Chapter:

Mass Spectrometry

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Chemistry with MJS

Chemistry Preparation by MJS

(MASS-SPECTROMETRY) - (M. Junaid SAHOO)

Mass Spectrometery → Quaulative & Semi-Quantitative technique.

Q = Why called mass spectrometery?

✓ Basic principle:

Electron beam is bombarded to molecule. ~~ionization~~ energy of electron beam should greater than the ionization energy of molecule. Thus electron is dislodge from the molecule and Molecular cation is formed. ($M^{\cdot+}$)

$$M + \bar{e} \longrightarrow M^{\cdot+} + 2\bar{e}$$

10ev Required. 70ev

The Further E → used for fragmentation of Molecular ions & used in K.E to accelarate

$M^{\cdot+}$ → cations & Radicals are formed.

★ Generally Singly charged cations are produced

m/z = Mass ⇒ bic $m/_{1Z} = m$

★ Some time $\bar{e}$ beam is captured → thus anions are produced (Less common phenomena)

↓ Molecular Anions

↳ Less common used Mode.

★ Some times Doubly charged cations ✓ produced.

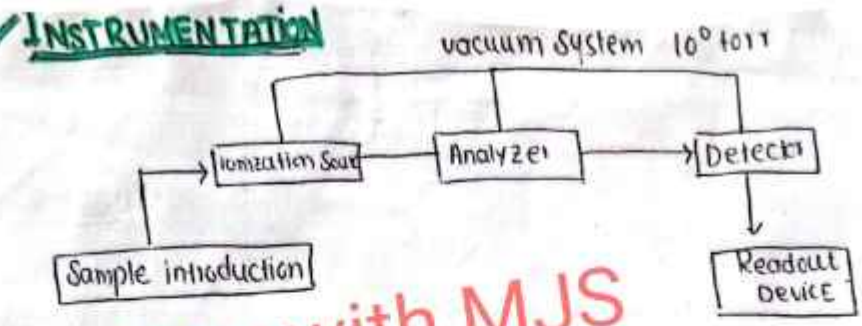
$M =$ $m/z \Rightarrow \frac{m}{2z}$ = Half m/z value.

e.g $m = 90 \Rightarrow m/z \Rightarrow 45$

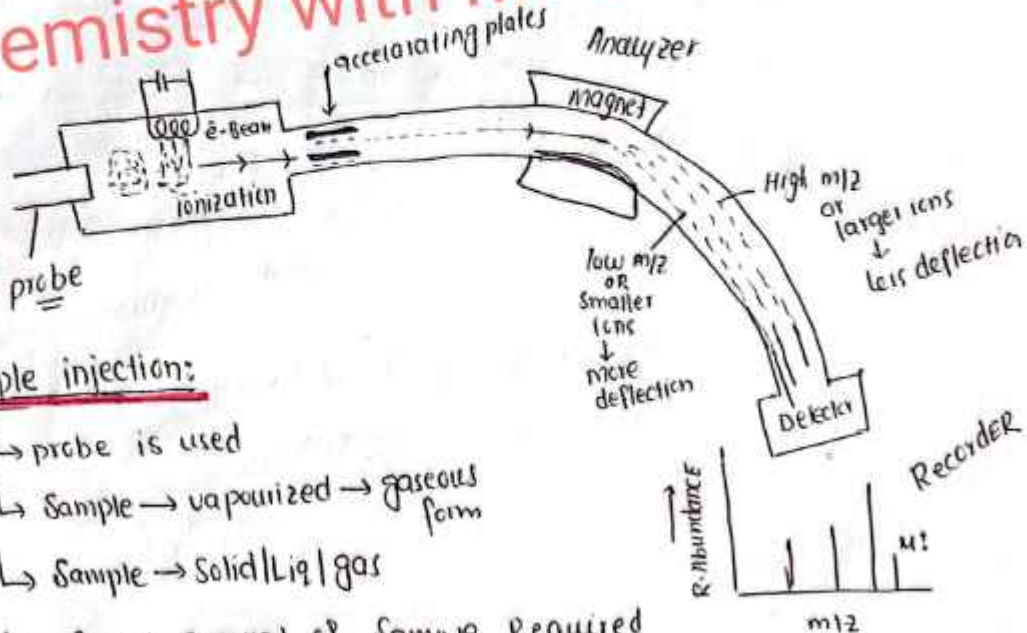
✓ These ions are separated by the Analzer & then detected by the detector

= **No. of ions ∝ current**

✔ INSTRUMENTATION



Components:



① Sample injection:

- ↳ probe is used
- ↳ Sample → vapourized → gaseous form
- ↳ Sample → Solid | Liq | gas
- ↳ Small Amount of Sample Reauired
  - $10^{-3} - 10^{-9}$ g (mg to ng)
  - ↳ v. Low (LOD)
  - ↳ Sensitive technique

② Ionization chamber → ionization occured → $M^{\pm}$ formed & Fragmentation → Daughter ions formed

↳ e-beams are bombarded

Methods:

- → ★ Electron impact (EI) (Hard ionization) → Most useful Method (70 eV) → E
- Soft:
  - → ★ Chemical ionization (CI)
  - → ★ Fast Atom bombardment (FAB)
  - → ★ plasma discharge
  - → ★ Field ionization
  - → ★ Laser ionization
    - ★ ESI (soft ionization)
    - ★ MALDI → soft ionization ↓ No Fragm ↓ For Bigger molecules ↓ protein
    - ★ LDI
      - ↳ Hard (Frag)
      - ↳ smaller molecules e.g. lipids & peptid

★ For ionization → 10 eV

★ Extra → used for Fragmentation & K.E

(Ionization Modes) → two modes

- +vely → M. cations formed → 90% useful & Easy way
- −vely → 10% (less common used) → molecular anions / Radical anions formed

3

$M + \bar{e} \longrightarrow M^{+\cdot} + 2\bar{e}$ (Radical cation)
↓ dislodged

$M + \bar{e} \longrightarrow M^{-\cdot}$ Radical anion)
↓
captured

@ low pressure ~10^{-6} torr kept ?
↓ B/c it minimize the chances of collision b/w ionized & unionized molecules.

③ Accelarating plates:

↳ -vely charged → depends upon the production of Molecular ions either cations or anions.
↳ These only attract the +vely charged.
↳ speed up.

④ ANALYZER:

↳ to separate the ions on the basis of m/z

- magnetic Analyzer → most commonly used.

modern ⇒ • Quadrapole, TOF, ion trap, FTICR
↓ Fourier transform ion cyclotron Resonance.

*Also evacuated → 10^{-7} torr

⇒ Magnetic Analyzer:

↳ Most commonly used.
↳ curved Metallic tube b/w poles of magnet.

$$m/z = \frac{H^2 r^2}{2E}$$

H → strength of M.F
r → Radius of curvature
E → Applied voltage (500–2000 V)

⇒ $m/z \propto r^2$

* larger ions ⇒ m/z ↑ ⇒ Follow a larger path ⇒ less deflection ⇓ Reach to detector later ↓ So Later Signal

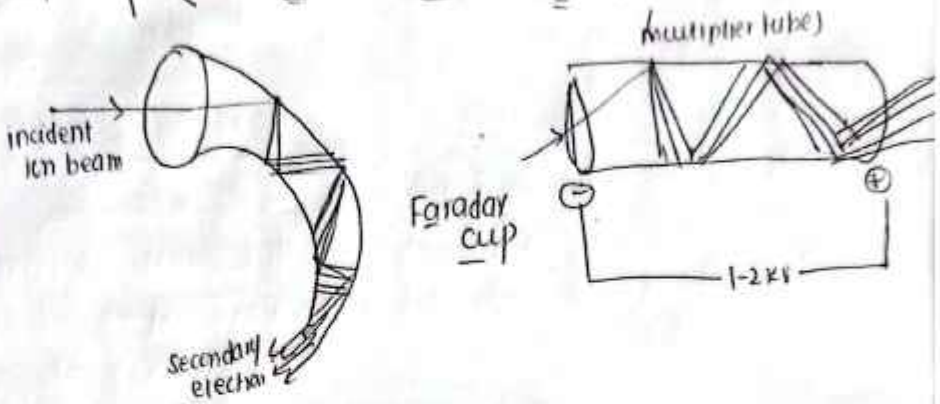
* Smaller ions ⇒ m/z ↓ ⇒ curvature ↓ more deflection ↓ 1st Signal.

* Efficiency of MS → measured from the ability of its analyzer to resolve (separate) the ions have closed m/z value.

