Lec- 1

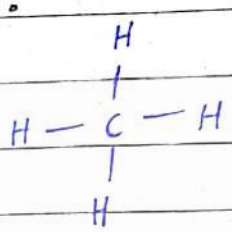
Date: _____ Chapter # 2

Chemical Bonding

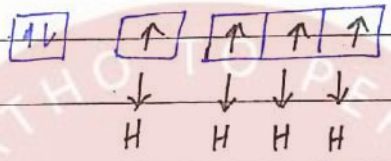
⊛ Hybridization:

pauling
slauter

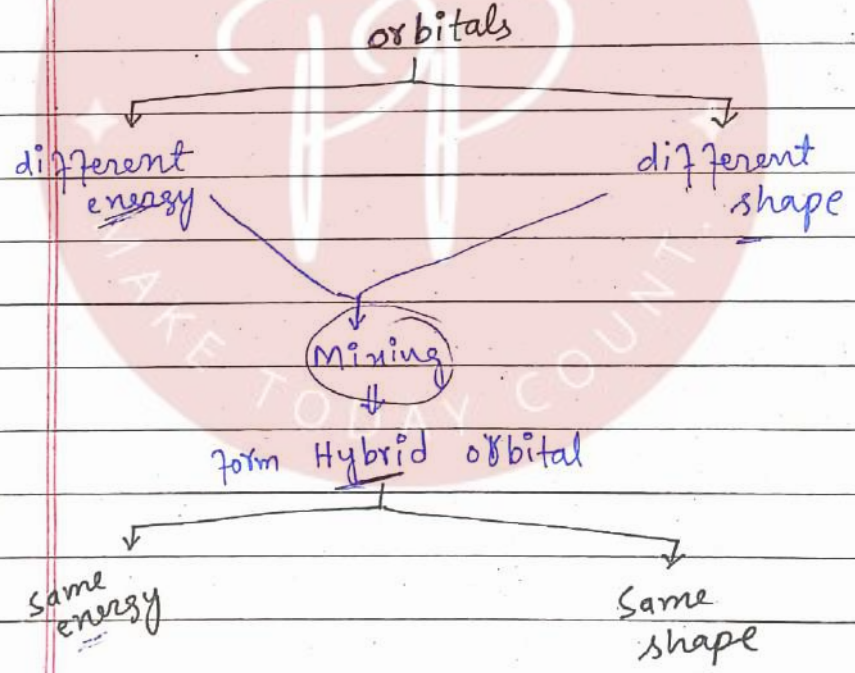
CH_4



C = $1s^2, 2s^2, 2p^2$



→ Same energy.



Date: M T W T F S

Mechanism:

* Mixing of orbital
* Excitation (may or may not)

simultaneous process

Facts:

* hypothetical or imaginary process.
* during the bond formation
* Monocentric atom
  - Related to one atom.
* Exothermic process.
* It imparts stability.
* occur in
  - => fully filled orbital
  - => half filled " "
  - => empty filled " "
  - (Transition elements)

degenerate orbitals.

* Hybrid orbitals:
  - in which hybridization occurs
  - Same energy & shape
  - (orientation is different)

* Monocentric → H_2O O = sp^3
* Max es = 2
* Min es = Zero

* H·O always form sigma bond.

Date: M T W T F S

No. hybrid orbitals = No # atomic orbitals combine

M·O → polycentric

in sp → 2 H·O

in sp^2 → 3 H·O

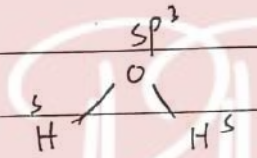
in dsp^2 → 4 H·orbital

⊛ unhybrid orbitals:

=> No hybridization.

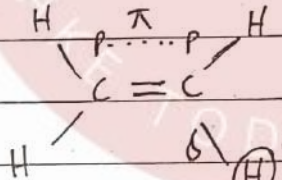
* also called atomic orbital.

* Mono centric → Relate to one atom.



* Max es⁻ = 02 * form σ & π-bond.

Min es⁻ = zero

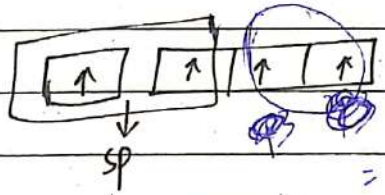


σ S orbital (H) ↳ No hybri

form pi bond.

No. unhybrid orbital = Total orbitals − hybrid orbital

e.g



Hybrid = 2

= 4 − 2

= (2)

sp^3d → (9) (5)

Date: M T W T F S

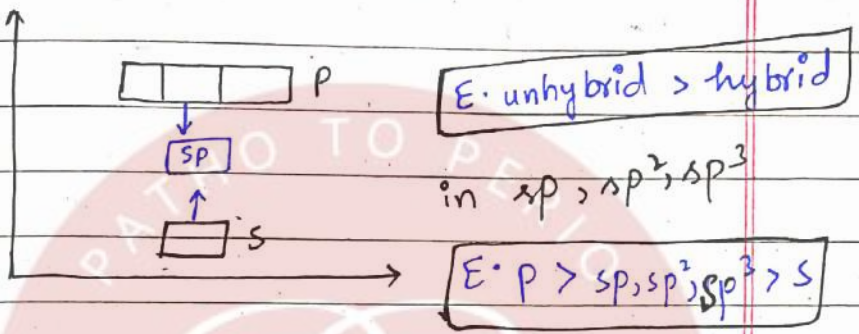
sp^3d hybrid = 5 ✓

unhy = 9 − 5 = (4)

sp^3d^3

9 − 7 = 2

Relative energy



E · unhybrid > hybrid

in $sp > sp^2 > sp^3$

$E \cdot p > sp > sp^2 > sp^3 > s$

Types

H·B — No# H·B (Steric No)

* sp — 02
* sp^2 — 03
* sp^3 — 04
* sp^3d — 05
* sp^3d^2 — 06
* sp^3d^3 — 07

Energy

$s < p < d < f$

R · energy

more d characters ↑

$sp < sp^2 < sp^3 < sp^3d < sp^3d^2 < sp^3d^3$

Date: M T W T F S

s- character:

b/c near to nucleus ← S - character ∝ E-N

s-contribution ↑ ← less

50% ← sp > sp^2 > sp^3 > sp^3d > sp^3d^2 > sp^3d^3 (50% 33 67 25% 75%)

R. Energy = 4s, 4p, 4d ← nd ← sp^2d > d^2sp^2 ← (n-1)d (lower shell) ← 3d, 4s, 4p

sp^3d^2 > d^2sp^3 ← no. shell ✓

↳ n ∝ E

sp^2d > d^2sp^2

sp^3d > d^2sp^3

Identification

① Neutral Molecule

$$H.B = \frac{V+M}{2}$$

e.g

* H_2O → $\frac{6+2}{2} = \frac{8}{2} = (4 = sp^3)$

* CCl_2 → $\frac{4+2}{2} = \frac{6}{2} = (3 = sp^2)$

* PCl_5 → $\frac{5+5}{2} = \frac{10}{2} = (sp^3d = 5)$

* H_2SO_4 → $\frac{6+2}{2} = \frac{8}{2} = 4 = sp^3$

Date: M T W T F S

H_3PO_4 $\quad \frac{5+3}{2} = \frac{8}{2} = sp^3$

SO_3 $\quad \frac{6+0}{2} = 3 = sp^2$

IF_7 $\quad \frac{7+7}{2} = \frac{14}{2} = 7 = sp^3d^3$

H_3PO_3 $\quad \frac{5+3}{2} = \frac{8}{2} = 4 = sp^3$

For Molecular Ion:

$$H.B = \frac{V+M-C+A}{2}$$

* OH^- $\quad \frac{6+1+1}{2} = \frac{8}{2}$ $\quad 4 = sp^3$

* NH_4^+ $\quad \frac{5+4-1}{2} = \frac{8}{2} = sp^3$

* CO_3^{-2} $\quad \frac{4+0+2}{2} = \frac{6}{2} = 3\ sp^2$

* ICl_4^- $\quad \frac{7+4+1}{2} = 6 = sp^3d^2$

* NH^{-2} $\quad \frac{5+1+2}{2} = \frac{8}{2} = 4 = sp^3$

* I_3^{-1} $\quad \frac{7+2+1}{2} = \frac{10}{2} = 5 = sp^3d$

$CH_3^+ \longrightarrow$ $\quad \frac{4+3-1}{2} = \frac{6}{2} = 3 = sp^2$

Date: M T W T F S

Free radical:

* having unpaired es̄.
* valence es̄ count = odd

* Central atom (O.S = +ve) → E.N ↑ → unpaired es̄ ✓ take part in H.B

H.B = 1 + atom attached to C. atom

* Central atom (O.S = -ve) → unpaired es̄

H.B = atom attached to C. atom

e.g

* $\overset{-}{C}H_3\overset{+}{} = ?$ 7 es̄

H.B = 3 = sp^2

* $\overset{+}{C}F_3$ 25 es̄

H.B = 1+3 = 4 = sp^3

FONCl

* $\overset{+}{Cl}\overset{-}{O}_2$ 7+12 = 19

H.B = 2+1 = sp^2

* ClO_3

H.B = 3+1 = sp^3

Date: M T W T F S

* NO_2^+ $\quad H\cdot B = 2+1 = sp^2$

Resonating lone pair

(π − δ − L·p) → No aromatic character

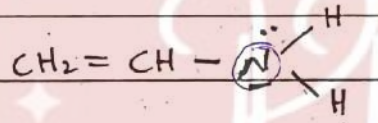
Aliphatic Compound:

H·B = L·p + atoms attached to C·atom

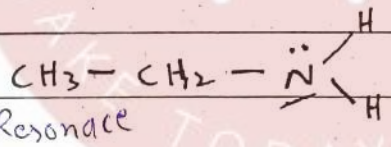
when L·p is in resonance

L·P → Not count

e.g.

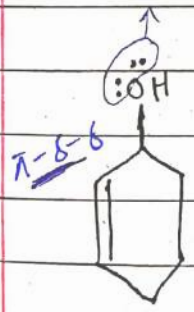


H·B = 3 = sp^2



No Resonace

H·B = 1 + 3 = 4 sp^3

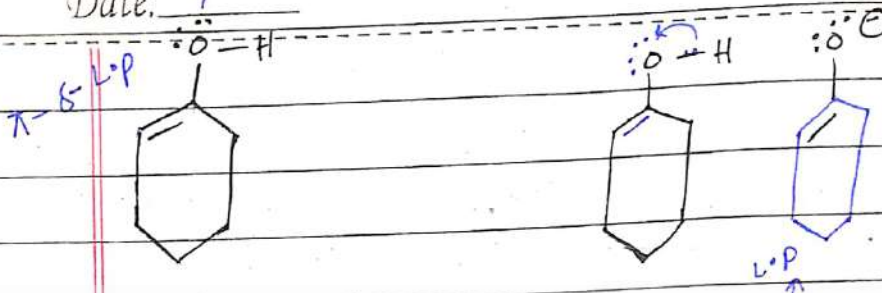


π − δ − 6

H·B = 2+2 = 4 sp^3

1 part in Resonance

Date: M T W T F S



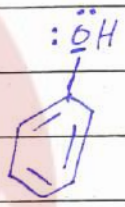
H·B = 1 + 2 = 3 sp^2

H·B = 2 + 1 = 3 = sp^2

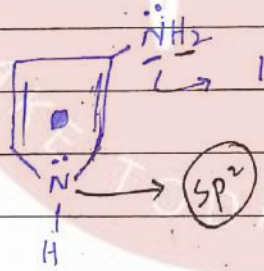
Aromatic Compound

When L·P as in resonance with aromatic Aromatic rings then they should be counted in formula H·B

aromaticity disturb.



H·B = 2 + 2 = 4 = sp^3



H·B = 1 + 3 = 4 sp^3

L·P

Aliphatic → Resonance → when L·P → not count

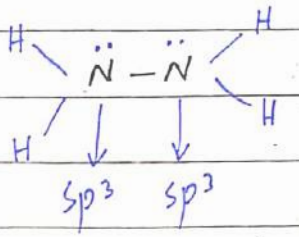
Aromatic → Resonance → in ⚠ (should count)

Date: M T W T F S

Multiple hybridization:

H·B = L·p + atoms attach to C·atoms

* N_2H_4, N = ?



* C_2H_2

$HC \equiv CH$

sp sp → sp^2

* $CH_2 = CH - C \equiv O\ddot{H}$ (Resonance)

sp^2 sp^2 sp^2 sp^2

* $CH_3 - CH = CH - \ddot{O}H$

sp^3 sp^2 sp^2 sp^2

Exception: → No H·B

① homodiatomic molecule (only overlapping) => No H·B

H_2, N_2, Cl_2, O_2.

② Heterodiatomic simple molecule => No H·B.

HF, HCl ↓

No → free radical

→ sp

Date: _____ V+M

M T W T F S

Hydrides

sp^3

Group V:	NH_3 (107.5°)	PH_3	AsH_3	SbH_3	BiH_3
Group VI:	H_2O (104.5°)	H_2S 93°	H_2Se 92°	H_2Te 91°	HgP 90°

sp^3 → No hybridization.

$sp^3 = 109.5^\circ$

Change in hybridization

alkene rxn + alkyne rxn

* Addition rxn.

$CH_2 = CH_2 + H_2 \longrightarrow CH_3 - CH_3$

(sp^2, sp^2 → sp^3, sp^3)

* Oxidation of alcohol

$CH_3 - OH \xrightarrow{[O]} H-\overset{\overset{O}{\|}}{C}-H$

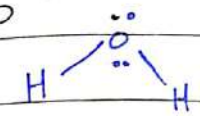
(sp^3, sp^3 → sp^2)

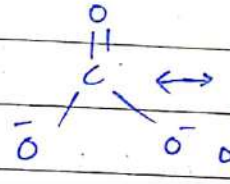
* Reduction of carbonyl Compound.

