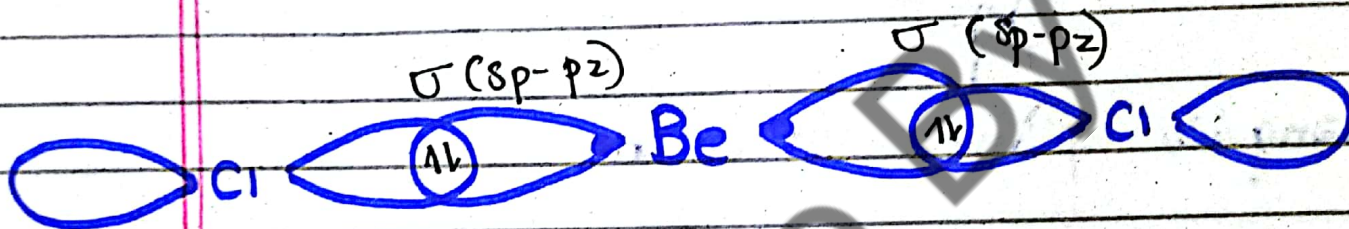
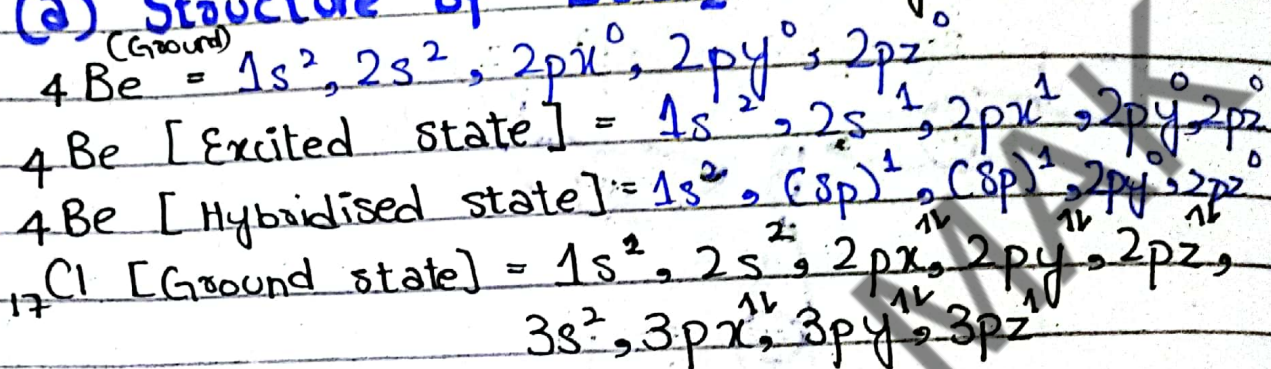
(b) Structure of Ethene, $CH_2 = CH_2$