⑤ ION collectors (Detectors)

↳ The most commonly used detector is

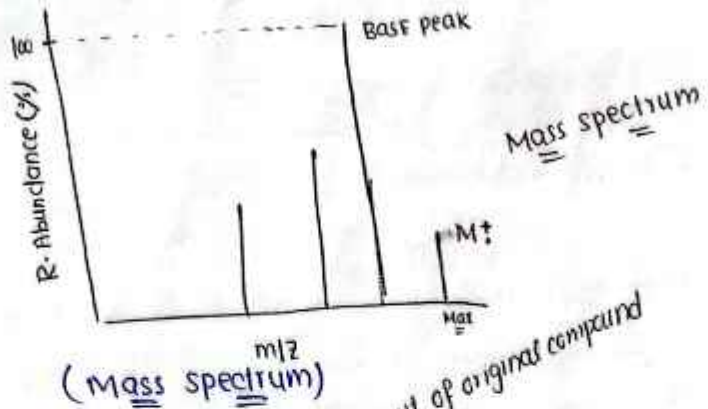
Faraday cup (electron multiplier tube)



Detector Signal ∝ no. of hitting ions

* By varying the M.F → ions of all masses are collected & counted.
* ionic current of even 10^{-15} A can be detected by Faraday Cup

⑥ Recorder: | Read out device



peaks

* Molecular ion peak (M^+) → M. wt of original compound → Also called parent ion peak
* Fragment ions peak (Daughter ions peaks)
  ↳ Reconstruct the molecular structure.
* Base peak (100% R.A) → most intense → show the stable cation
* Isotope peaks: → with Molecular ion peak one or two small peaks at one or two mass units higher than M. ion peak
  ↳ Arises due to their isotopes

Metal ion Metastable peak:

↳ occasionally low intensity broad peaks at non-integral m/z value.

↳ This happened when a metastable ion of mass m_1 undergo fragmentation after acceleration But Before entering the M.F to mass m_2 ↓ will This have lower K.E

⇒ It gives valueable information about the Mode of Fragmention.

Example; Toulene  show strong peaks at m/z = 91 & 65 → m_2 ↓ m_1

↓ Also shows broad peak of metastable ion.

$$m^* = \frac{(m_2)^2}{m_1} = (65)^2/91 = 46.4$$ non integral

Broad less intense peak.

⇒ INFORMATIONS BY MASS SPECTRUM:-

Following information/ Application,

✓ ① Determination of Molecular weight

✓ ② Determination of Molecular Formula → By M.wt, By isotopic peaks

✓ ③ Determination of structure.

⇒ 1) Determination of Molecular weight:

* Molecular ion peak → gives the information of M.wt of compound (↓ m/z)

* Sometime molecular ion peak is not Recognized due to isotopic peaks or unstability of Molecular cation- Then best way is (Nitrogen Rule)

✓ Nitrogen Rule:

① * If molecule contain odd No. of N (N atoms) → M.wt will be odd

If molecule contain No Nitrogen or even No. of Nitroger

⇓

Then M.wt even

OR

② * If Molecular weight odd → Fragments mass No → even (All)

* If Molecular weight even → All Fragments mass No → odds.

Example: ① CH_3 (15) CH_2 (14) NO_2 (46) m/z M.wt = 75 odd

Fragments 60, 46, 14 etc

② CH_3 (29) CH_2 (15) CH_3 M.wt = 44

2) Determination of Molecular Formula:

- Isotopic peaks
- * Molecular weight
  - Actual Atomic Masses → Determine
  - Gives the Molecular Formula
  - ↓ BIC Actual → not integers
- DBE
- C-13 Rule

$C_2H_6 \rightarrow 30$	CH_2O (30)
$2C \rightarrow 24.0000$	$C \rightarrow 12.00000$
$6H \rightarrow 6.04695$	$2H \rightarrow 2.01565$
$C_2H_6 = 30.04695$	$O \rightarrow 15.99492$
	$CH_2O = 30.01057$

* C-13 Rule is used to guess the Molecular Formula

✓ C-13 Rule:

Example: M.wt = (121) → odd Mass → odd No. of Nitrogen

$\frac{121}{13} = 9$

$C_9H_{9+4} = C_9H_{13}$

$\downarrow -CH_2$

$C_8H_{11}N$

$\downarrow -CH_4$

$\rightarrow C_7H_7NO$ (Molecular Formula)

∴ N → CH_2 Remove

∴ O → CH_4 Remove

O

||

C-NH_2

⇒ DBE (Double bond Equivalent)

$$DBE = C - \frac{H+X}{2} + \frac{N}{2} + 1$$

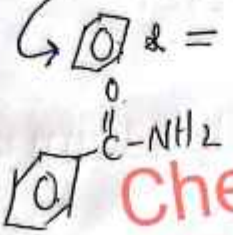
Example 121

C_7H_7ON

$$D.B.E = \frac{7}{1} - \frac{7}{2} + \frac{1}{2} + \frac{1}{1}$$

$$D.B.E = \frac{14 - 7 + 1 + 2}{2}$$

$D.B.E = 10/2 = 5$ →



* DBE ⇒ 1 ⇒ =, Ring
* DBE ⇒ 2 ⇒ 2 =, ≡, 2 Ring
* DBE = 3 ⇒ 2 D.B & 1 Ring
  OR
  ≡ & = or Three D.B
  OR
  3 Ring & =
* DBE ⇒ 4 Benzene Ring

⇒ Isotopic peaks

* to measure the Relative intensities of the isotope peaks

~~Example~~

3) Determination of Molecular structure:

* Molecular weight m/z of molecular ion peak
* Fragmentation peak
* Base peak
* To confirm the structure
  * apply C-13 Rule
  * N-Rule
  * DBE

* ——— *

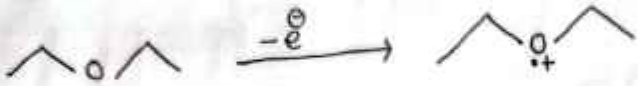
FRAGMENTATIONS

Ease of removal of $\bar{e}$

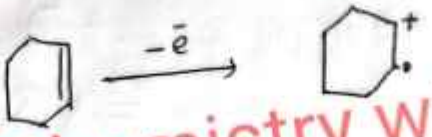
&

non-B-$\bar{e}$ > π-$\bar{e}$ > σ-$\bar{e}$

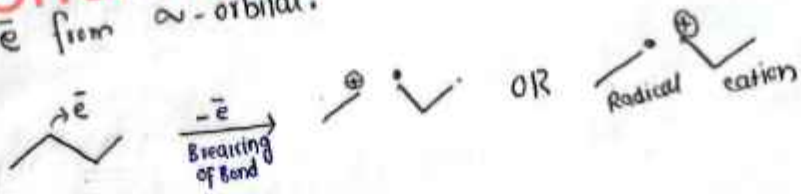
* Loss of $\bar{e}$ from non-bonding orbital



* loss of $\bar{e}$ from π-orbital:



* loss of $\bar{e}$ from σ-orbital:



Fragmentation process

① Stevenson's Rule | simple cleavage

→ Most probable fragmentation → cations form → with lowest i.E → Mean stable cation

stability order

$H_3C^{\oplus} < RCH_2^{\oplus} < R_2CH^{\oplus} < R_3C^{\oplus} < CH_2=CH-CH_2^{\oplus}$ Allylic cation

$< CH\equiv C-CH_2^{\oplus} < C_6H_5CH_2^{\oplus}$

propargyl

② α- cleavage: (More E·N or Heteroatom Attached to C)

↳ (Alkyl Halides & Ethers)

e.g $R\{\overset{\alpha}{CH_2}-Cl \longrightarrow \overset{\oplus}{CH_2}-Cl$ cation $+ \dot{R}$ ↓ larger part Radical

e.g $R\{\overset{\alpha}{CH_2}-O-R \longrightarrow \dot{R}$ Radical $+ \overset{\oplus}{CH_2}-O-R$ cation

β-cleavage: (Gen-in Alkenes) → Allylic cation formation

$$R\{CH_2-CH=CH_2 \longrightarrow \overset{\oplus}{C}H_2-CH=CH_2 + R^{\bullet}$$

4) **Elimination:** (α-β) → Alcohols & Halides
(Removal of H_2O & Alkene)

(i) $R-\underset{\beta}{CH_2}-\underset{\alpha}{CH_2}-OH$

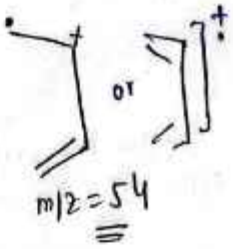
$$R-\underset{H}{\underset{|}{CH}}-\underset{OH}{\underset{|}{CH_2}} \longrightarrow R-CH=CH_2]^{+\cdot} + H_2O$$

(ii) $$R-\underset{H}{\underset{|}{CH}}-\underset{X}{\underset{|}{CH_2}} \longrightarrow R-CH=CH_2]^{+\cdot} + HX$$

5) **Dields-Elder cleavage:** → elimination of neutral Alkene Molecule.