Aldehyde/ketone ⟶ alcohol

Date: M T W T F S

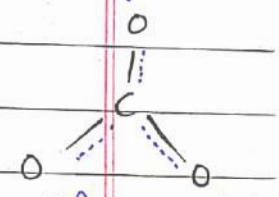
Resonance

H_2O 

CO_3^{-2} 

which have more than one structure.

Delocalization


(Resonance hybrid)

Shifting of electron (Pi & δ)

δ-delocalization
⇓
(hyperconjugation)

π - delocalization
⇓
Resonance
(It is the shifting of πe^-)

(define for those compounds which have more than one structure.)

Resonating / Limiting / Contributing / Canonical Structure
⇓
⇒ imaginary structures.

⇒ have same or different energy.

⇒ R.s may have same or different contribution in Resonance hybrid.

Date: _____ M T W T F S

* contribution in Resonance hybrid ∝ stability of R.structure

Resonance hybrid:

=> Real / Actual structure of Molecule

=> R.hybrid ⟶ more stable R.s than any due to more bond formation (π)

=> R.hybrid ⟶ Lower energy than any R.s.

Condition for Resonance

* delocalization => π es will shift
* position of atom same
* donot vilate octect rule.
* Total charge on R.s => Same.
* unpaired es in R.s => Same.
* Resonance impart energy.

effect:

* Aromaticity * position of atom same * No. nuclei same
* Resonance * position of nuclei same.
* hyperconjugation * position of π-es
* inductive effect not same

Date: M T W T F S

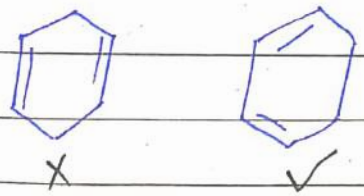
How to find Resonance

① Major Resonance:

↳ involve more than one atom or bond.

minor ← $\overset{-}{C}-\overset{+}{O}$ $\quad$ $CH_2=CH-\overset{-}{O}$ → major.

* π − δ − π
* π − δ − +ve charge
* π − δ − −ve
* π − δ − L.P
* π − δ − unpaired e⁻s
* π − π − L.P
* π − π − −ve
* π − π − +ve
* π − π − unpaired e⁻s



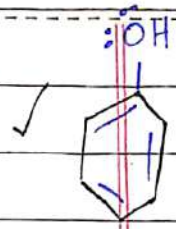
X ✓

$CH_2=CH-CH_2^+ \leftrightarrow {}^+CH_2-CH=CH_2$ (+1)

$CH_2=CH-\overset{-}{O}$ (−1) → this e⁻ move

$\leftrightarrow \overset{-}{C}H_2-CH=O$ (−1)

Date: _____ M T W T F S



π - π̄ - L·p involve in Bond

O ch. O ch.

$CH_2 = CH - \dot{C}H_2 - CH = CH_2$

$CH_2 = CH = \overset{+}{C}H$ $CH_2 = \dot{C} = CH$

$CH_2 = C = \overset{\ominus}{C}H$ $CH_2 = C = \ddot{N}H$

$\dot{C}H_2 - C \equiv CH$ $\dot{C}H_2 - C \equiv \overset{+}{N}H$

Minor Resonance

involve in one bond.

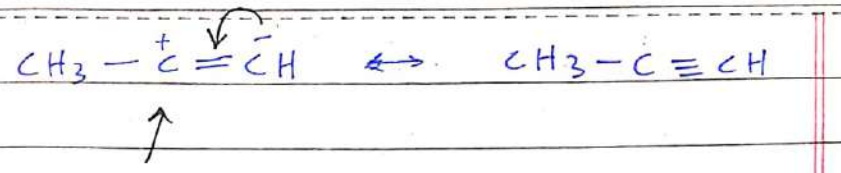
① +ve — δ — -ve

$\overset{+}{C}H_3 - \overset{-}{C}H_2 \leftrightarrow CH_2 = CH_2$

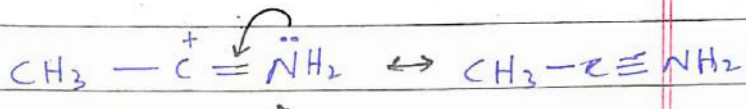
② +ve — δ — L·p

$CH_3 - \overset{+}{C}H - \ddot{N}H_2 \leftrightarrow CH_3 - CH = \overset{+}{N}H_2$

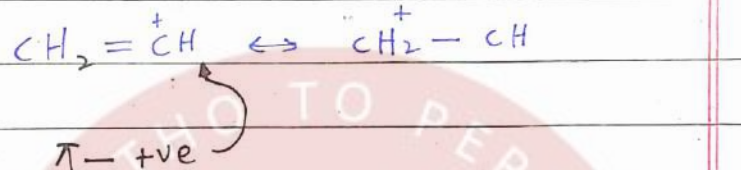
Date: M T W T F S



③ +ve — π — -ve



④ +ve — π — L·p



⑤ π — +ve

⑥ π — L·p

Stability of R· structure

Priority:

① Stability ∝ No. π bonds

② Stability ∝ Neutral as compared to charge.

$O^{+1} < Na^{+1}$

$O^{-1} > Na^{-1}$

③ Stability ∝ +ve on (when on E·positive) E·P ∝ -ve on E·N atom E·N

④ Stability ∝ $\frac{1}{\text{distance b/w charges}}$

Stab ↑↑ cont in hy ↑↑

Date: M T W T F S

Neutral — Neutral but individually charge

① $CH_2 = CH - \ddot{N}H_2 \longleftrightarrow CH_2^- - CH = \overset{+}{N}H_2$

↓

=> stable

=> more contribution in R·hybrid

② $CH_2 = CH - O^- \longleftrightarrow CH_2 - CH = O$

↓

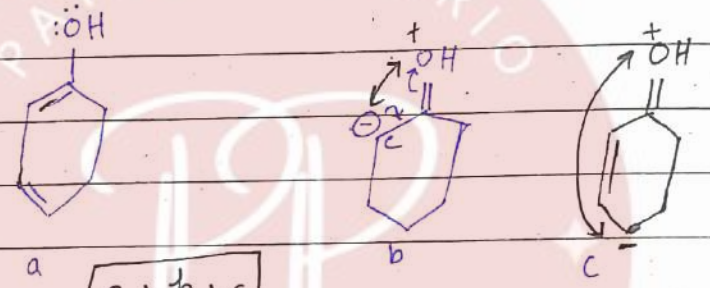
=> stable

③ $CH_2 = CH - \overset{+}{N}H \longleftrightarrow \overset{(+)}{C}H_2 - CH = NH$

∴ at this C·P is present

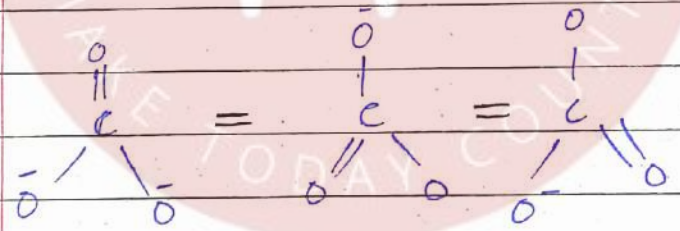
↓

=> more stable



a > b > c

CO_3^{-2}



Same Contribution in R·H·

Date: M T W T F S

=> e⁻ donating group

(+)

=> +ve charge

stability ∝ 1/charge

e⁻ ⇑

$CH_3 - \overset{+}{C}H - CH = CH_2$ (Less charge)

more stable

e⁻ ⇓

$CH_3 - CH = CH - \overset{+}{C}H_2$ (More charge)

stability ∝ 1/(distance of E·D·G from +ve)

=> -ve charge

$CH_3 - \overset{\ominus}{C}H - CH = CH_2 \leftrightarrow CH_3 - CH = CH - \overset{\ominus}{C}H_2$

More Negative

(Less stable)

Less -ve

(stable)

stability ∝ distance of E·D·G from -ve

NO_2, NO_2^+

=> e⁻ with drawing group

(+ve)

e⁻ ⇑

$Cl - \overset{\oplus}{C}H - CH = CH_2 \leftrightarrow Cl - CH = CH - \overset{\oplus}{C}H_2$

more +ve

unstable

Less +ve

(stable)

$Cl - \overset{-}{C}H - CH = CH_2 \leftrightarrow Cl - \overset{-}{C}H = CH - CH_2$

Less -ve

(stable)

more -ve

Date: M T W T F S

⇒ stability $\propto$ E·D·G distance +ve

⇒ stability $\propto \frac{1}{\text{distance b/w E·D·G (-ve)}}$

VSEPR Theory

Geometry of molecule.

Postulates:

① Arrangement of e⁻s → arrange to max e⁻s ⇓ repulsion ⇓ → stability ⇑ ⇒ form geometry.

Monocentric

② Volume

L·P > B·P → Bicentric

b/c under control of one nucleus

Repulsion $\propto$ e⁻ density $\propto$ V

Repulsion order:

L·P − L·P > L·P − B·P > B·P − B·P

due to max V

③ Multiple bond → consider as a single bond

Why:

Geometry depends upon sigma bond not π-bond.

H − H linear

O = O linear

N ≡ N Linear

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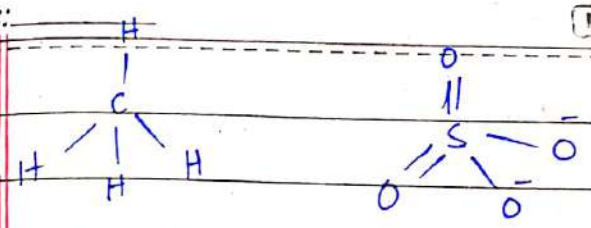
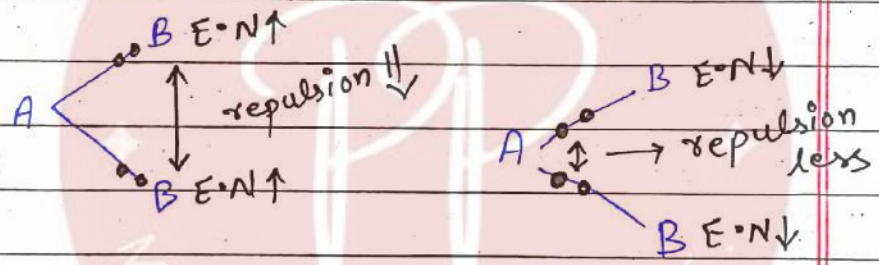


* Geometry → not depend on $\overline{\Pi}$ – bond.
→ depend on (δ-bond + L·P)

effect of Bond pair:
↳ repulsion

effect of B·P or repulsion $\propto \frac{1}{\text{E·N of attached atom}}$



overall geometry:

* depend on valence e⁻s.

Concept

Geometry / electronic Geometry:
⇓
depend on electron pair
↓ ↓
L·P B·P

Date: M T W T F S

Monovalent atom:

(E·P = Hybridization)

Polyvalent atom

having valency = 1

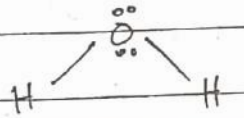
Mono Valent

H & Halogen

other → poly

E·P → from structure

e·g H_2O



sp^3 → 4 → pair

NH_3 → sp^3 → 4 E·pair

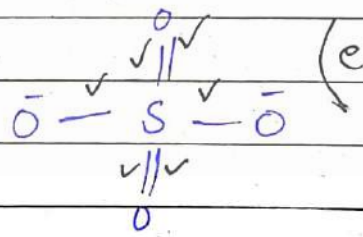
PCl_5 → sp^3d → 5 e·p

H_3O^+ → sp^3 → 4 l·p

Q# According to VSEPR theory e·pair in SO_4^{-2}.

→ sp^3 H·B → 4 e·pair

Q# E·P in SO_4^{-2} is:



(e·pair = 08)

Date: M T W T F S

Shape / Molecular geometry:

→ depend on bond pair.

e.g H_2O → 2 B.P → Bent.

→ Bond pairs are arranged by l.p & other B.pair

⇒ Monovalent atom / According to VSEPR Theory:

B.P = atom attach to C.atom

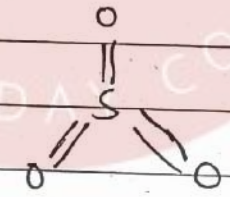
Polyvalent atom / structure

B.P → structure.

H_2O = 2 B.P PCl_5 = 5 B.P NH_4^+ = 4 B.P

Q# According to VSEPR Theory B.P in SO_3 is

B.P = 3



* B.P in SO_3 → 06

Lone pair

L.P = H.B - B.P

H_2O = 4 - 2

= 2

Date: M T W T F S

* H_3O^+ ⟶ 4-3 = 1 L·P

* SO_4^{-2} ⟶ 4-4 = 0 L·P

* ICl_4^- ⟶ 6-4 = 2 L·P

* I_3^- ⟶ 5-2 = 3 L·P

* XeF_2 ⟶ 5-2 = 3 L·P

* OH^- ⟶ 4-1 = 3

Iso-structural Specie:

↳ compound having same structure.

Condition:

H·B = Same
L·P = Same
B·P = Same

NH_4^+	CH_4
* sp^3	* sp^3
* 0 L·P	* 0 L·P
* 4 B·P	* 4 B·P

SO_2 ↓ sp^2 1 L·P

H_3O^+ ↓ sp^3 1 L·P

Not iso-structure.

Date: M T W T F S

iso-structural

H_3O^+	NH_3
sp^3	sp^3
1 L·P	1 L·P
3 B·P	3 B·P

· Central atom

→ which can form maximum bonds.

Conditions:

⇒ Low E·N

⇒ vacant orbital present

⇒ Less in formula.