Linear structure

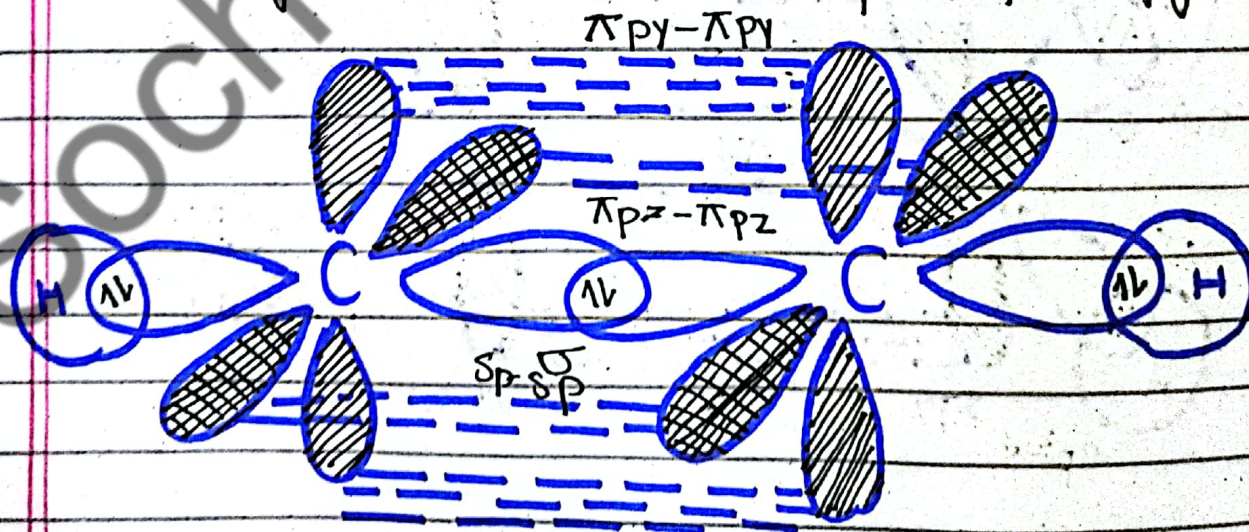
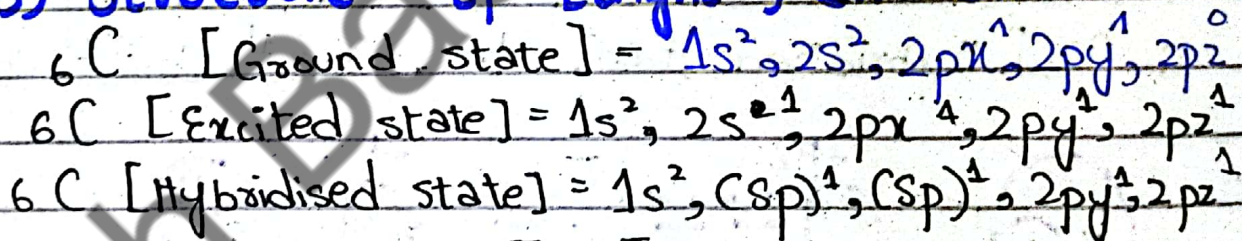
SP HYBRIDIZATION

(a) Structure of BeCl_2 [Beryllium Chloride]



Linear structure

(b) Structure of Ethyne, $\text{CH}\equiv\text{CH}$

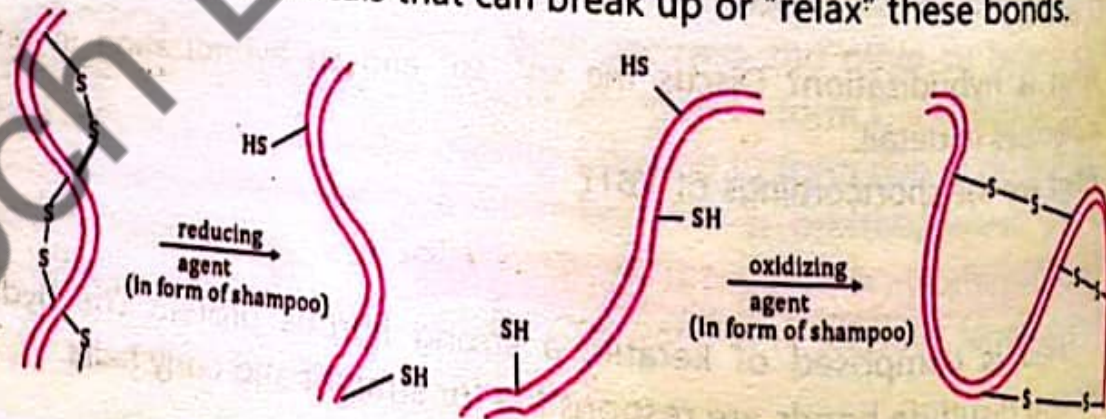
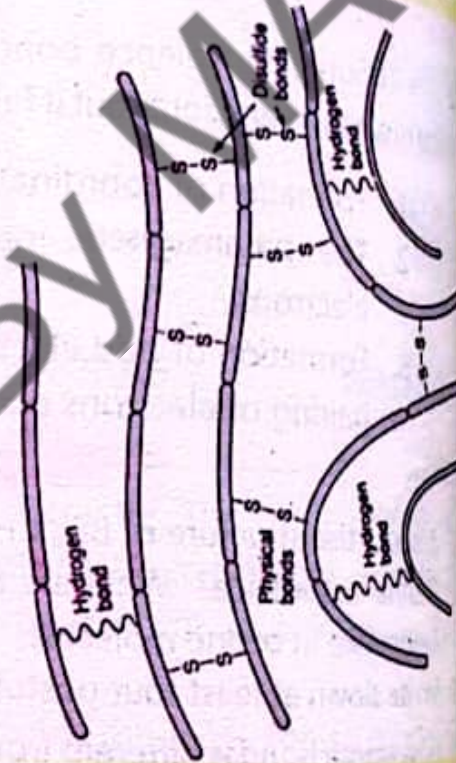