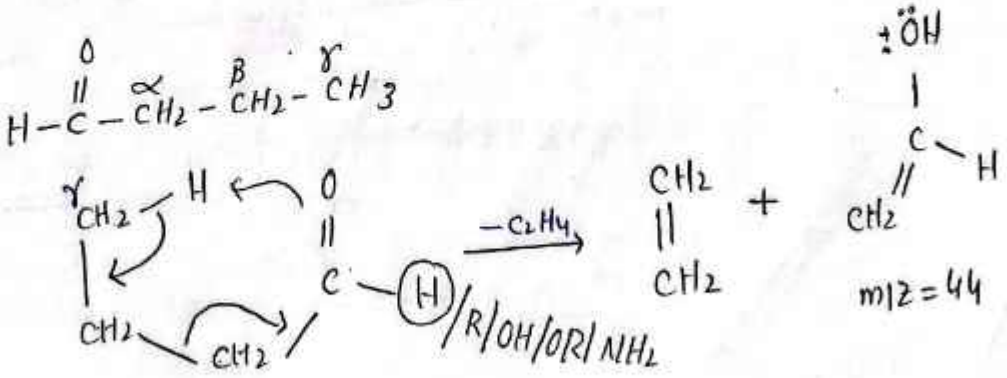
$m = 82$

$M-28$



6) **McLafferty rearrangement:** → (Carbonyl compounds & Alkenes) (If γ-H available)

↳ transfer of γ-H to unsaturated system



Alkanes (DBE=0) → Successive loss of CH_2

- Generally M^+ peak is less intensed in Alkanes
  - *Comparatively simple Alkane's M^+ intensity is more as compared to the Branched Alkanes.
    - more portion of original molecule will exposed to $\bar{e}$-beam more will be the Fragmentation thus M^+ peak intensity decreases e.g in Branched Alkanes.
    - Simple Alkanes → less portion exposed to $\bar{e}$-beam so Fragmentation unfavourable thus M^+ peak intensity higher than Branched.
    - in branched more chances of 2^0 or 3^0 carbocation → more stable cation gives Base peak.

Example;

Butane

$CH_3-CH_2-CH_2-CH_3$

M.W = 58

$\oplus CH_3$ m/z = 15

$CH_3-\overset{\oplus}{C}H_2$ m/z = 29

$CH_3-CH_2-\overset{\oplus}{C}H_2 \longleftrightarrow CH_3-\overset{\oplus}{C}H-CH_3$

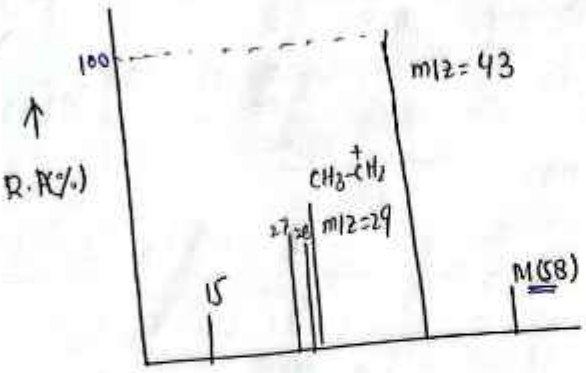
1^0 → 2^0 → more stable

BASE PEAK

m/z = 43

$CH_3-\overset{\oplus}{C}H_2 \xrightarrow{-H} \dot{C}H_2-\overset{+}{C}H_2$ m/z = 28 $\xrightarrow{-H}$ $\dot{C}H_2-\overset{+}{C}H \longleftrightarrow CH_2=\overset{\oplus}{C}H$

m/z = 29 m/z = 27



Butane

*Isobutane $CH_3-\overset{CH_3}{\overset{|}{\overset{+}{C}}}H-CH_3$ (M^+ → less intense than butane)

M.wt = 58

→ B.peak m/z = 43

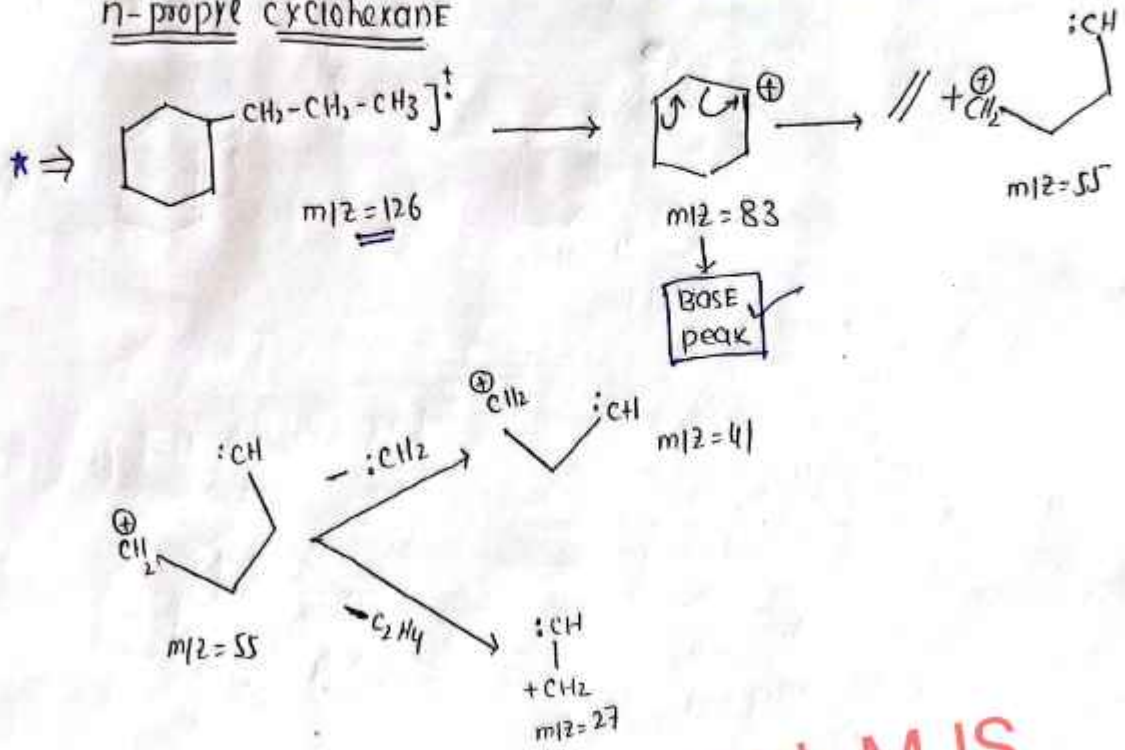
M(58)

Cycloalkanes (DBE=1) → Successive loss of ethene (M-28)

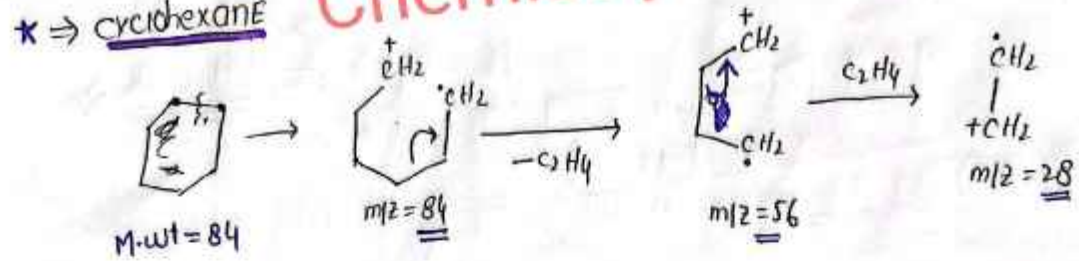
↳ Gen. More intense M^+ peak than Aliphatic Alkanes.

⇒ Here cleavage of C-C Bond difficult. so intense peak.
↓ So M-structure less Fragmented.

n-propyl cyclohexane



* ⇒ cyclohexane



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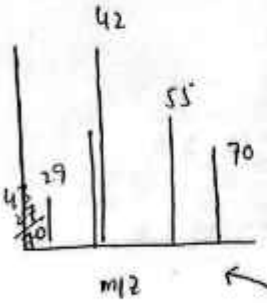
(2) ✓ Alkenes → (DBE = 1) → prominant M^+ peak

↳ Distinct M^+ peak

↳ Fragments ARE DUE TO β-cleavage → Allylic cation $CH_2=CH-\overset{\oplus}{C}H_2$

↳ If γ-H available → Mclafferty rearrangement

↳ Generally BASE peak due to Allylic cation ~~of~~ If γ-H not available otherwise due to MCLAFFERTY B.peak

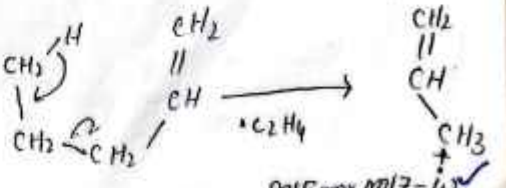


$CH_2=CH-\overset{\alpha}{C}H_2-\overset{\beta}{C}H_2-\overset{\gamma}{C}H_3$ → $CH_2=CH-\overset{\oplus}{C}H_2$ m/z = 41 ✓

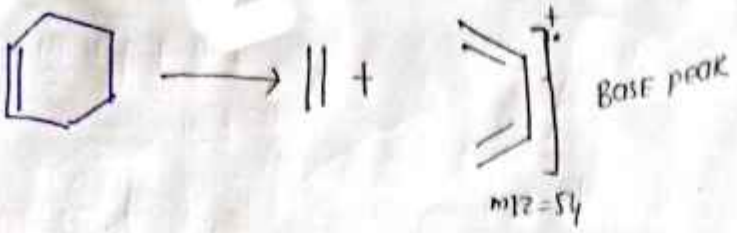
$CH_2=CH-\overset{\alpha}{C}H_2-\overset{\beta}{C}H_2-\overset{\gamma}{C}H_3$