Note:

* (H) & (F) can never be central atom.

* No Central atom in diatomic molecule.

e.g

HF → X HCl → X

* H_2SO_4 → S * C_3H_8 → C

* H_3PO_3 → P

* $CH_3-\overset{O}{\overset{\|}{C}}-O-H$ → C_2H_2O

Note:

VSEPR not valid for simple diatomic molecule not ion & free radical

atom

H—H $\ddot{O}=\ddot{O}$ $:\ddot{F}-\ddot{F}:$

b/c it is linear

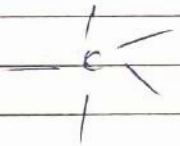
Geometry not depend on L·pair

Date: M T W T F S

H·B	L·P	Shape
sp	0	Linear
sp^2	L·P = 0	Trigonal planner
	L·P = 1	Angular planner (H–O–H)
sp^3	L·P = 0	Tetrahedral
	L·P = 1	Trigonal pyramidal
	L·P = 2	Angular (Non-planner)
	L·P = 3	Linear
sp^3d	L·P = 0	Trigonal bipyramidal
	L·P = 1	See saw
	L·P = 2	T- shape
	L·P = 3	Linear
sp^3d^2	L·P = 0	octahedral
	L·P = 1	Square pyramid
	L·P = 2	Square planner
sp^3d^3	L·P = 0	pentagonal bipyramidal
	L·P = 1	pentagonal monopyramidal

Date: M T W T F S

Geometry	Bond angle
Linear	180° $BeCl_2$
Trigonal planner	120° BF_3
" "	Less than 120 (118°)
Tetrahedral	109.5° (CH_4)
	107.5° (NH_3)
	104.5° (H_2O)
	180°
Trigonal bipyramidal	
octahedral	
pentagonal bipyramidal	



Date: _____ M T W T F S

MCQs

shape

* OH^-:

sp^3 → Tetrahedral

4 - 1 = 3 L.P

Linear shape

* CCl_2:

sp^2 → Trigonal planner

1 L.P → Angular planner

* ClF_3:

sp^3d → Trigonal bipyramidal

2 L.P → T- shape

* ICl_4^-

sp^3d^2 → octahedral

2 L.P → square planner

* I_3^-

sp^3d → Trigonal bipyramidal

3 L.P → Linear

* SeF_4 → F — Se — F (F, F)

sp^3d → Trigonal bipyramidal

1 L.P → See saw

* SO_4^{-2}

sp^3 → Tetrahedral

0 L.P

4 4

Date: M T W T F S

Resonating Lone pair

★ When L·p is in resonance then it should not be counted while determine geometry & Shape.

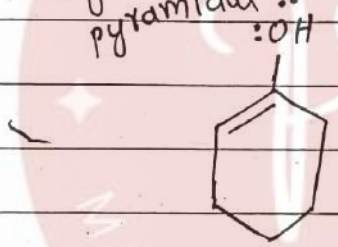
$CH_2 = CH - \ddot{N}H_2$ → Trigonal planner (shape)

H·B = 0+3 = sp^2 → Trigonal planner (Geo)

aliphatic Ring ← $CH_3 - CH_2 - \ddot{N}H_2$

H·B = 4 = sp^3 (Geo) → Tetrahedral

Trigonal pyramidal



H·B = 1+2 = sp^2 → Trigonal planner

S → Angular planner

Aromatic Ring → having = – = – bonds.

★ L·p → count when determine shape & Geometry.

H·B = 2+2 = 4 → sp^3 → Tetrahedral (Geo)

→ Angular (shape)

Free radical

Date:

M T W T F S

* CF_3 O.S of C.atom +ve

⇓

then unpaired es will be considered as lone pair

O.S = -ve

⇓

unpaired es not counted as L.P.

$\overset{+}{C}F_3^-$ → 1+3 = 4 = sp^3 → Tetrahedral

contain one unpaired es → 1 L.P → Trigonal pyramidal

* $\overset{-}{C}H_3$: → sp^2 = Trigonal planner

→ O=L.P → Trigonal planner.

* $N^{+b}O_2^{-b}$ → sp^2 = Trigonal planner.

→ 1 L.P → Angular planner.

L.P کو consider کرنا ہے unpair

* $\overset{+}{Cl}O_3^-$:

1+3 = 4 = sp^3 → Tetrahedral

1 L.P ⇒ Trigonal pyramidal

Multiple Geomtries

Resonance

$CH_3 - CH = CH - \ddot{N}H_2$

Tetrahedral ← sp^3 sp^2 sp^2 sp^2

L.P = 0 L.P = 0 L.P = 0 L.P = 0

⇓

Trigonal planner

Date: M T W T F S

Bond Angle

repulsion ↑↑ B.A ↑↑

Facts:

$$B.A \propto \frac{1}{L.P}$$

when attach atoms same

B.A ∝ E.N of C.atom

B.A ∝ size of attached atom

For same group element or when C.atom same

B.A ∝ "s" character

different group & period

B.A ∝ $sp > sp^2 > sp^2 > sp^3 > sp^3 > sp^3$

L.P = 0, L.P = 1, L.P = 0, L.P = 1, L.P = 2

Ions:

when (H.B = same)

B.A = +ve > Neutral > -ve

Q#

which one has Max B.Angle?

(a) NH_3 > (b) PH_3 > (c) AsH_3 → (B.A ∝ E.N)

$OF_2 < OCl_2 < OBr_2 < OI_2$ (B.A ∝ size)

$NCl_3 > NH_3$

different group & period

Date: M T W T F S

$BeCl_2 > AlCl_3 > CCl_2 > \overset{+}{N}H_4 > H_3O^+ > H_2O$

sp | sp^2 0 L·P | sp^2 L·P = 1 | sp^3 0 L·P | sp^3 1 L·P | sp^3 L = 2 P

$\overset{+}{C}H_3 > CH_4 > \overset{-}{C}H_3$

sp^2 0 L·P | sp^3 0 L·P | sp^3 L·P = 1

more S ↑

$\overset{+}{N}H_4 > NH_3 > \overset{-}{N}H_2$

sp^3 L·P = 0 | sp^3 L·P = 1 | sp^3 2 L·P

B·A is decreased by L·P as compared to unpaired es

← Lone pair & unpaired es

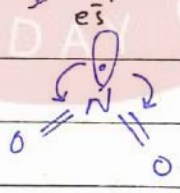
$\overset{+}{N}O_2 > \overset{\pm\delta - \delta}{N}O_2 > NO_2^-$ (ion)

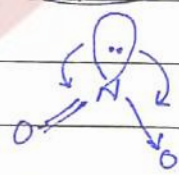
2 = sp | 3 = sp^2 | 3 = sp^2

L·P = 0 | 1 unpaired es | L·P = 1

B·A decrease due to L·P

$O = \overset{+}{N} = O$





Change in Bond angle

$NH_3 + H^+ \longrightarrow \overset{+}{N}H_4$

sp^3 107.5° → sp^3 109.5°

109.5° − 107.5° = 2°

with 1 L·P ⟶ ↓2° change occur in B·A

Date: M T W T F S

MCQs $H_2O + H^+ \longrightarrow H_3O^+$

104.5° 107.5°

$\Delta B \cdot L = 107.5° - 104.5° = 3°$

MCQs $H_2O \longrightarrow OH + H^+$

sp^3	sp^3
L·P = 2	L·P = 1
104.5°	180°

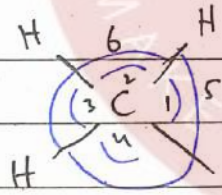
$\Delta B \cdot L = 180° - 104.5° = 75.5°$

⇒ No # Bond Angle

$B \cdot A = \frac{n(n-1)}{2}$ n = No attached atom

★ CH_4

$= \frac{4(4-1)}{2} = \frac{12}{2} =$ 6 Bond angle



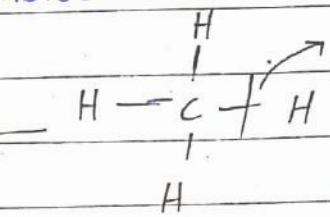
★ PCl_5

$B \cdot A = \frac{5(5-4)}{2} = \frac{20}{20} =$ 10

Date: _____ dissociation M T W T F S

Bond energy

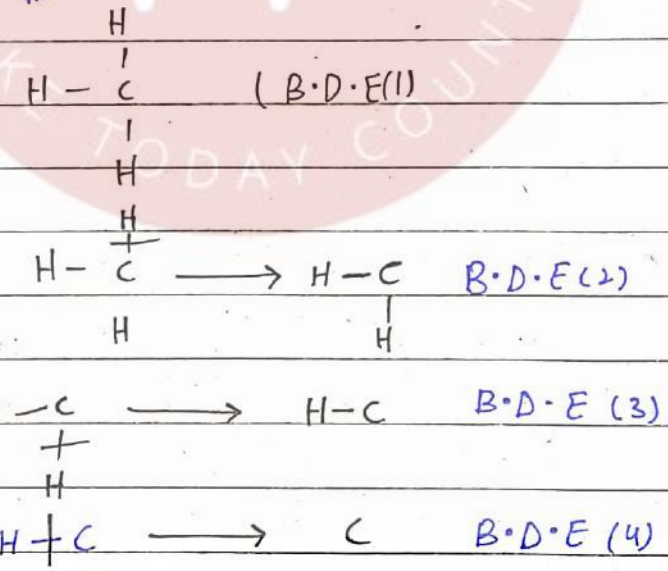
amount of energy required to break a specific bond in a molecule.



⇒ (B·D·E) for same bond in a molecule is different.

average of ← Bond energy
BDE

Amount of energy required to break all the bond in one mole of a molecule.



Date: M T W T F S

$$B.E = \frac{BDE(1) + BDE(2) + \cdots BDE(n)}{N \text{ (No \# bond)}}$$

* B.E for covalent compound

* B.E for ionic compound → Lattice energy

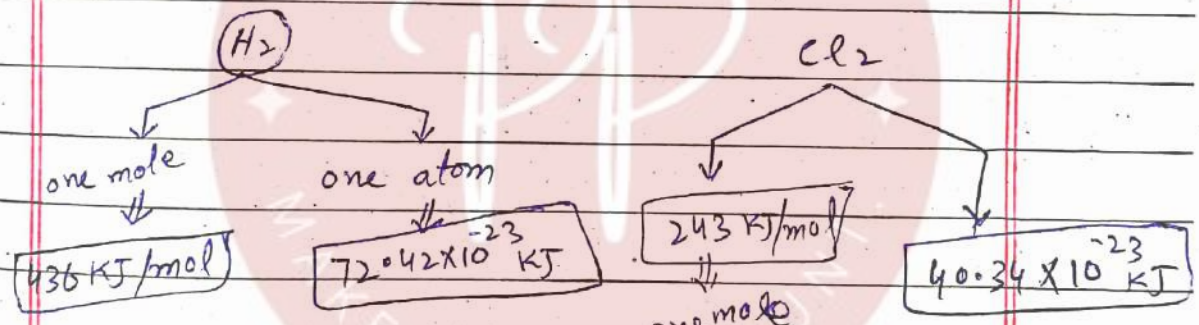
In diatomic molecule

$$B.E = B.D.E$$

$H \{ H$

unit: KJ/mol

B.E → endothermic or exothermic



Date: Lec # New

M T W T F S

Per mole:

$$B.E = \text{"x"}\ KJ/mole$$

Per molecule:

$$B.E = \frac{x}{N_A}\ KJ$$

Contribution per atom:

$$B.E = \frac{x}{N_A \times atomcity}\ KJ$$

Q# B.E of A_3 is 18.066×10^{23} KJ/mol then B.E of each A:

$$B.E = \frac{18.066}{6.023 + 3} = 1\ KJ$$

(#) Exp ≠ Theor B.E

Heteroatoms:

Theoritical B.E → Not consider ionic character

$(+\delta)\ A$ —— $(\delta)\ B$

Exp: consider ionic character

Hetero atom:

$(+\delta)\ A$ —— $(-\delta)\ B$

ionic character

Exp B·E ∝ difference in E·N

Date: M T W T F S

Exp B·E > T·B·E

Homoatomic: A — A

Exp B·E = Theoritical B·E

MCQs

The B·E of A is 60J and B is 40J. then B·E of AB will be.

(a) 100J (b) 95J

(c) 105J (d) None

Hetero

Exp > Theor

For B_2 ⟶ 100J

Factor affecting B·E

① E·N

(*) when C· atom different / attach atoms same

B·E ∝ difference in E·N

NH_3 > PH_3 > AsH_3

H_2S < H_2O > H_2Se

(*) when C· atom same

B·E ∝ E·N of attach atom

B·E ∝ No. of attached atoms E·N

CH_4 < CCl_4 C_2H_6 < C_2F_6

CH_4 < CH_3Cl < CH_2Cl_2

Date: M T W T F S

Bond order:

B.E ∝ B. order

B.E ∝ multiplicity of bond

B.E ∝ ≡ > = > −

H_2 < O_2 < N_2

− = ≡

Bond length:

$B.E \propto \frac{1}{B.L}$

Size of atom

$B.E \propto \frac{1}{size}$

C−Cl > C−I → size ⇑

F_2 Cl_2 Br_2 I_2

Small size ← F_2 but having 3 L.P ↓ cause repulsion ⇒ B.E ⇓

$Cl_2 > Br_2 > F_2 > I_2$ Trend

− cause B.L ⇑

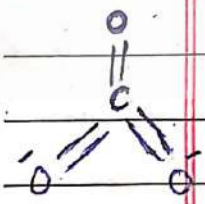
Resonance:

B.E ∝ Triple > Double Bond > Partial > Single

Q# B.E b/w C & O.

$CO > CO_2 > CO_3^{-2} > C-O$

$C \equiv O$ $O = C = O$ partial bond.