Linear Structure

The hair will remain in the new "shape" until it is wetted with water again and that can occur either through shampooing/conditioning or through humidity.

Disulphide bonds

Disulphide bonds are also known as Cysteine bond, Sulphur bond or S-bond. There is a formation of a covalent bond called a disulphide bridge between the sulphur atoms on two cysteines on separate chains of keratin. These bonds are stronger than hydrogen bond. The more disulphide that occurs in the fiber, the curlier and kinkier the hair. These bonds cannot be broken by water or heat treatment. Only chemical agents can break these bonds. Therefore, if a person with curly hair wants straight hair, he/she would need to use chemicals that can break up or "relax" these bonds.



bonds, the curlier the hair. The fewer the number of disulphide bonds, the straighter the hair. It depends upon the number of disulphide bonds between cysteine molecules of keratin whether your hair is curly, wavy or straight. A disulphide bonds imbalance causes the hair to appear straight in certain areas and curly in other areas. People with straight hair can change their hair to force it into curly state by using chemicals. They are chemically forcing the making of strong disulphide bonds. The waves do not stay for all time, because the new hair grows in, which is straight, and only the ends curly.

Soch

Table 3.2: Difference between Sigma and Pi Bonds

Sigma Bond	Pi Bond
A covalent bond formed by linear overlap of two half-filled atomic or hybrid orbitals is called sigma bond.	A covalent bond formed by parallel overlap of two half-filled atomic orbitals is called pi bond.
It has electron density around the bond axis.	It has electron density above and below the bond axis.
All single covalent bonds are sigma bonds.	In a multiple bond, one is essentially a sigma bond which is formed earlier than pi bond.
It is stronger due to greater overlap of orbitals.	It is weaker due to lesser overlap of orbitals.
It is less reactive than pi bond.	It is more reactive than sigma bond.
Its formation does not depend on pi bond.	It is formed after the formation of sigma bond.
The shape of a molecule is determined only by the orbitals forming sigma bonds	The shape of a molecule is not determined by the orbitals forming pi bonds.
We can easily rotate the atoms around the bond axis of sigma bond.	Rotation about the double bond is not possible. The rotation is restricted because pi bond has two regions of electron density.
Example: In the molecule of NH_3 , all bonds between nitrogen and hydrogen are sigma bonds.	Example: N_2 molecule has one sigma and two pi bonds.

m) The shapes of molecules having delocalized π -electrons.

3.2 Resonance

The process in which two or more structures are written for a compound which differs only in the arrangement of electrons is called resonance. The different structures obtained are called resonance structures. Resonance structures are not actual structures. They are hypothetical and exist only on paper. They are, therefore, cannot be prepared or isolated in the laboratory. The real or actual structure is a hybrid of all the resonance structures. The resonance is represented by a double-headed arrow (\longleftrightarrow). There are some molecules and polyatomic ions for which no single Lewis structure can be written. Let us take the example of oxygen. It exists in two allotropic forms; the dioxygen, O_2 (oxygen molecule) and the trioxygen (ozone). Ozone is present in larger amounts in the upper atmosphere where it shields life on earth from harmful UV radiation from the sun. It is also present in trace amounts in the lower atmosphere where it may damage plants and animal tissues. There are two possible Lewis structures "A" and "B" for Ozone which are