Pentene

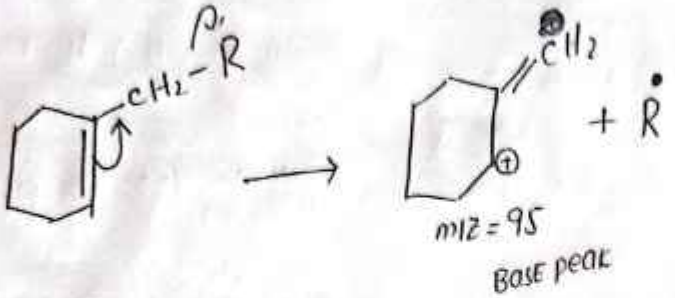
M.wt = 70



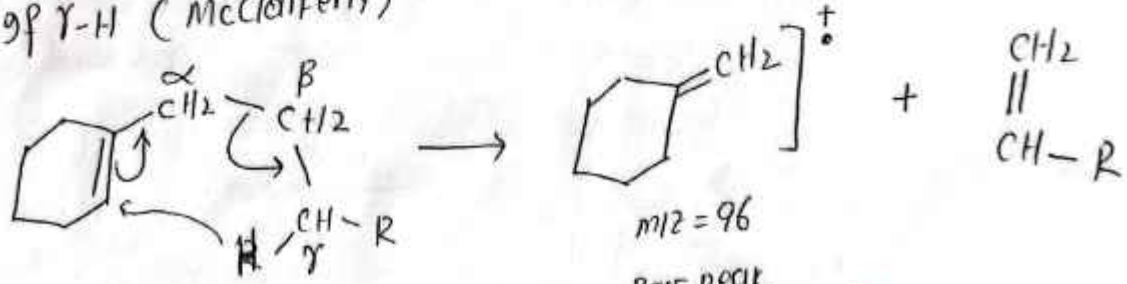
Cycloalkene



(ii)



(iii) of γ-H (McClafferty)



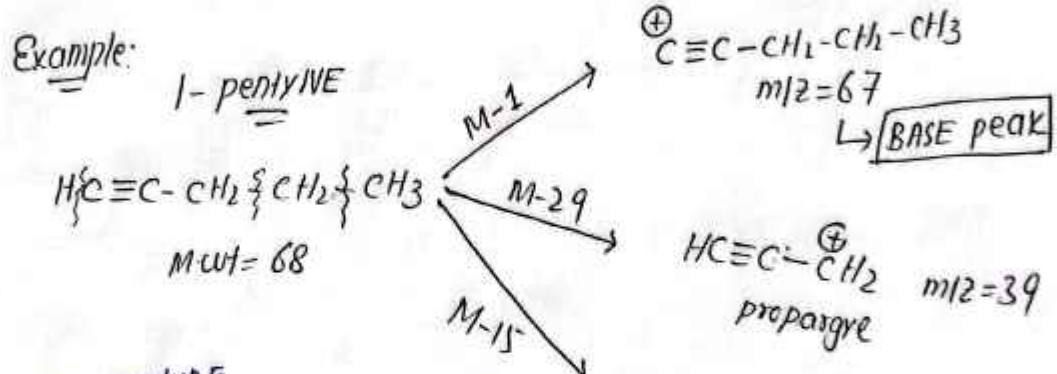
(3) ✓ ALKYNES → (DBE = 2)

* ↳ Base peak in ALKYNES due to M-1 peak

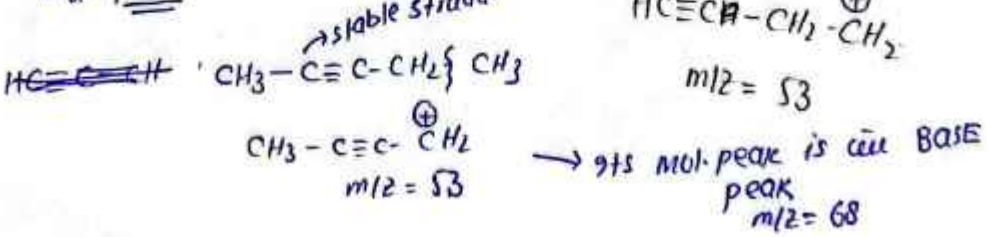
* Also strong peak due to → propargyl ion (m/z = 39)

Example:

1- pentyne

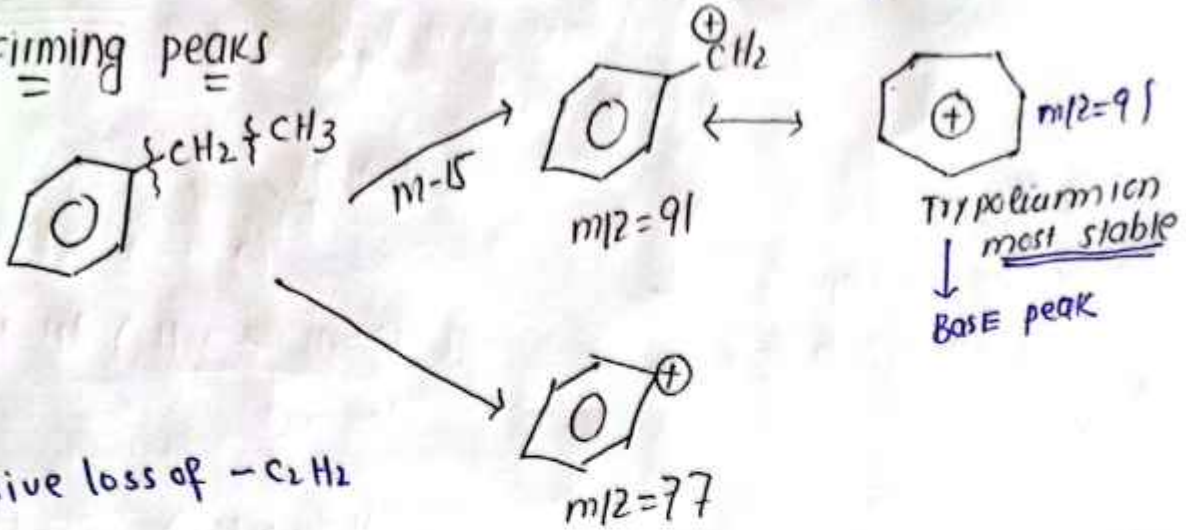


* 2- pentyne

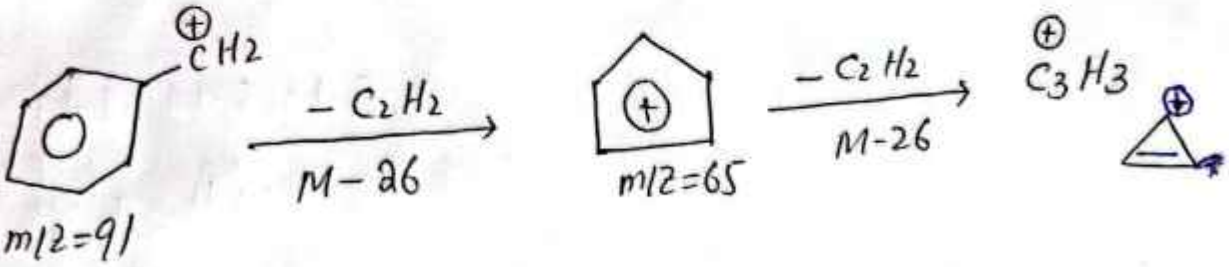


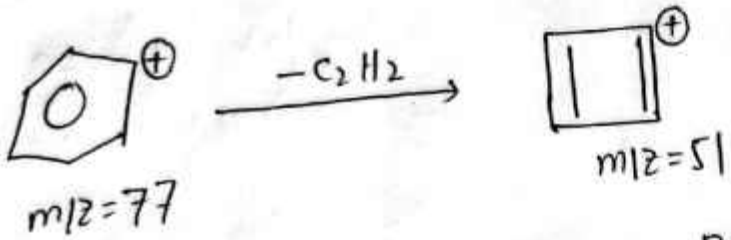
Aromatic Hydrocarbons: (DBE = 4) → strong M^+ peak

Confirming peaks

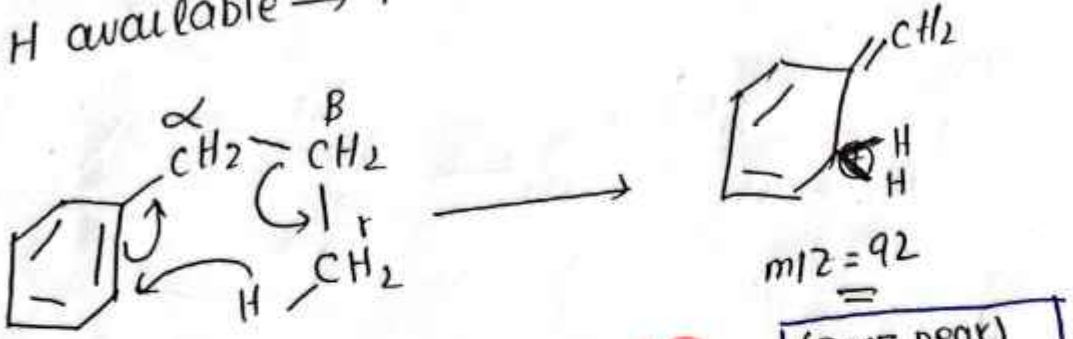


*Successive loss of $-C_2H_2$





⇒ If γ-H available → Mcclafferty Rearrangement



* ——— *

Alcohols ⟶ * M^+ peak in 1° & 2° alcohol → ↓ loss
** absent sometimes
↓ in 3° alcohol