Date: M T W T F S

C = N B·E

double → NH > partial → NH > single → NH_2

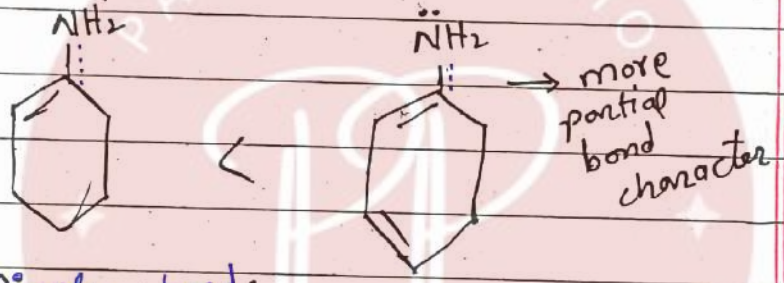
C–N B·E

$CH_2=CH-\ddot{N}H_2 \;<\; \ddot{O}=CH-\ddot{N}H_2$

$\bar{C}H_2-CH=\overset{+}{N}H_2 \;<\; \bar{O}-CH=\overset{+}{N}H_2$

Note:

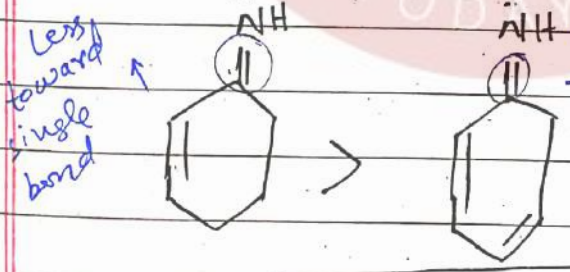
B·E ∝ stability of R·S (when resonance same)



Single bond:

B·E ∝ Magnitude of Resonance

Double bond:



$B \cdot E \propto \frac{1}{\text{Magnitude of Resonance}}$

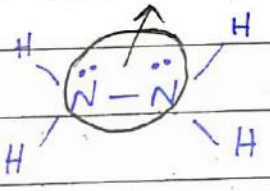
Date:_____ M T W T F S

* $\bar{e}-\bar{e}$ repulsion:

$$B.E \propto \frac{1}{e\text{-}e \text{ repulsion}}$$

cause repulsion

$NH_3 > N_2H_4$



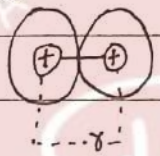
H_2O_2

$H_2O > H_2O_2$

Bond length

calculated by

X-ray diffraction or analysis of molecular spectra



Average equilibrium bond distance b/w two nuclei

Why called average

⇓

b/c atom every time vibrate due to which bond vibrate.

Why called equilibrium

⇓

bond is formed at specific distance.

⇒ combined state

- M.B
- C.B
- I.B
- V.R.B

Date: M T W T F S

Hetero atomic Molecule:

Theoritical B.L A — B

Exp B.L $A^{\delta+} \cdots B^{\delta-}$ → due to ionic character ⇓ attract B.L ⇓

T.E B.L > Exp B.L

Homo atomic Molecule:

A — A T.E B.L = Exp B.L

Q#

in AB molecule the radius of A is 6nm and B is 4nm then B.L of AB is:

(a) 10 nm (b) 12nm (c) 8nm ✓ (d) None

Hetero

Factor affecting

$$B.E \propto \frac{1}{B.L}$$

Date: M T W T F S

Valence Bond Theory

* It deals bonding
* es⁻ is a particle
* based on classical Mechanics

Concepts:

* Concept of orbital
* Concept of B E·C
* overlapping

Postulates:

① A bond is formed when atom approach each other.

② both orbital will half filled.

A	B		A	B	
☐	☐	X	↑↓	↑↓	X
↑↓	↑	X	↑	↑	X

=> Spin of es⁻ in orbital must be **opposite**

↑ ↓

③ Orientation of orbital = Symmetrical

=> Px → Px ✓

=> Px → Py X

=> Pz → Py X

=> s-Px s-Py s-Pz

Date: M T W T F S

* (S) can overlapp with any orbital because it is spherical

* Direction of Bond = direction of overlapping.

=> pattern of overlapping → Linear
→ Bent (Cycloalkane)
→ Sidewise

Overlapping:

It is mixing of e⁻ density

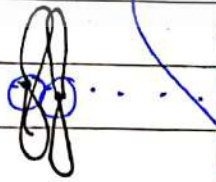
depends on * directional character of orbital
* direction of overlapping
* Type of orbital

On Basis of overlapping

Max e⁻ density → Linear overlapping → strong → σ-bond

Min e⁻ density → Side wise → weak → π-bond

internuclear axis



Date: Linear

side wise

M T W T F S

* aver B.E = 80-85 KJ	* avg B.E = 65 KJ
* es density on internuclear axis	* es above or below internuclear axis
* es density ↗ at one place co-planner	* not coplaner
* es density symmetrical	* unsymmetrical
δ	π
* S-S	* Pπ - Pπ
* S-P	* Pπ - dπ
* P-P	* dπ - dπ → delta bond
* hybrid-hybrid	
* hybrid - atomic	* Min π-bond = 0
* sp^2 - sp^2	* Max π-bond = 2
Max δ bond = 1	* No free rotation.
Min π bond = 1	
* free rotation ⇓ wagging	* Geometry not depend on π-bond
* Geometry depend on δ-bond.	* dependant bond.
* independant bond	

Date: M T W T F S

* The angle b/w σ & π is 90°

σ

π

stability ∝ No. bond	Reactivity ∝ No π bonds

Exceptions of VBT:

=> VBT not obey when excitation of e⁻ occur.

⇓

when no. bonds > unpaired e⁻

eg

* CH_4

not obey

$C = 1s^2, 2s^2, 2p^2$ — 2 unpaired e⁻

(No bond > un·e⁻)

4 > 2

* $BeCl_2$

$Be = 1s^2, 2s^2, 2p^0$

obey

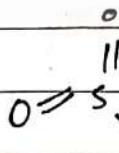
* H_2O:

$O = 1s^2, 2s^2, 2p^4$

unpaired = bond

e⁻ 2 = 2

* SO_3:



$S = 1s^2, 2s^2, 2p^6, 3s^2, 3p^4$

$3d^0$

2 unpaired e⁻

6 - bonds.

π- bond → always directional

σ → may directional or non-directional

Date: M T W T F S

(*) VBT not explain co-ordinate C.B.

(*) Not explain de-localized bonding
↳ Resonance.

e.g CO_3^{-2}, C_6H_6 → not explain by VBT.

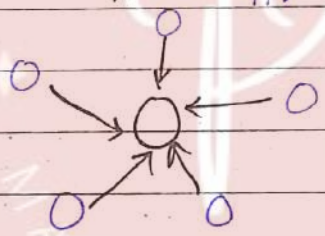
Types of overlapping

(*) S-S:

* always form Sigma bond.

* Non-directional bond.

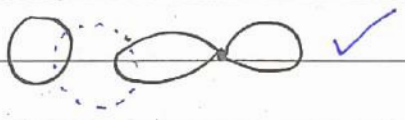
* H_2

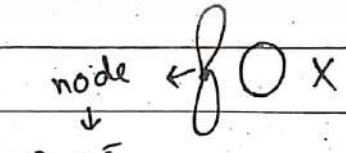


(*) S-p:

* always sigma bond

* always directional





Date: M T W T F S

* p-p overlapping

$P_\delta - P_\delta$

* Directional
* Sigma bond

$P_\pi - P_\pi$

* π-bond
* Directional

Strength:

$P_\pi - P_\pi$ < S-S < S-p < $P_\delta - P_\delta$

Extent of overlapping $\propto$ Bond strength

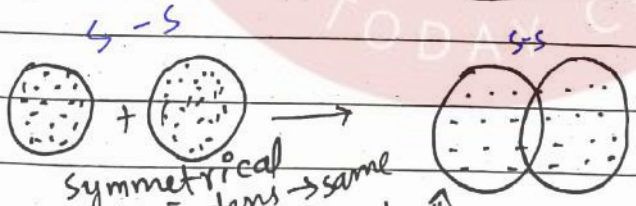
$\propto$ B.E

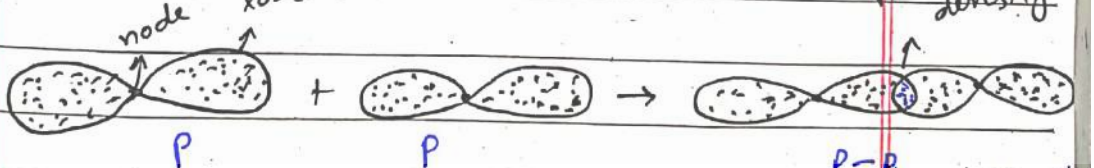
$\propto \frac{1}{B.L}$

$\propto$ stability

$\propto \frac{1}{\text{Reactivity}}$

$\propto \frac{1}{P.E}$





overl ⇑ energy ⇑ rele

Date: _____ M T W T F S

Hybrid- Hybrid overlapping:

* always σ- bond.
* Directional overlapping.
* Linear + Bent

e.g.

$sp-sp$, sp^2-sp^2 , sp^3-sp^3.

Bond strength / Bond energy

Strength $\propto$ E.N $\propto$ s-character

$sp-sp > sp-sp^2 > sp-sp^3$

$> sp^2-sp^2 > sp^2-sp^3$

B. length , P.E:

$sp-sp < sp-sp^2 < sp-sp^3 < sp^2-sp^2 < sp^2-sp^3$

$< sp^3-sp^3$

* Hybrid & atomic Orbital:

* always σ- bond
* directional bond.

Order

Hybrid-hybrid > Hybrid-atomic > atomic-atom-

Date: M T W T F S

$s-sp$ $p-sp^3$

strength ∝ E·N ∝ "s" character

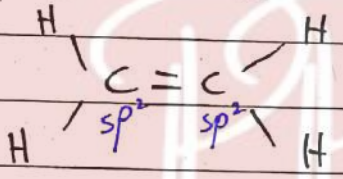
Bond strength / B·E

$s-sp > s-sp^2 > s-sp^3 > p-sp > p-sp^2 > p-sp^3$

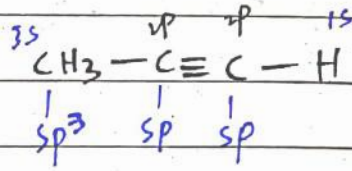
$BeCl_2 > AlCl_3 > CCl_4$

$p-sp$ $p-sp^2$ $p-sp^3$

No # orbitals



* Hybrid orbitals = 6
* unhybrid / atomic orbitals = 6
* p- orbitals = 6
* s- orbitals = 4



* hybrid = 8
* unhybrid / atomic = 8
* total orbitals = 16

p = 4

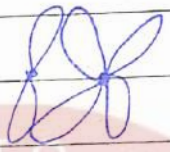
s = 4

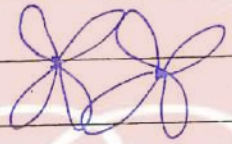
Date: _____ M T W T F S

$CH_3-\overset{\overset{O}{\|}}{C}-OH$

Formation of π-bond:

$P\pi - P\pi$ 

$P\pi - d\pi$ 

$d\pi - d\pi$ 

Period #2:

as central ↙ only $P\pi$ & $P\pi$ overlapping.

other period elements:

$P\pi - P\pi$ & $P\pi - d\pi$

($2P\pi - 2p\pi$ overlapping)

e.g. ① CO_2:

$O \overset{\uparrow}{=} C = O$

↓

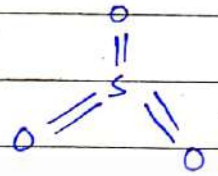
p#2

②

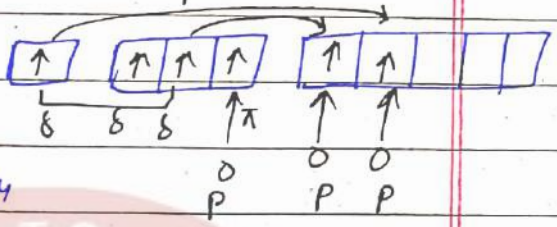
Date: M T W T F S

Formation of π- Bond

① SO_3:



S = $1s^2, 2s^2, 2p^6, 3s^2, 3p^4, 3d^0$



H·B = sp^2

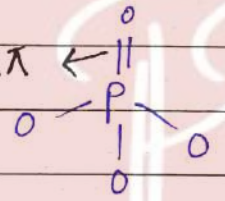
O = $1s^2, 2s^2, 2p^4$

1 $p\pi - p\pi$

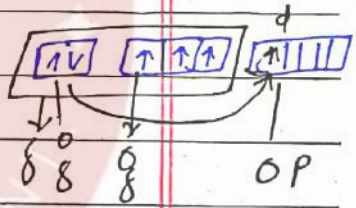
2 $p\pi - d\pi$

★ PO_4^{-3}:

↓ $p\pi - d\pi$ ←



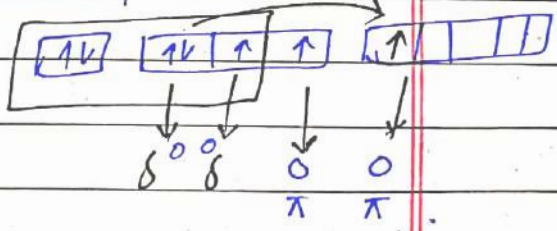
P = $1s^2, 2s^2, 2p^6, 3s^2, 3p^3, 3d^0$



H·B = sp^3

★ SO_2 → 4 bonds.