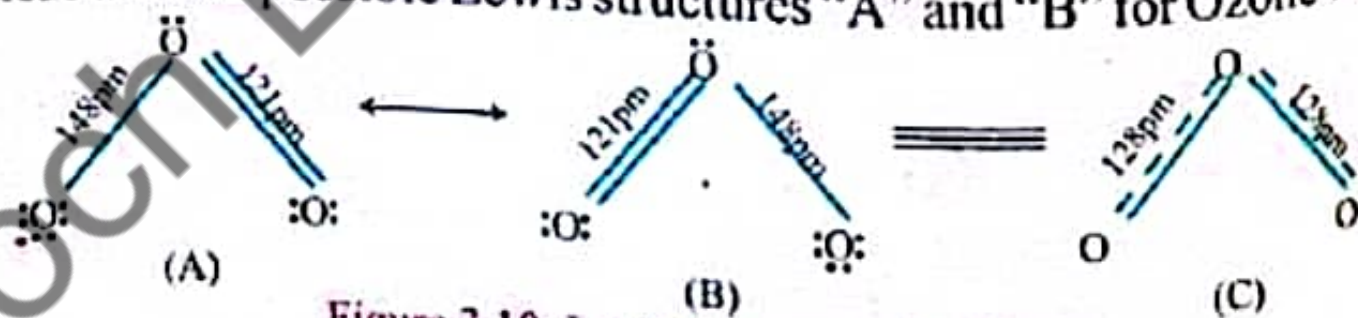


Figure 3.10: Lewis structures for Ozone

14) The number of electrons in the molecular orbitals is equal to the sum of electrons on the bonding atoms.

The molecules are said to be diamagnetic if they have paired electrons in the molecular orbitals (bonding and antibonding molecular orbitals) and they are said to be paramagnetic if they have unpaired electrons in the molecular orbitals. Paramagnetic substances are attracted by a magnetic field whereas diamagnetic substances are slightly repelled by a magnetic field. Paramagnetic character is directly proportional to number of unpaired electrons in the molecular orbitals and increases as number of unpaired electrons increases.

Relative Energies of Molecular Orbitals

Keep in Mind

You can think of two groups (say one group belongs to first year and the other belongs to second year) of students in a tug-of-war. The first year students are at one end of the rope and the second year students are at the other end. Each group pulls the rope towards itself. There is no movement, because each group pulls on the rope with the same force but in the opposite direction. Hence, the net force is zero.

Figure 3.27: Linear overlap of $2p_x$ - $2p_x$ orbitals

Keep in Mind

If atomic orbitals do not have the same symmetry then they will not combine. For example, $2p_x$ orbital of one atom can combine with $2p_x$ orbital of the other atom but not with the $2p_y$ or $2p_z$ orbital due to their different symmetries.

The other two sets of $2p$ orbitals ($2p_y$ and $2p_z$) are perpendicular to the x -axis, and they will overlap sidewise to give two bonding and two anti-bonding π -

weighted average of these Lewis structures.

The phenomenon in which two or more structures can be written for a compound, which involves identical positions of atoms, is called resonance. In other words, you can simply say that, a molecule or ion that has multiple correct Lewis structures shows resonance. Each of these Lewis structures is called a resonating structure. The actual structure of the molecule is said to be a resonance hybrid of all possible structures.

This led to the idea that such molecules exist in the state, which is combination of two or more electronic structures.

Tidbit

Resonance Hybrid

The weighted average of resonance contributors, which best represents, the reality. Demonstrating the molecule the way it is observed in lab.

Science, Technology and Society

Hair is composed of keratin, a strong fibrous protein. The hydrogen bonds and disulfide bonds are responsible for straight and curly hairs.

Hydrogen bonds

These bonds are the most flexible. Hydrogen bonds are easily broken in the presence of water and heat. They are the primary bonds responsible for changing our hair's overall shape. Hydrogen bonding allows our hair to change shape temporarily and produces a strong hold. When the hair is wet by either shampooing/conditioning or in the presence of humidity, the molecules enter the fibers, break up the hair's preset hydrogen bonds, and form new bonds. For example, hair is usually set in rollers while wet. The hair is then held in position until it dries. As the hair dries, hydrogen re-bonding occurs, but in the new "shape".

Tidbit

Many boron compounds are electron-deficient, meaning that they lack an octet of electrons (mostly have six electrons) around the central boron atom. This deficiency of electron is responsible for acidic nature of boron compounds.

b. Two Bond Pairs and One Lone Pair