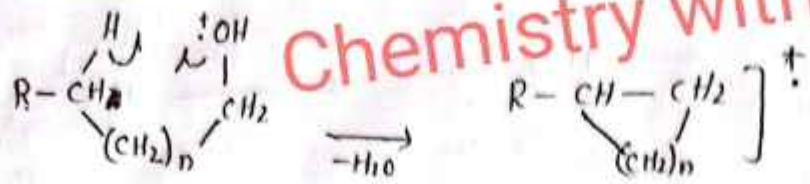
CH_3-CH_2-OH 1° alcohol

* 1° alcohol → m/z = 31 ($CH_2=\overset{+}{O}H$)
* 2° alcohol → 45 → $CH_3-\underset{\oplus}{CH}=OH$
* 3° alcohol → 59 → $(CH_3)_2\overset{\oplus}{C}=OH$

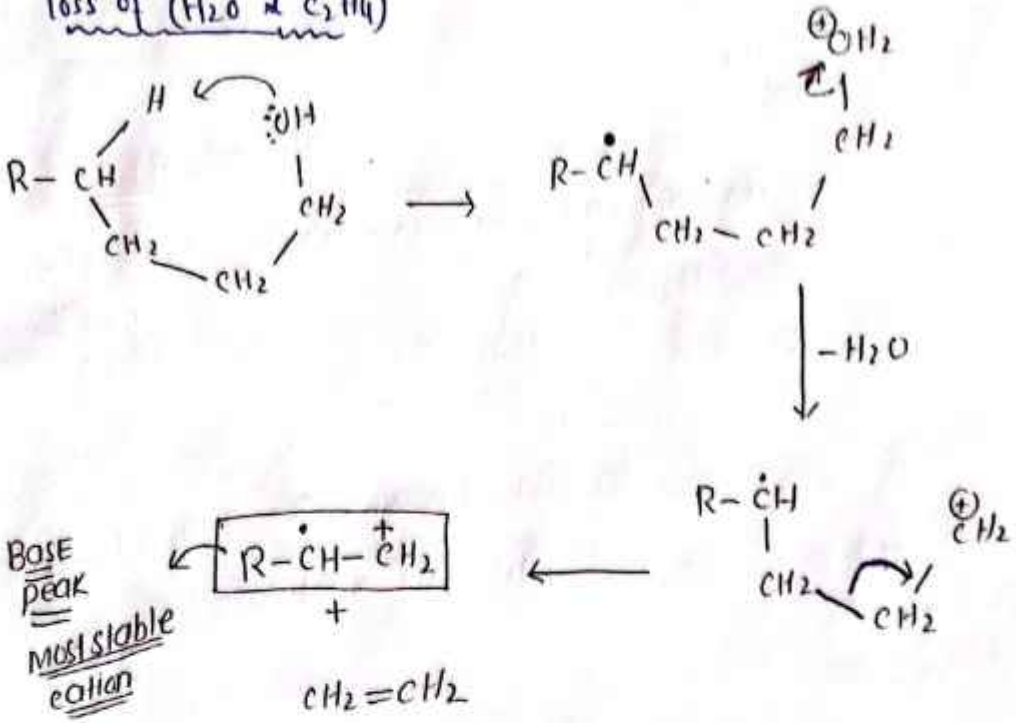
✓ Fragments formed due to

* M-18 ($-H_2O$)
* M-46 (H_2O & $CH_2=CH_2$) ← Removal
* M-33 (H_2O+CH_3)
* M-1, M-2, M-3

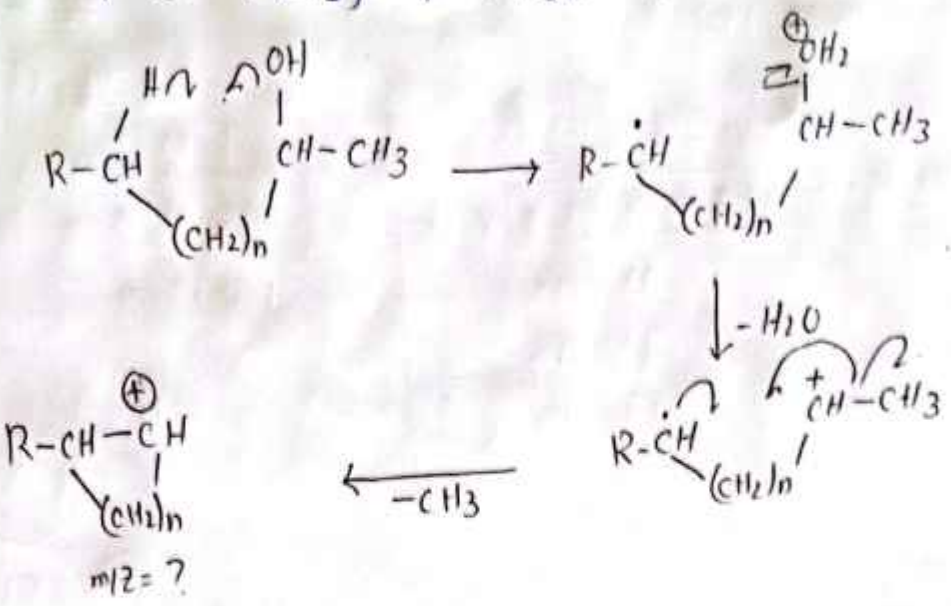
(i) Loss of H_2O: (M-18)



(ii) loss of (H_2O & C_2H_4)

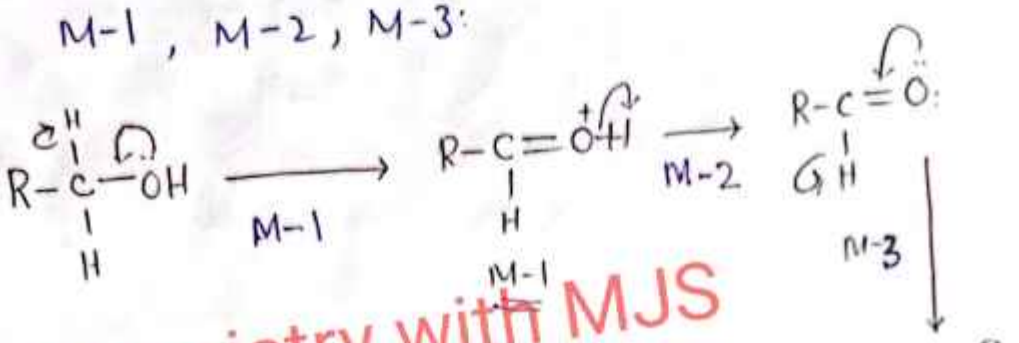


Loss of $(H_2O + CH_3) \longrightarrow M-33 \longrightarrow$ Generally in 2° Alcohol.



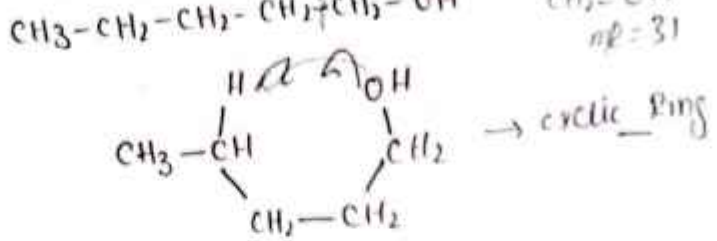
m/z = ?

* M-1, M-2, M-3:

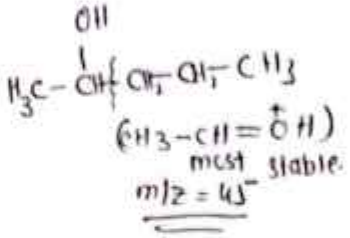


Example:

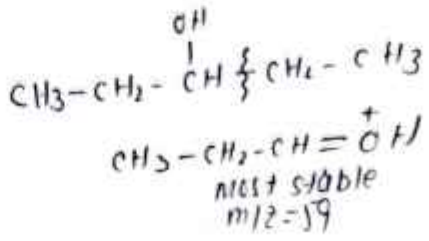
* 1- pentanol → v.v. small M^+ peak



* 2- pentanol → M^+ peak not observed
  → B-peak m/z = 45



* 3- pentanol → M^+ peak not observed
  B-peak m/z = 59



phenols: M^+ - peak v.v. strong → Also give the Base peak

★ Fragments

- ★ M-1
- ★ M-28
- ★ M-29

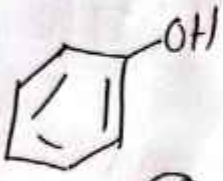
confirming peaks

m/z = 94 → B. peak → M^+ peak

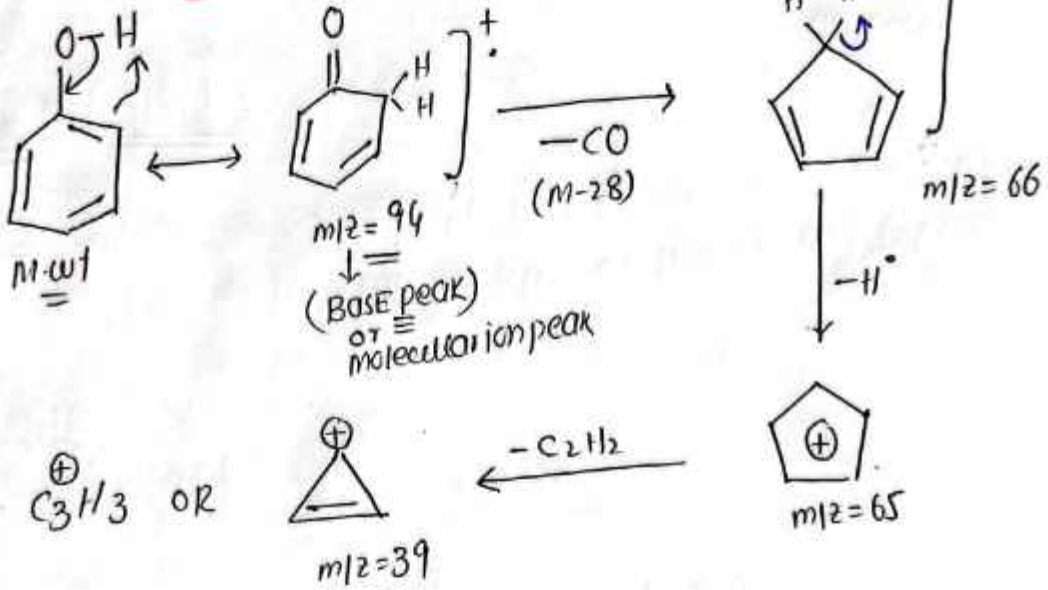
m/z = 66

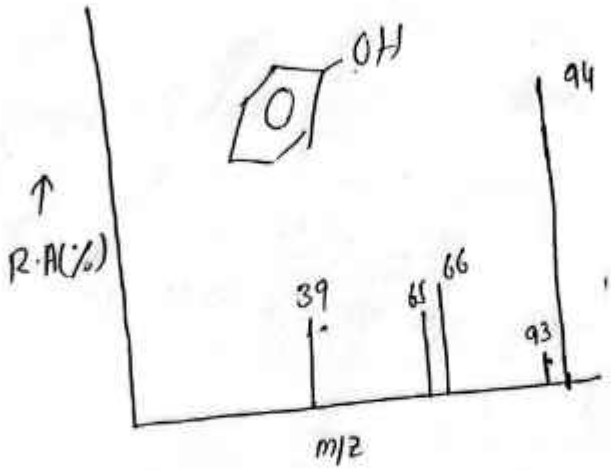
m/z = 65

m/z = 39



77+17 = (94)





* ——— *

Thiols: ($R-CH_2-SH$)

* Molecular ion peak is more intense than Alcohols. It show M+2 peak due to the presence of Heavy isotope ^{34}S

* Here M-34 peak occur due to the Loss of H_2S as compared to the H_2O in Alcohols

Example; $CH_3-CH_2-CH_2-SH$ M.wt = 76

M-34 → CH_2-CH_2 / CH_2

M-15 → $CH_3-\overset{+}{C}H-CH_3$ m/z = 43 Base peak

(9) Ethers & Sulfides:

Ethers → M^+ peak of Alephatic Ethers are intense than Alcohols, but still v. low → Difficult to observe.

Fragments α-cleavage m/z = 43, 59, 73 etc

Example; $CH_3-CH_2-CH_2-O-CH_2-CH_2-CH_3$

α-cleavage

$\overset{+}{O}H_2-O-CH_2-CH_2-CH_3$ m/z = 73

$CH_3-\overset{+}{C}H-CH_3$ m/z = 43

$\overset{+}{O}=CH_2-CH_2-CH_3$ m/z = 59 Stable cation

Base peak

* Aromatic Ethers → show intense M^+ peak

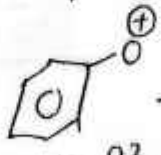
possibilities

(i) 

Stable

108 (Anisole)

M^+ → peak show Base peak



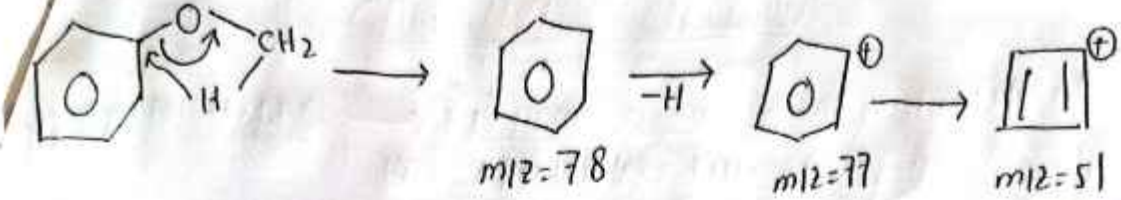
m/z = 93

$-CO$

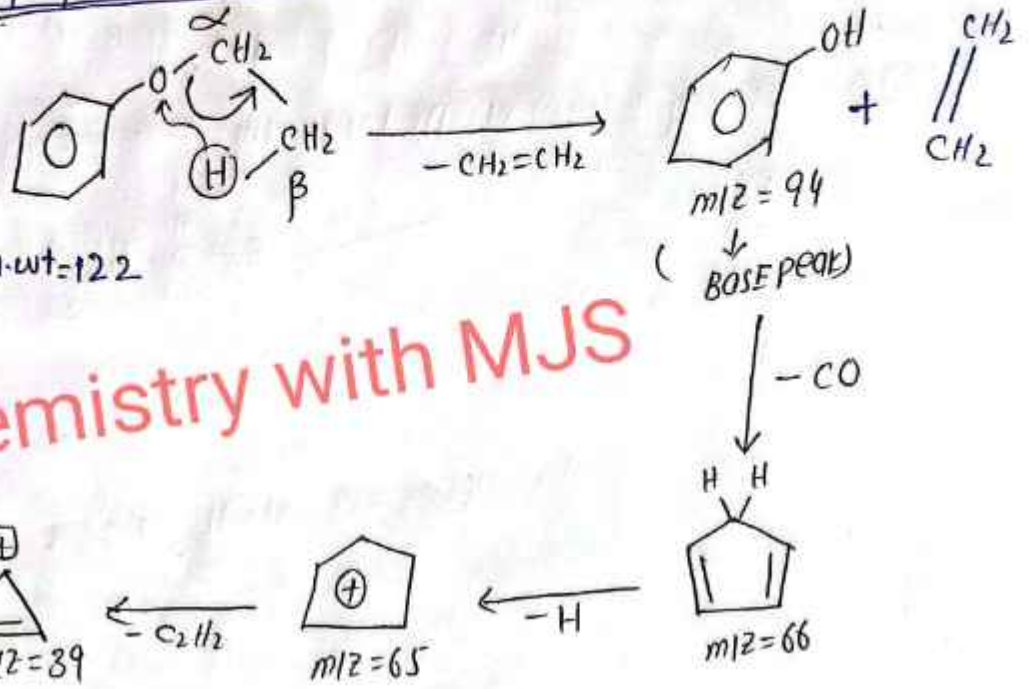
m/z = 65

$-C_2H_2$

m/z = 39



(iii) If β-H available → then β-H transfer → gives BASE peak

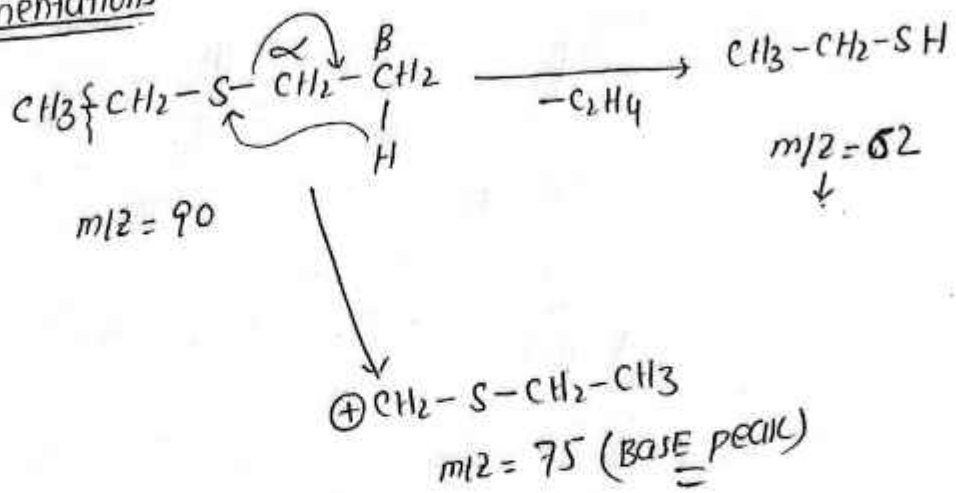


(10) Sulfides (R-S-R)

↳ Thioesters

↳ more intense M^+ peak than ETHERS.