S = $3s^2, 3p^4, 3d^0$



O = S = O

H·B = sp^2

① $P\pi - P\pi$

② $p\pi - d\pi$

Date:

M T W T F S

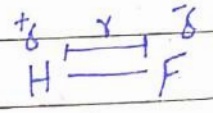
Dipole moment"

explain

=> polarity of molecule

=> not explain polarity of bond.

M. Form:



$\mu = q \times r$

unit:

* Cm * Debye

Direction:

Vector quantity

Direction

↳ From Less E.N toward more E.N atom

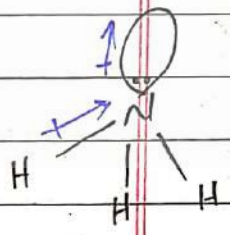
↳ From atom → to L.P

Same atoms (C-C)

$E.N \propto sp > sp^2 > sp^3$

$CH_3 - C \equiv CH$

sp^3 sp



$CH_2 = CH - C \equiv CH$

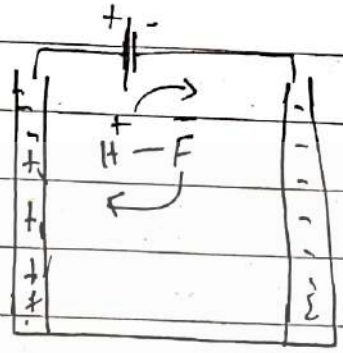
sp^2 sp

Less E.N

Date: M T W T F S

Measurement:

electric condensor



polarity ∝ decrease in P.D

* Solution ⟶ Should be . Non-polar .

* experimental dipole moment

identification of polarity of Molecule

* Diatomic Molecule

- Homo
  - ⇓
  - * $\mu = 0$
  - * non-polar
  - O_2, N_2, Cl_2, F_2
- Hetero
  - $\mu \neq 0$
  - => polar
  - => $\mu \propto$ diffe E.N
  - * HCl, HF, NO, CO

HF > HCl > HBr > HI

Date: _____ M T W T F S

Polyatomic

① Same atom attached to c. atom

② different atoms attached to c. atom.

From Geometry

L.P ≠ 0 ⇓ μ ≠ 0 * polar e.g. $\ddot{P}Cl_3$

t.p = 0 ⇓ μ = 0 * non-polar e.g. PCl_5, SO_3, CCl_4, NH_4^+, SO_4^{-2}, CO_2, CO_3^{-2}, CH_4

sp (Linear): (polar)

atoms different attach.

BeClBr ↓ sp

Br ← Be → Cl

$\ddot{S}O_2$ $\ddot{N}H_3$ $H_2\ddot{O}$ H_3O^+ $:\ddot{N}H_2^-$

sp^2 (Trigonal planner): (polar)

different atoms to c. atoms.

$AlCl_2Br$ ⇒ polar

↓ sp^2

sp^3 (Tetrahedral):

different atoms to c.a

c. atom

CH_3Cl → polar

CH_2Br_2 → polar

$CHCl_3$ → polar

all polar ← $CH_3Cl > CH_2Cl_2 > CHCl_3$

μ ≠ 0

μ ∝ ΔE.N

μ ∝ NO E.N atoms

H:B ⇒ same

μ ∝ E.N

μ ∝ NO E.N atom

CH_3F $CH_3Br > CH_3I$ X

CH_3Cl

Date: M T W T F S

exceptional:

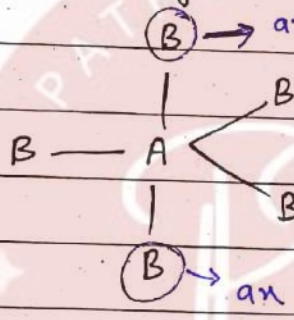
$CH_3Cl > CH_3F > CH_3Br > CH_3I$

$\mu = q \times r$ $\quad \mu \propto q$ $\quad \mu \propto r$

C–Cl: $q \Downarrow$ $r \Uparrow$ $\Rightarrow$ r dominant factor

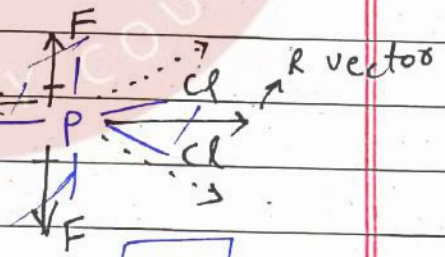
C–F: $q \Uparrow$ $r \Downarrow$ size small so cause

sp^3d (Trigonal bipyramidal)



* More E·N atom → occupy Axial
* Less E·N atom → equitorial

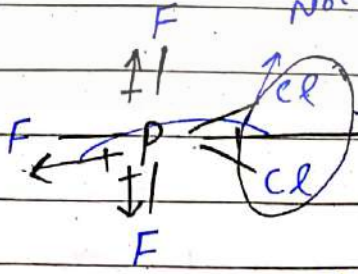
PF_2Cl_3: sp^3d



$\mu = 0$

PF_3Cl_2

sp^3d



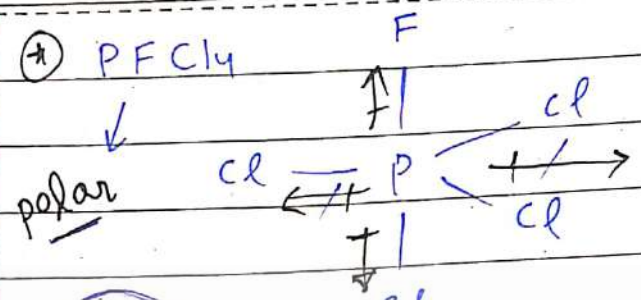
Not equally cancel each other as one consider

polar

Date:

M T W T F S

(*) $PFCl_4$

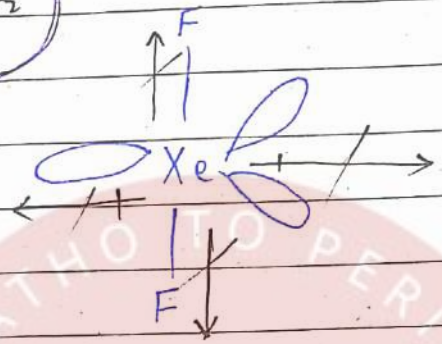


polar

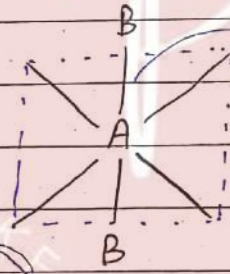
$:XeF_2$

Non-polar

$\mu = 0$



Sp_3d^2 (octahedral)

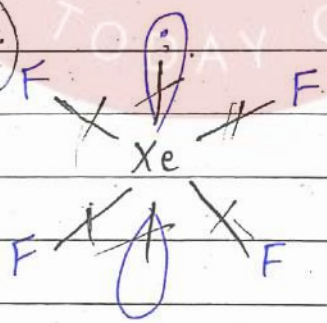


Axial = lone pair

XeF_4

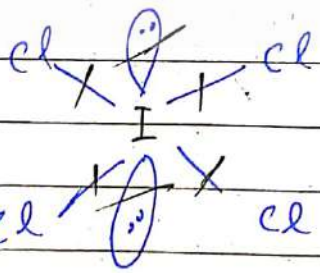
Non-polar

$\mu = 0$



ICl_4^-

$l.p = 2$



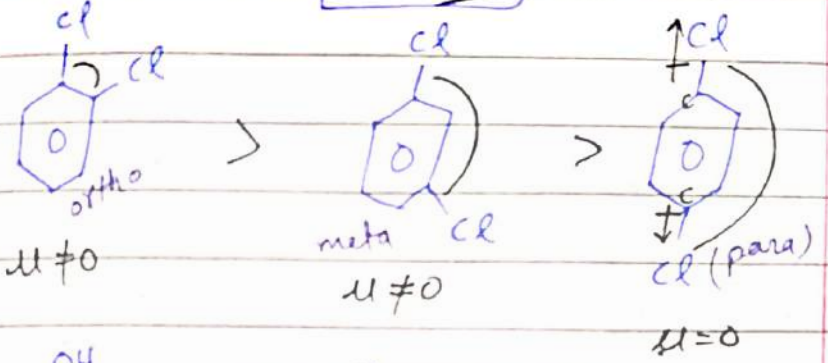
Non-polar

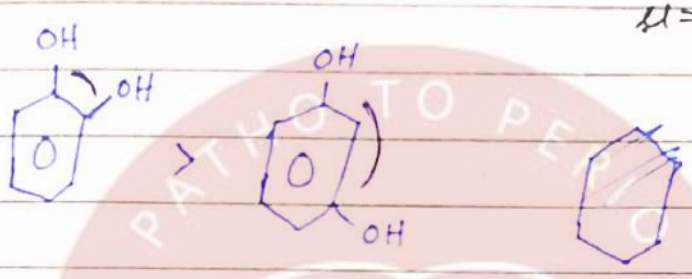
sp^2

Date: M T W T F S

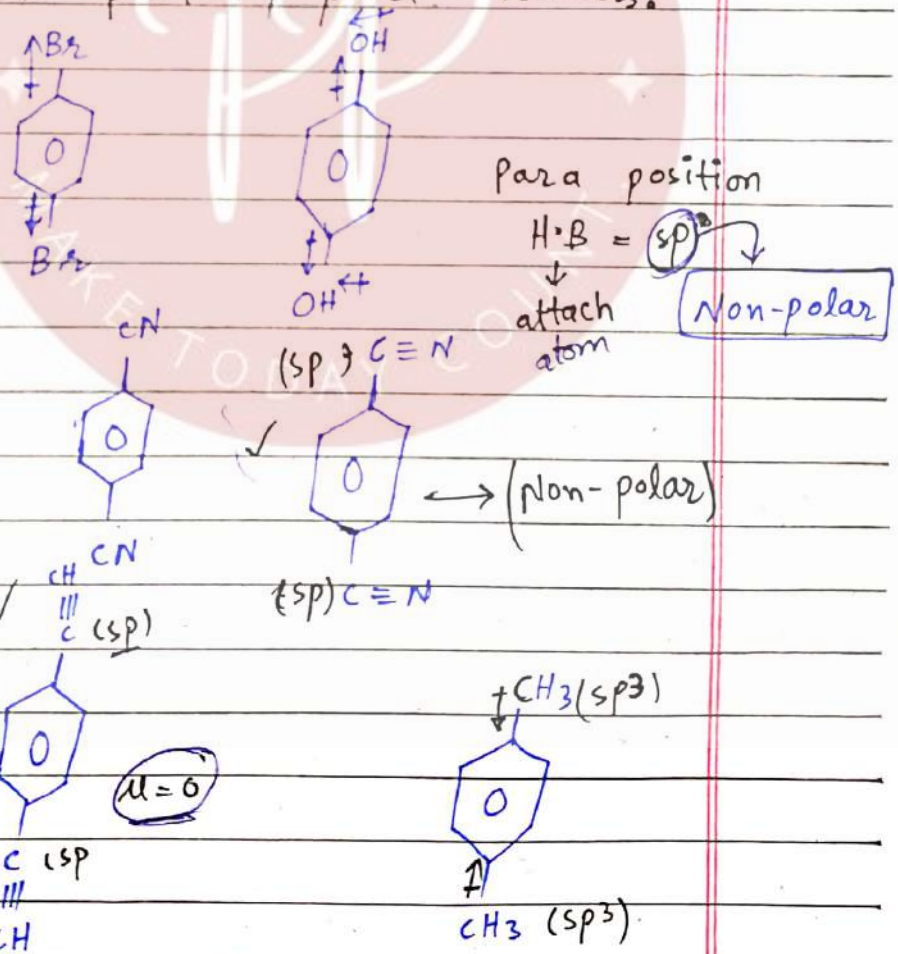
Planner Ring

$\mu \propto \frac{1}{B.A}$ → external

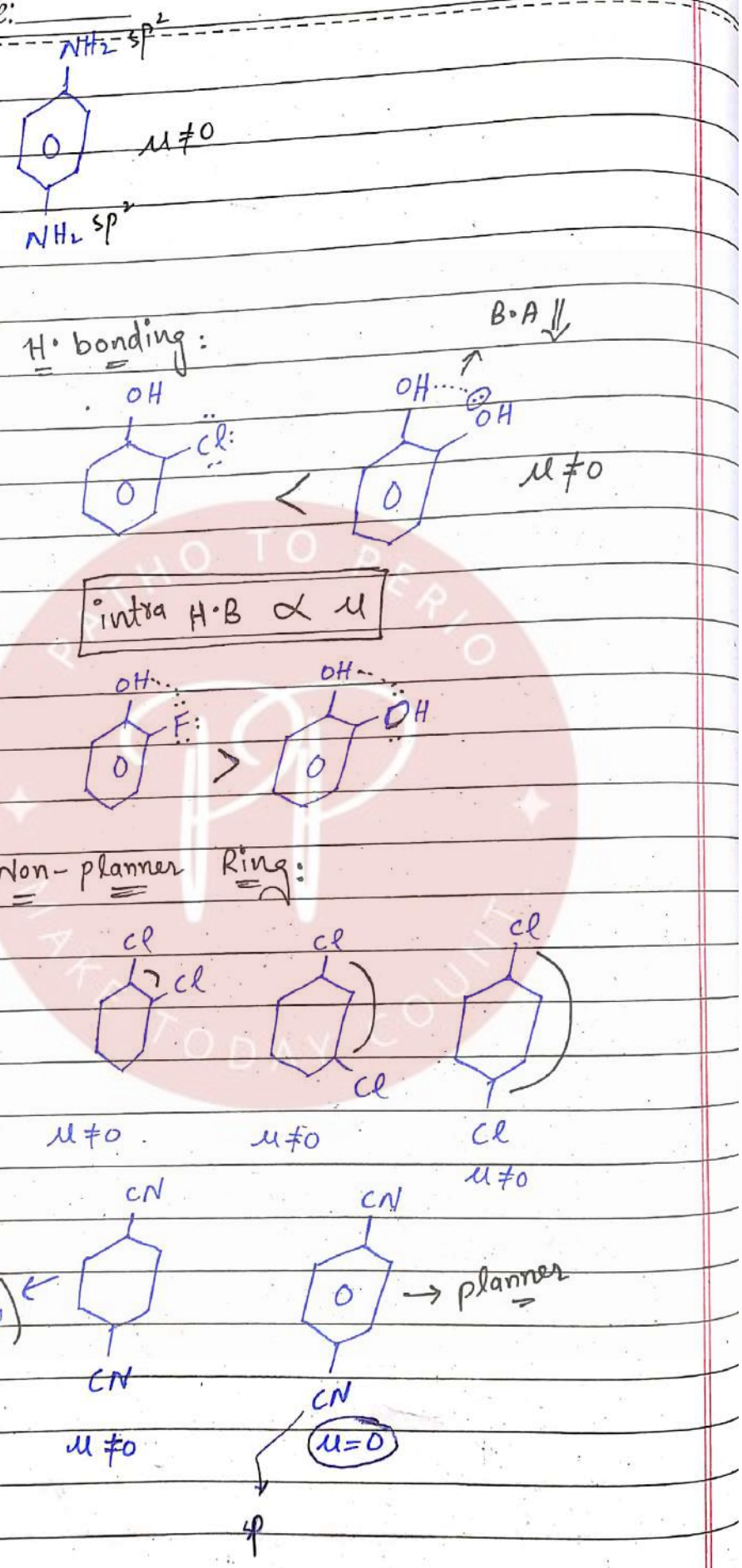




Para position / para isomers:



Date:

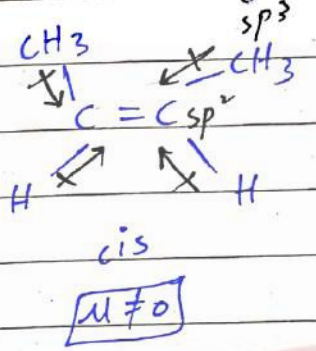


same groups at one side.