Fragmentations



CARBONYL COMPOUNDS

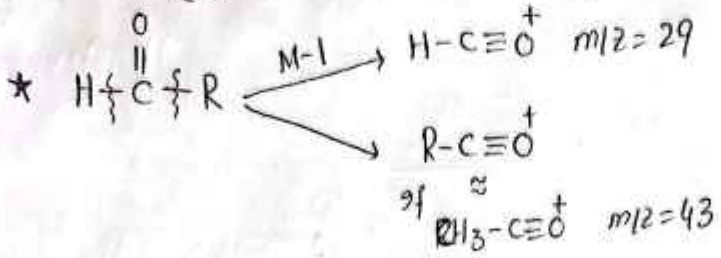
ALDEHYDES: → M^+ peak weak in Alephatic Aldehydes But observable. But strong in Aromatic Aldehydes.

Fragments

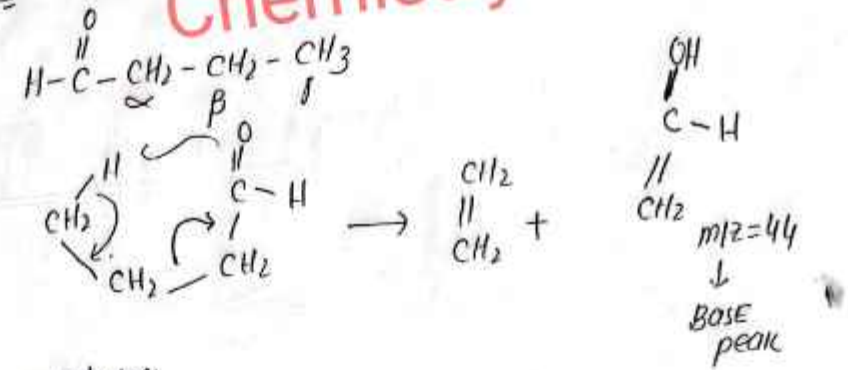
(i) ∝-cleavage.

(ii) β-cleavage.

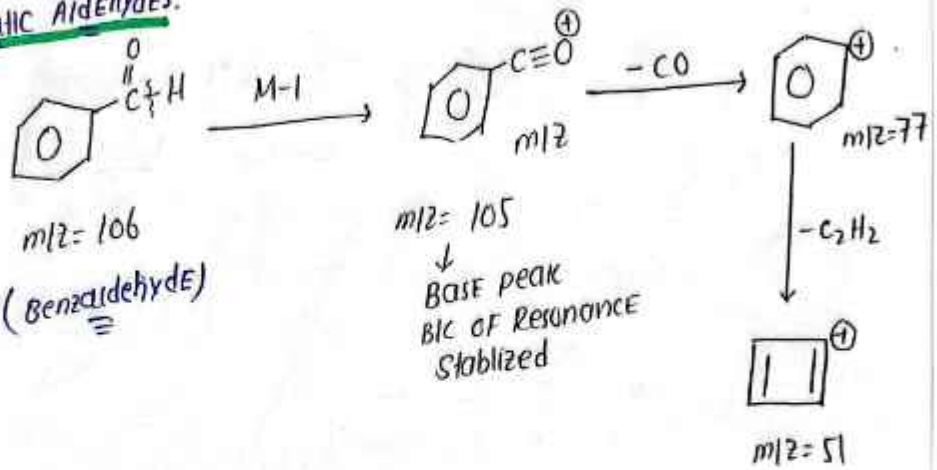
(iii) McLafferty Rearrangement. (BASE PEAK)



* McLafferty Rearrangement:



⇒ Aromatic Aldehydes:

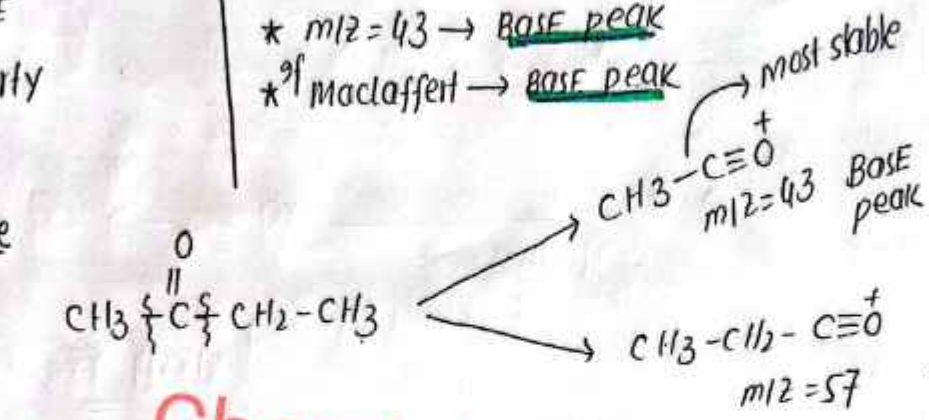


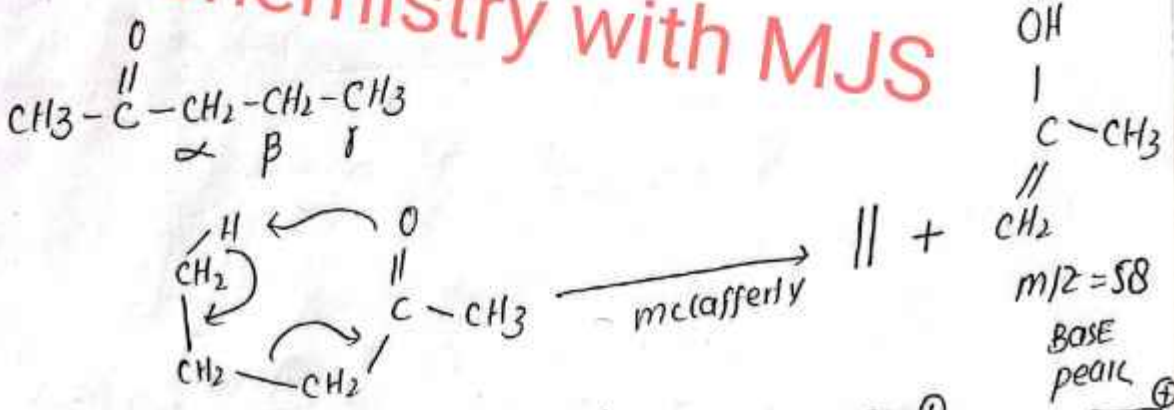
KETONES → M^+ → strong

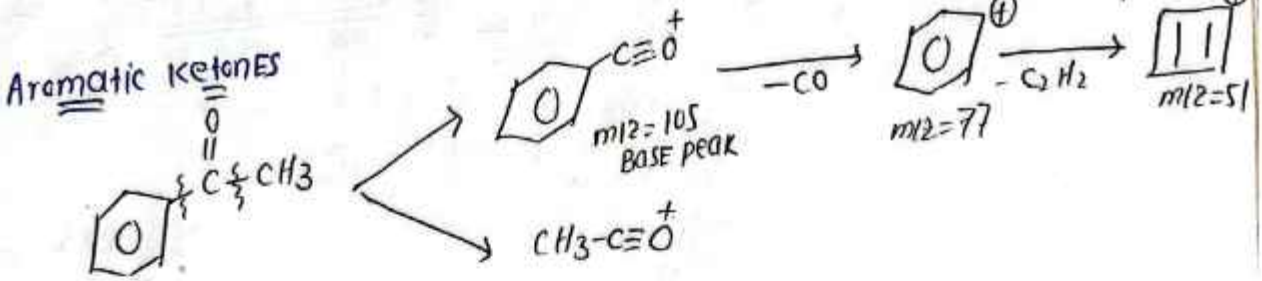
α-cleavage
β-cleavage
Mcclafferty

M-15, M-29, M-43

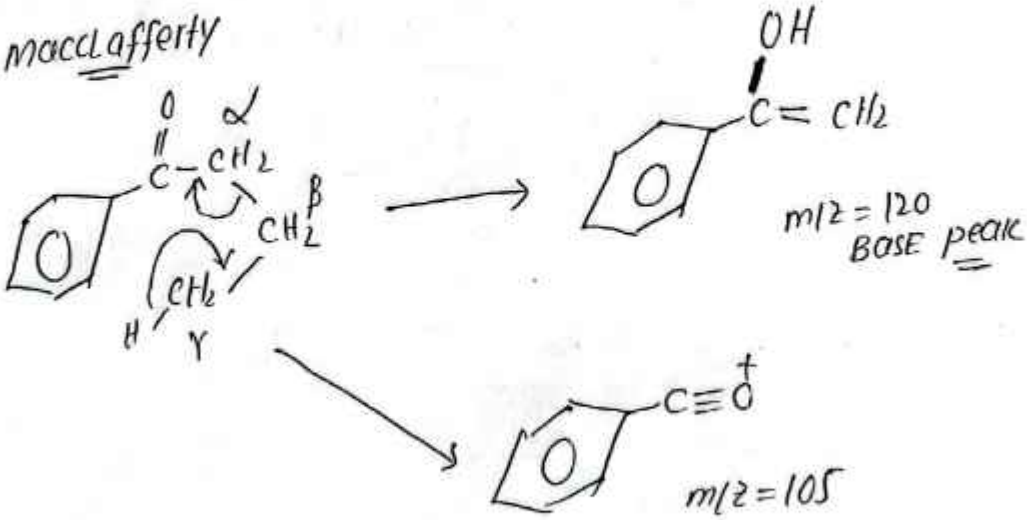
* m/z = 43 → Base peak
* If Maclafferh → Base peak