Date: M T W T F S

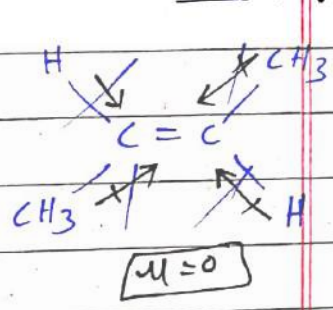
Cis & **Trans:**

* when two types of atoms/group:



cis

$\mu \neq 0$

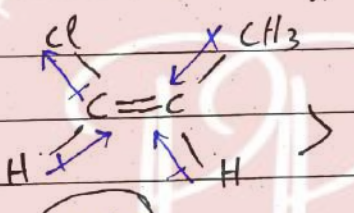


$\mu = 0$

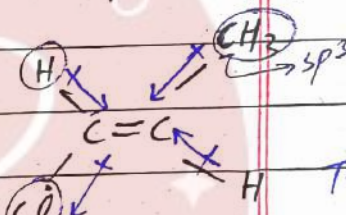
cis = polar

trans = Non-polar

* when three types of atoms/group.



Cis $\mu \neq 0$ more polar



Trans $\mu \neq 0$ polar

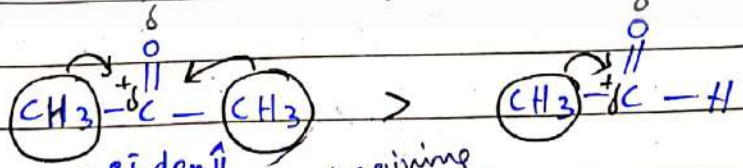
* es donating & es with drawing group.

$\mu \propto r$

es donating group

E·Den ↑ r ↑ μ ↑

E·Dens ↓ r ↓ μ ↓



Start repulsion ← es·den ↑ for gaining

B·length ↑ ↘ stability

r = ↑↑ for

Date: M T W T F S

$\mu \propto$ E·D·G $\propto$ No. E·D·G $\propto$ strength $\propto \frac{1}{\text{dist}}$

$C_2H_5-\overset{O}{\overset{\|}{C}}-C_2H_5 > C_2H_5-\overset{O}{\overset{\|}{C}}-CH_3 > CH_3-\overset{O}{\overset{\|}{C}}-CH_3$

(4) (3) (2)

$Cl-\overset{O}{\overset{\|}{C}}-H > Cl-\overset{O}{\overset{\|}{C}}-Cl$

more polar

es den ⇓

To attain stab B·L ⇓

γ ⇓

$\mu \propto \frac{1}{\text{E·D·G}} \propto \frac{1}{\text{strength}} \propto \frac{1}{\text{No}} \propto \frac{1}{\alpha}$ distance

$Cl-\overset{O}{\overset{\|}{C}}-H < Br-\overset{O}{\overset{\|}{C}}-H$

Br ⇓ streng ⇓ B·L ⇑ γ ⇑

$Cl-CH_2-\overset{O}{\overset{\|}{C}}-H < CH_2(Cl)-CH_2-\overset{O}{\overset{\|}{C}}-H$

2 gps. (2) gps. μ = more

$\mu \propto$ distance of with E·D·G

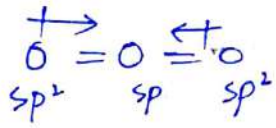
(#) Resonance

Nature of Bond:

=> Bond polar → Molecule polar

→ Molecule Non-polar (PCl_5 → (E-N diff present))

=> Bond Non-polar → Molecule Non-polar (Cl_2) (O=O)



Date: M T W T F S

Resonance:

Resonating + Non-Resonating

$CH_2 = CH - \ddot{N}H_2$ < $CH_3 - CH_2 - \ddot{N}H_2$

partial bond — single bond

$\mu \alpha R$

B.L α → ⋯ > = > ≡ $\alpha \mu$

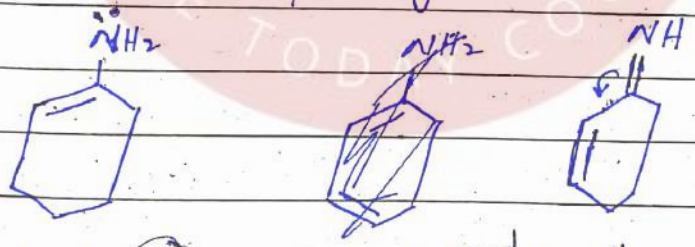
$\mu \propto \frac{1}{R.S}$

Two R. structures

⊛ Single bond → Resonance → ↓ B.L ↓

↓ μ = ↓

C – N bond polarity

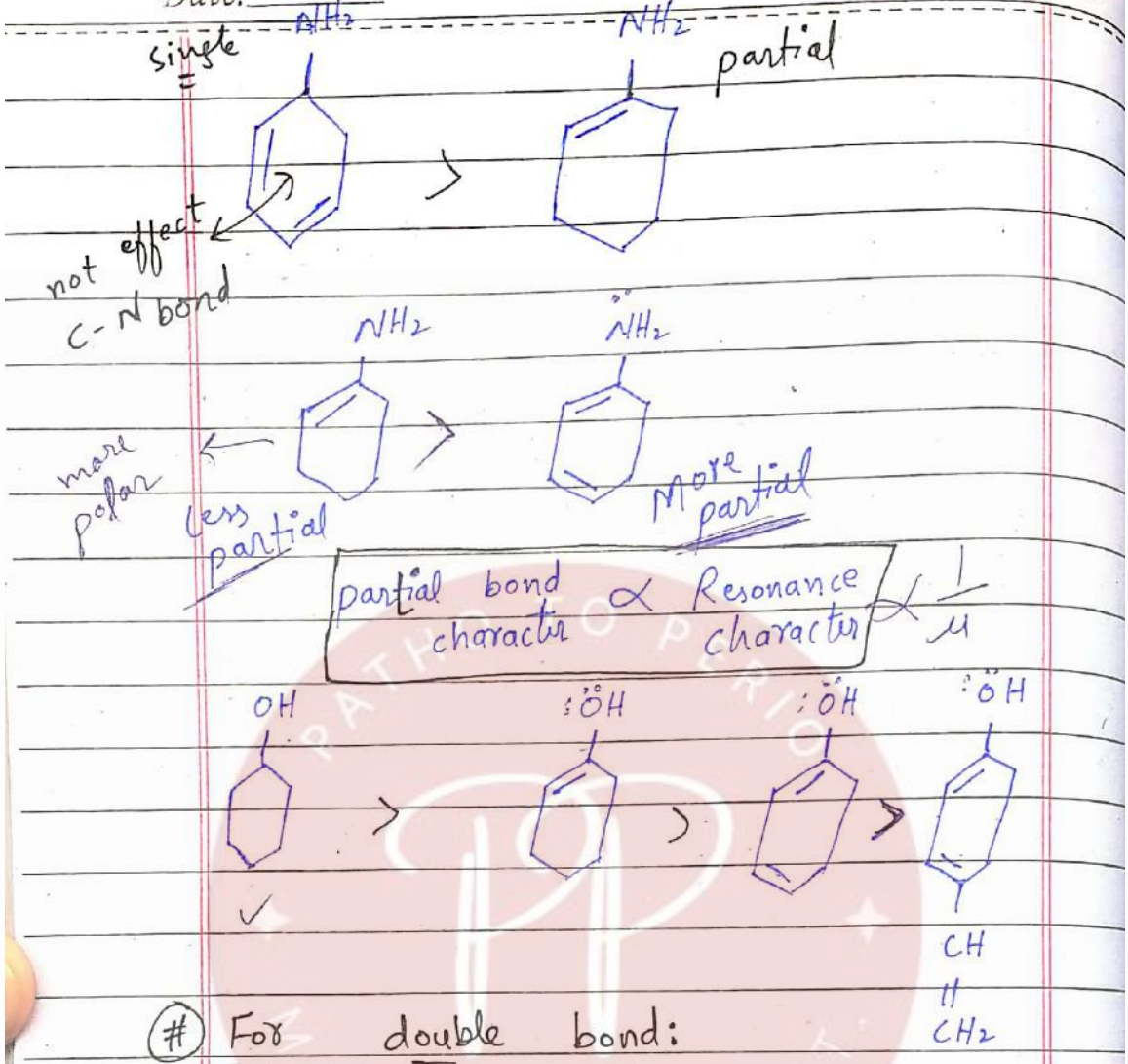


Single ↑ → convert to partial ↓

Double bond = ↓

partial = ↑

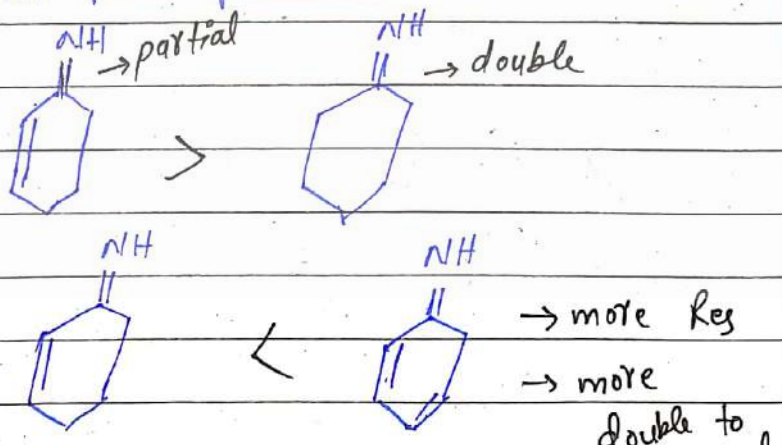
Date:



(#) For double bond:

d. bond → Resonance → convert to partial

C-N polarity



Date: M T W T F S

μ(single) $\propto$ 1/Resonance $\propto$ 1/partial bond

μ(double) $\propto$ Resonance $\propto$ partial bond.

Resonance occur due to which change is produced.

↑

HydroCarbon

$CH_2 = CH - CH = CH_2$ $\mu \neq 0$ ↓ polarity produced. $\mu \propto q$

$CH_3 - CH_2 - CH_2 - CH_3$ $\mu = 0$

less polar ②

$CH_2 = CH - CH = CH_2$

① more polar

$CH_2 = CH - CH = CH - CH = CH_2$

non-polar ③

$CH_2 = CH - CH_2 - CH_2 - CH_3$

$\mu \propto$ Resonance ✓

$CH_2 = CH - CH_2 - CH = CH_2$ No Reson

$CH_2 = CH - CH = CH - CH_3$ (Resonance)

Date:

M T W T F

* Alkyne:
  - Linear molecule ✓
  - slightly polar ✓

$H - C \equiv C - H \quad \mu = 0$

$CH_3 - C \equiv C - CH_3 \quad \mu = 0$

$CH_3 - C \equiv C - H \quad \boxed{\mu \neq 0}$

$CH_3 - C \equiv C - C_2H_5 \quad \boxed{\mu \neq 0}$

* Ionic character:

present in covalent compound.

$H \overset{\delta^+}{\cdots\cdots} F \overset{\delta^-}{}$

$\boxed{I.C \propto \Delta E.N}$

* $I.C \propto$ Bond strength
* $I.C \propto$ Bond energy
* $I.C \propto \frac{1}{B.L}$
* $I.C \propto$ stability
* $I.C \propto \frac{1}{\text{reactivity}}$
* $I.C \propto \frac{1}{\text{covalent character}}$

Date: M T W T F S

% age ionic character: electric condenser

$$\%\text{ age I.C} = \frac{\mu_{obse}/\mu_{exp} \times 100}{\mu_{ionic}/\mu_{theo}}$$

μ_{ionic} →

consider C.B. 100% ionic

$H^{+\delta}F^{-\delta} \longrightarrow H^{+}F^{-1}$

* μ_{ionic} (100%) = μ_{exp} (100%) → for I.C = possible (I.B present)
* μ_{ionic} (100%) > μ_{exp} (<70%) = possible (ionic = above 50%, covalent = below 50%)
* $\mu_{ionic} < \mu_{exp}$ => Not possible

on Basis of E.N & % age I.C

ΔE.N → 0 ↔ 0.4 (covalent) (non-polar)

ΔE.N → 0.4 ↔ 1.7 (covalent) (polar)

Al_2Cl_6

ΔE.N = 1.7 → covalent (50%) + ionic (50%)

ΔE.N > 1.7 → ionic

* % I.C < 50% = C.B
* " " = 50% = C.B + I.B
* " " > 50% = ionic bond.

Date:

M T W T F S

MOT

e⁻ (as wave)

(#) Based on Quantum Mechanics

Concept:

explain

* magnetic behavior
* Feasibility of Molecule
* Stability of Molecule
* Bond strength
* Bond order

Postulate:

(1) Atomic orbital combine → Molecular orbital

combine → Molecule

(2) Atomic orbital will lose identity ($\pi, \pi^*, \delta, \delta^*$)

No concept of s,p,d,f

(3) Max e⁻ in MO = 2

(4) Min e⁻ in MO = 0

(5) M.O orbital is delocalized

⇓

spread on more than one nuclei

Atomic orbital

↓

(localized)

Date: M T W T F S

M.O ⟶ polycentric

* probability of es around many Nuclei → Molecular orbital.

* " " " " around one Nuclei → A.orbital

* No # M.orbital = No # atomic orbital.

* All es take part in bonding.

No # M.orbital in CO:

C ⟶ $1s^2, 2s^2, 2p^2$

O ⟶ $1s^2, 2s^2, 2p^4$

5 + 5 = (10)

N_2^{+2}

N = 7 ⟶ $1s^2, 2s^2, 2p^3$

N = 7 ⟶ $1s^2, 2s^2, 2p^3$

5 + 5 = (10)

Those atomic orbital form Molecular orbital having

* Same shape ✓

Same symmetry ✓

Same or nearly same energy except 1s.

Date: M T W T F S

(x-plane) symmetry different (y-plane)

$n \propto E$

2px - 2py ✗

E=same shape=same

2px - 2s ✓

1s - 5px (weak bond)

Homo (bond only weak)

2px - 2s

2py - 2py

x-plane

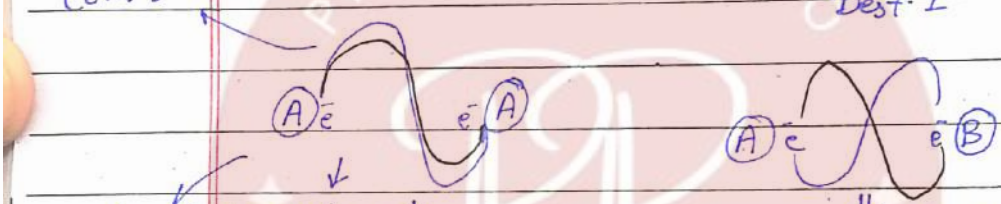
Types of M.O

1. * BMO
2. * ABMO
3. * NBMO

e⁻s → wave → const. In / destr. In

Cons. I

Dest. I



Bond ⇑

Support each other

(BMO)

cancel each other

(ABMO)

* Form at Constructive interfe

* Form at destruct

* attractive force

* Support bond

* Repulsive forces.

* oppose bond.

show probability of e⁻s

$\psi = \Sigma ie$

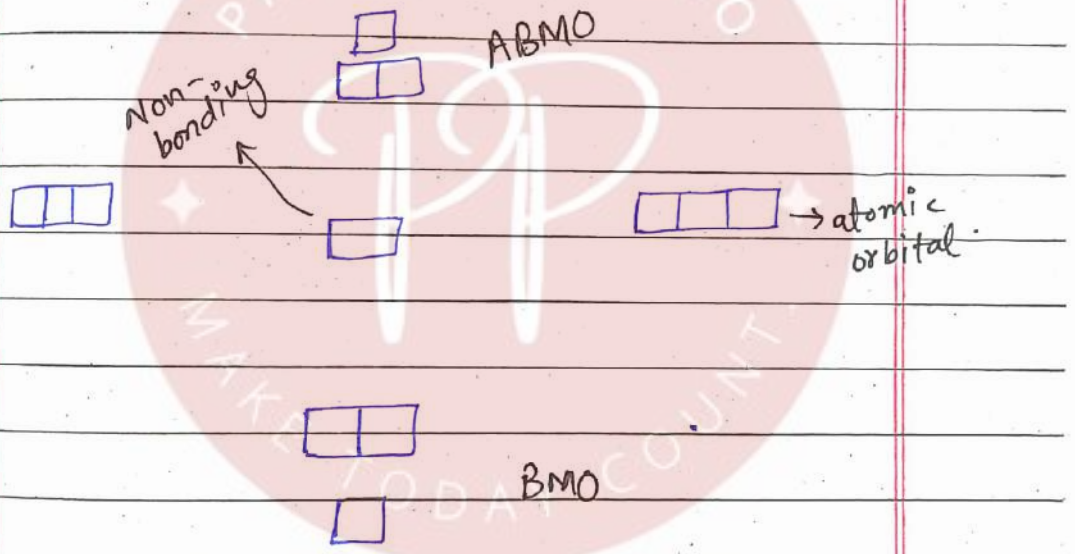
$\psi_{ABMO} = \psi_A + \psi_B$

$\psi_{ABMO} = \psi_A - \psi_B$

Date: M T W T F S

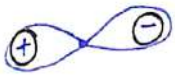
BMO	ABMO
* Low energy ✓	✓ * High energy.
* May or may not have node	* always have node
* Stable ✓✓	* unstable. ✓
* HOMO ↓ Highest occupy Molecular orbital	* LOMO * Lowest occupy Molecular orbital.

Energy order

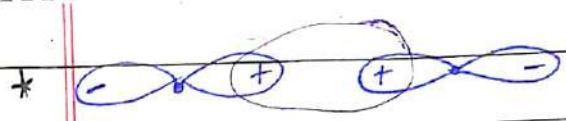


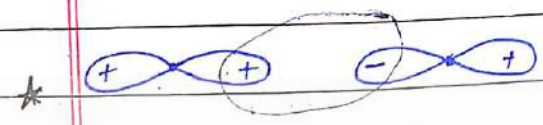
ABMO > NBMO = Atomic orbital > BMO

* Lobes = Same sign	* Lobes = opposite sign.



Date: _____ M T W T F S

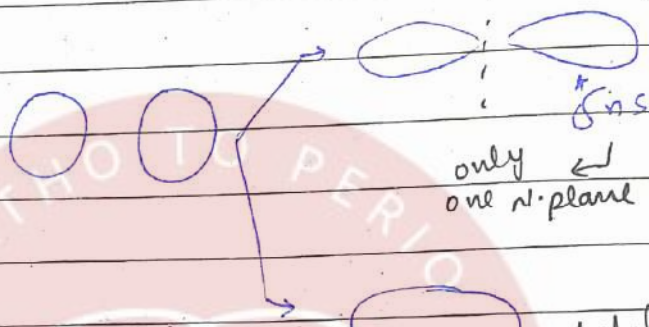




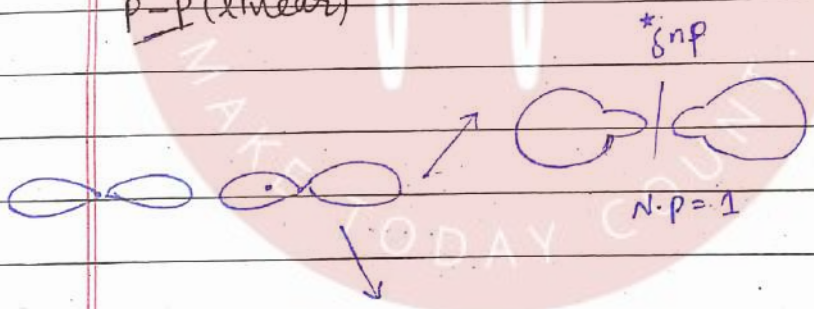
Types of overlapping in M.orbital

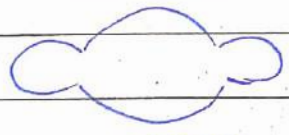
node / Nodal plane

S-S:



P-P (linear)





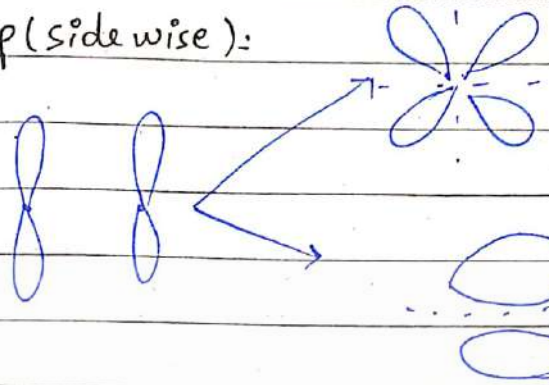
N.P = 0

δnp = 0 N.P

Date: M T W T F S

π^*np

p- p (side wise):



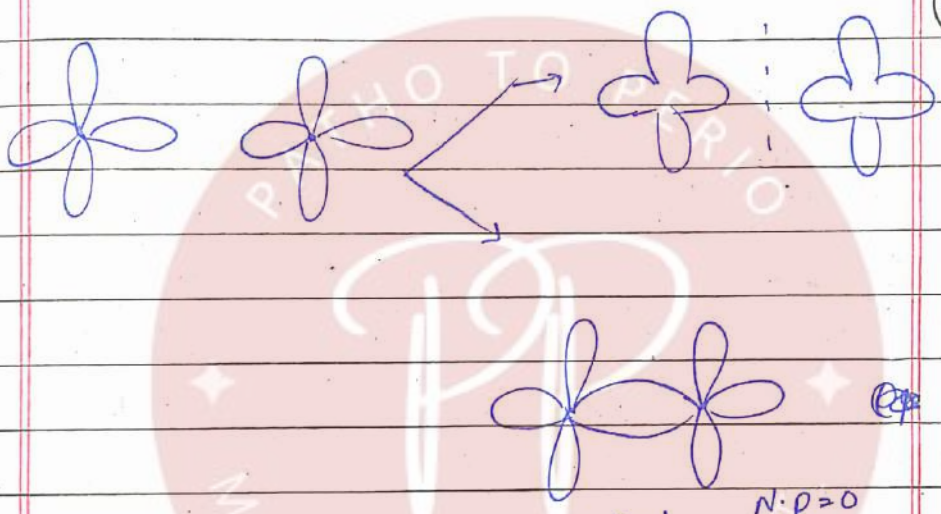
N·p = 2

N·p = 1

πnp (BMO)

d- orbital:

n·d = 1



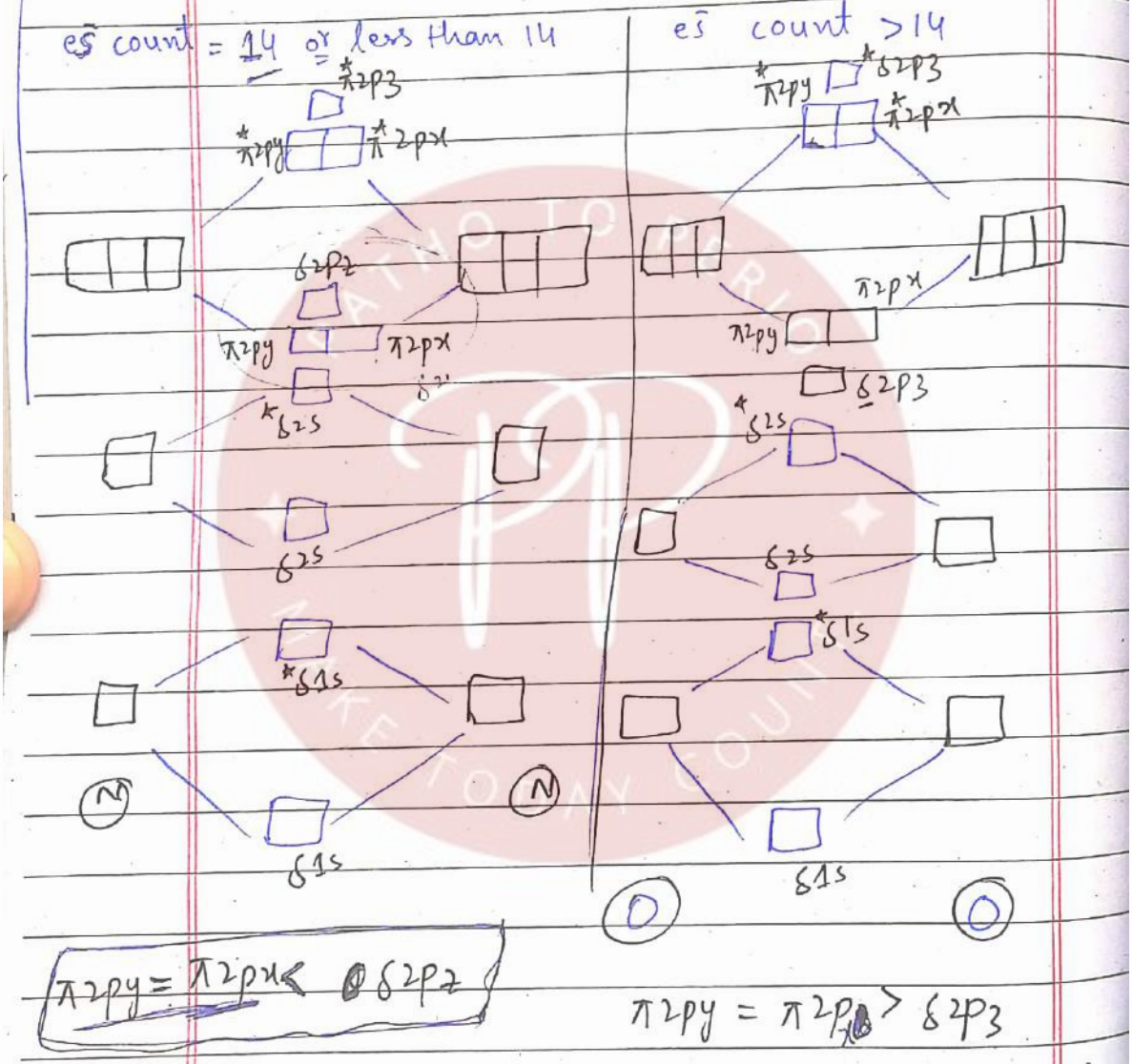
σ^*nd N·p = 0

Date: M T W T F S

Energy level diagram

* Homoatomic molecule
* overlapping: Same energy orbital.
* Symmetrical energy level diagram.

energy



π2py = π2pz < δ2p2

π2py = π2pz > δ2p3

Bp δ2pz < π2py = π2p3

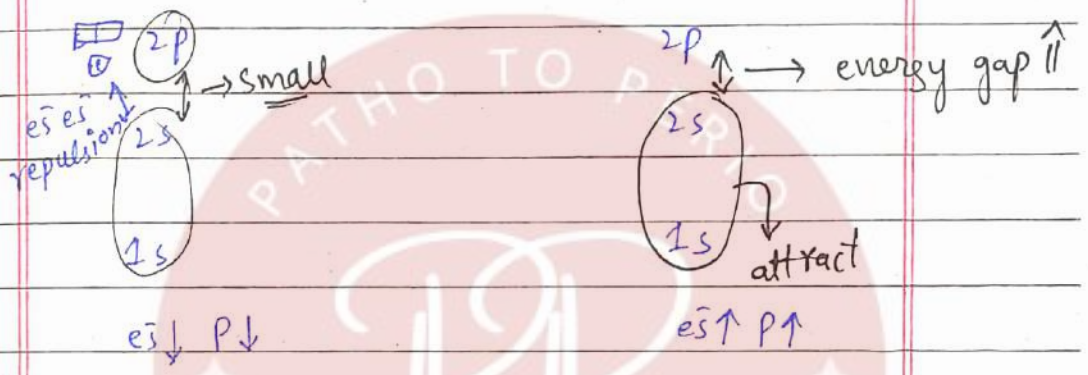
Date: M T W T F S

$e\bar{s} = 14 < 14$ ✓ | $e\bar{s}$ count > 14

Energy of $\delta > \pi$ ↕ orbital intermixing $\pi > \delta$ | energy of $\pi > \delta$ | $\delta > \pi$

Stable = bond strong

when $e\bar{s} < 14$ | $e\bar{s} > 14$.



Q#

$e\bar{s} = 15$

Which one is true for N_2^{-1}?

(*) $\pi 2px = \pi 2py > \delta 2p3$ X

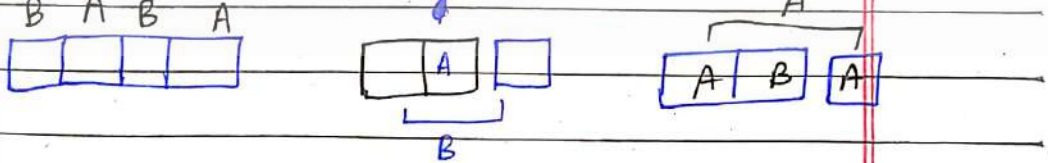
(a) ✓ $\pi 2px = \pi 2py < \delta 2p3$

$e\bar{s}$ should be counted in Neutral form

count not Neutral

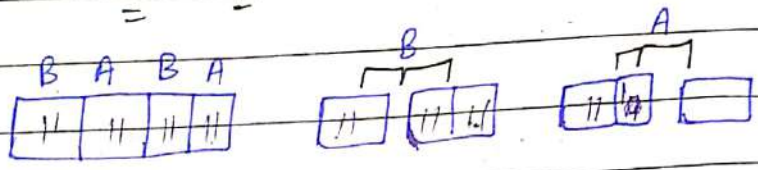
$N_2 = 14$

(*) $e\bar{s}$ count = 14 or less than 14



Date: M T W T F S

e⁻ count = 14 :

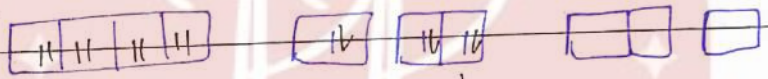


Q# How many e⁻ are present in BMO of F_2^{-1}?

* e⁻ in BMO = 10
* " " ABMO = 04

* How many e⁻ are present in degenerate orbitals of O_2^{+2}?

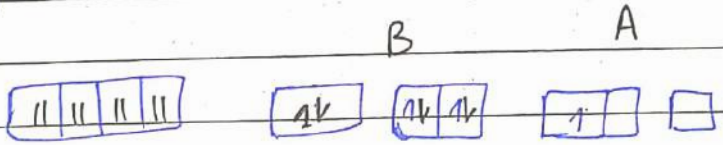
O = 16
O^{+2} = 14



These are degenerate orbitals.

* e⁻ in d.O = 4

Q# How many unpaired e⁻ are present in O_2^{+1}?



1 unpaired e⁻
⇓
present in ABMO

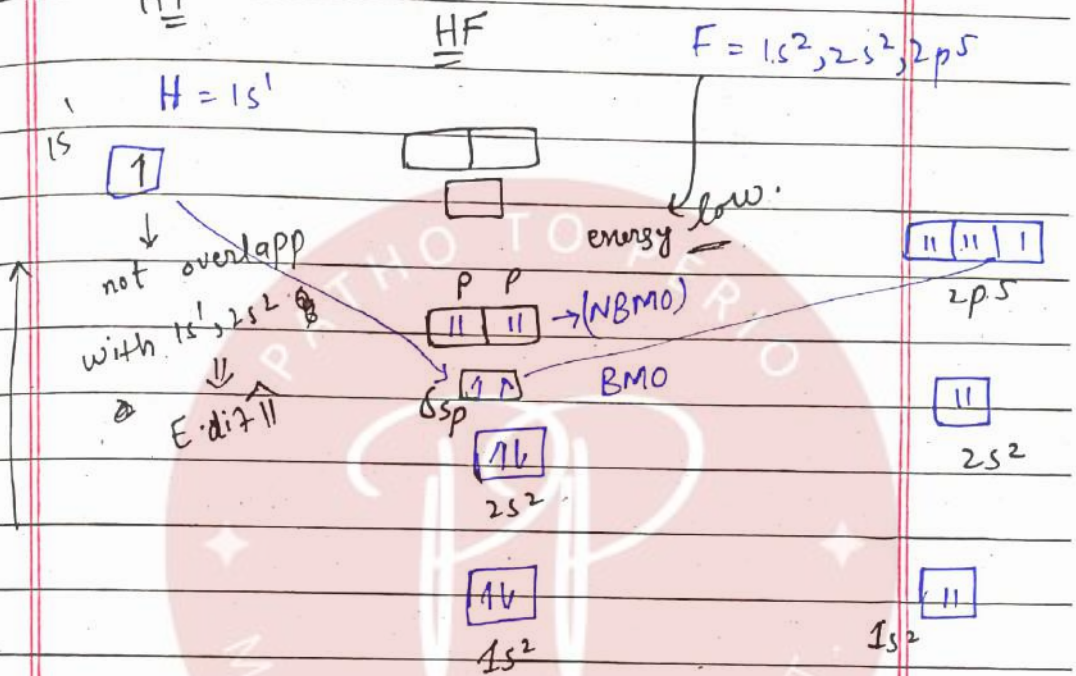
Date: M T W T F S

Energy level diagram

↳ For heteroatomic unsymmetric

* More E.N atom orbital energy low.

HF



Bond order

* No. bonds formed b/w two atoms.

* B.O = 1 → 1 bond.

* B.O = 2 → 2 bonds.

* B.O = fraction → partial bond → (Resonance occur)

* B.O = 0 → No bond

* B.O = -ve → Not possible

Date:

M T W T F S

⊛ Possibility:

BMO $e\bar{s}$ = $e\bar{s}$ ABMO → No bond.

$e\bar{s}$ BMO $e\bar{s}$ > $e\bar{s}$ ^{B}AMO → bond form.

$e\bar{s}$ BMO $e\bar{s}$ < $e\bar{s}$ ABMO → Not possible.

Stability ∝ $e\bar{s}$ in BMO

Stability ∝ $\frac{1}{e\bar{s} \text{ in ABMO}}$

Factors:

B.O ∝ stability

B.O ∝ B.E

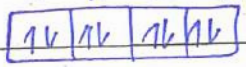
B.O ∝ $\frac{1}{\text{B.L}}$

B.O ∝ $\frac{1}{\text{reactivity}}$

Calculation:

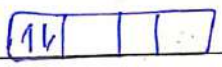
① up to 8 $e\bar{s}$:

B A B A



$$B.O = \frac{BMO_{e\bar{s}} - ABMO_{e\bar{s}}}{2}$$

H_2



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

Date: M T W T F S

+ e⁻ removal from BMO → weak bond

e⁻ removal from ABMO → break bond

* H_2^{+1}

B A

↑ | | |

$\frac{1}{2} = 0.5$

* H_2^{-1}

B A

↑↓ | ↑ | | |

$\frac{2-1}{2} = 0.5$

Stability:

$H_2 > H_2^{+1} > H_2^{-1}$

Bond length:

$H_2 > H_2^{+1} = H_2^{-1}$

Be_2

↑↓ | ↑↓ | ↑↓ | ↑↓

B.O = 0

* e⁻ 9 - 20

B.O = 3 - 0.5(x)

x = A number which is greater or less than (14) any sig

O_2:

O_2 = 16 e⁻ ← (2) 14

B.O = 3 - 0.5(2)

3 - 1 = (2)

O_2^{+2}:

e⁻ = 14

3 - 0.5(0)

= (3)

Date:

O_2^{+1}: $e\bar{s} = 15$

B.O = 3 - 0.5(1)

= 2.5

O_2^{-1}:

= $e\bar{s} = 17$

B.O = 3 - 0.5(3)

= 1.5

O_2^{-2}:

= $e\bar{s} = 18$

B.O = 3 - 0.5(4)

B.O = 1

$3-2$

1

Stability:

$O_2^{+2} > O_2^{+1} > O_2 > O_2^{-1} > O_2^{-2}$

For Hetero:

CO: $e\bar{s} = 14$

3 - 0.5(0)

CO = 3 B.O

NO: $e\bar{s} =$ ~~14~~ 15

= 3 - 0.5(1)

= 2.5

NO^+:

B.O = 3

(*) one e⁻ can change B·O by 0·5:

Date: M T W T F S

NO^{+2}:

B·O = 2·5

NO^{-1}:

B·O = 2

NO^{-2}:

B·O = 1·5

stability:

$NO^{+1} > NO > NO^{+2} > NO^{-1} > NO^{-2}$

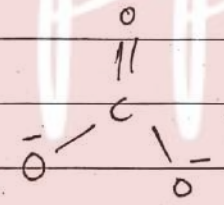
Stabi when B·O same

Neutral > +ve > -ve

(#) Poly atomic Molecule

$$B{\cdot}O = 1 + \frac{No.\ \pi\ bond}{No.\ \delta\text{-}bond}$$

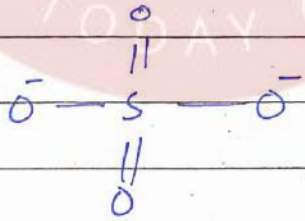
* CO_3^{-2}:



B·O = $1 + \left(\frac{1}{3}\right)$

B·O = 1·33

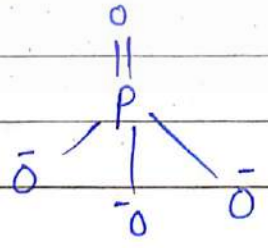
* SO_4^{-2}



B·O = $1 + \frac{2}{4}$

= 1 + 0·5 = 1·5

* PO_4^{-3}



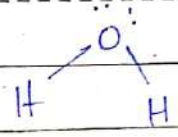
B·O = $1 + \frac{1}{4}$

1 + 0·25

= 1·25

Date: _____ M T W T F S

H_2O:



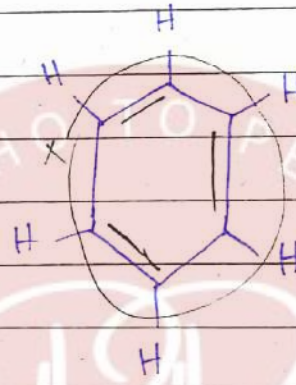
$B.O = \frac{1+0}{2} = 1$

CO_2:

$O = C = O$

$B.O = \frac{1+2}{2}$ $1+1 = 2$

Benzene:



$B.O = \frac{1+3}{6}$

$B.O = 1.5$

$3 - 0.5(x)$

$\frac{BMO - ABMO}{2}$

$1 + \frac{no\ \pi\ Bond}{no\ \sigma\ bond}$

Date: New lec M T W T F S

* e^- count → even → Diamagnetic

* e^- count → odd / 10, 16 → paramagnetic

=> N_2 → $e^- = 14$ (Dia)

=> CO → $e^- = 14$ (Dia)

=> B_2 → $e^- = 10$ (Para)

=> O_2 → $e^- = 16$ (para)

=> NO^{+1} → $e^- = 14$ (Dia)

=> NO_2^{+1} → $e^- = 13$ (para)

NO
7 (15) (14)