Acetophenone

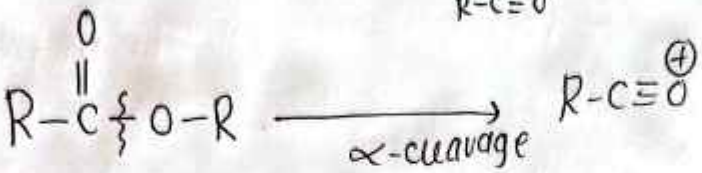


⇒ **Esters** → M^+ → weak

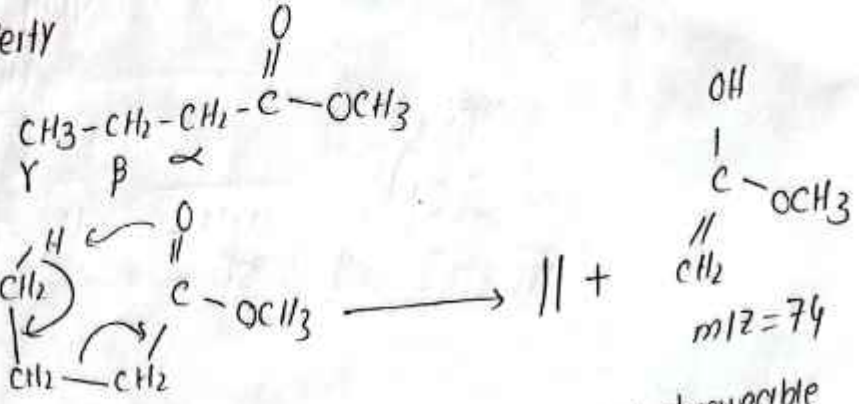
↳ Most imp. Fragmentation of Ester is α-cleavage.

↓

Loss of Alkoxy group → Acylium ion Formation $R-C\equiv O^+$



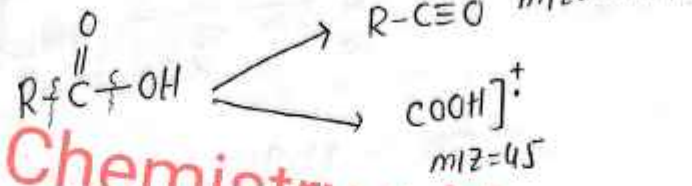
McLafferty

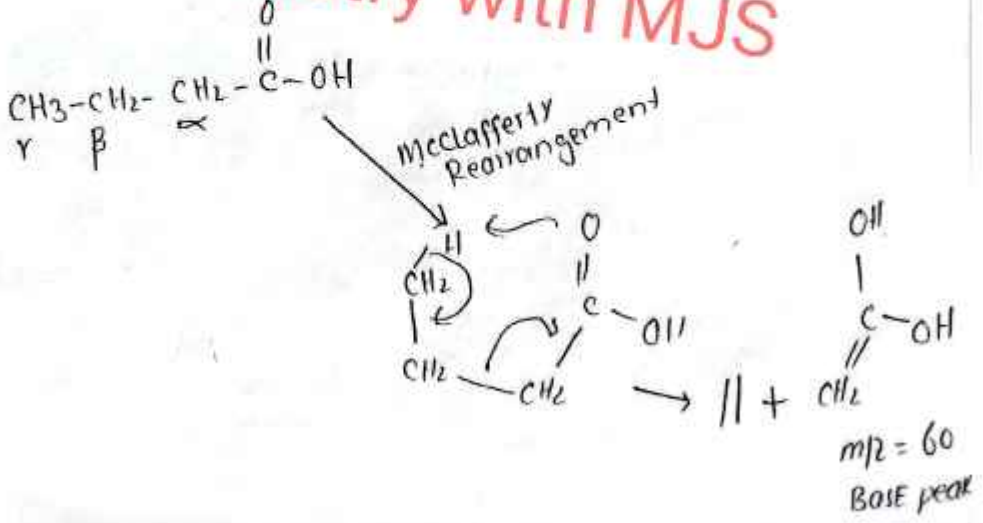


⇒ **Carboxylic Acids** → Alephatic M^+ → weak but observeable
→ Aromatic M^+ → strong

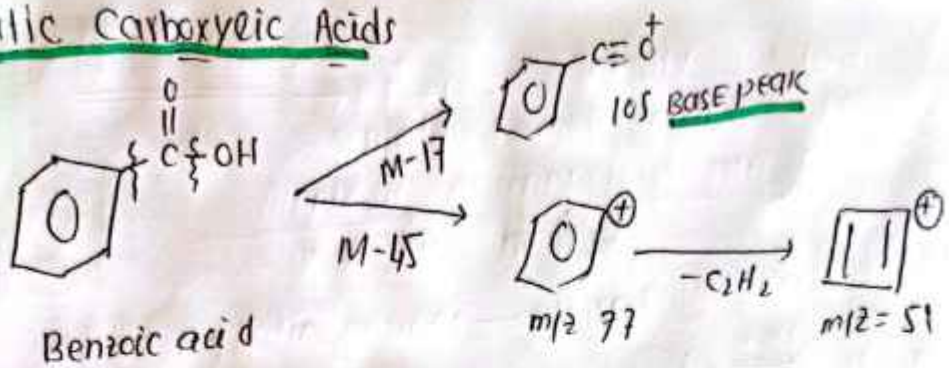
↳ confirming peaks
* M-17
* M-45

* α-cleavage
* McLafferty



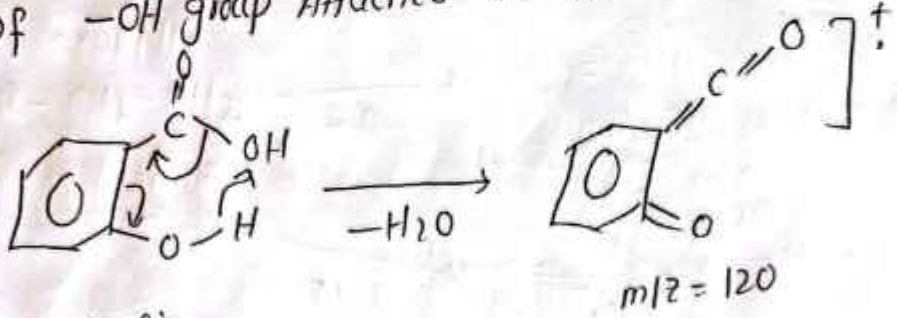


Aromatic Carboxylic Acids



Benzoic acid

⇒ If –OH group Attached at ortho- to C_6H_5COOH

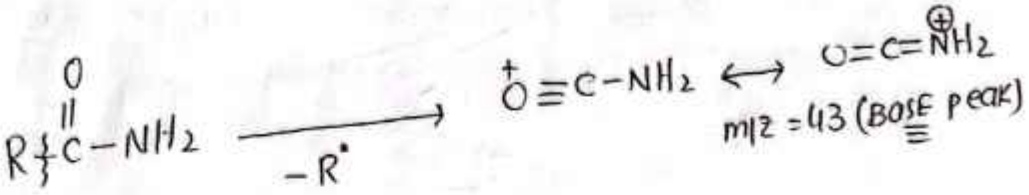


Salicylic acid

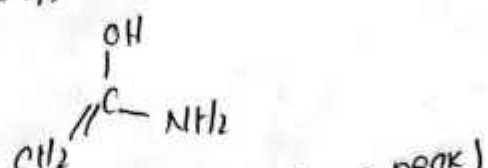
(14) ✓Amides

confirming peaks (i) m/z = 43 α-cleavage

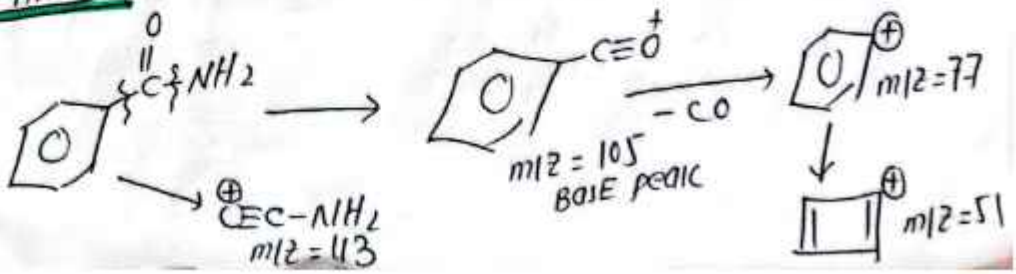
(ii) m/z = 59 Maclafferty



✓ If γ-H ⇒ mcclafferty Rearrangement



✓Aromatic Amides



(15) ✓ **AMINES:** → M^+ → peak usually weak, sometimes undetectable for Aliphatic amines but intense for Aromatic Amines.

⇒ In Aliphatic Amines → Base peak occurs due to α-cleavage.

Base peaks: ∴ 1° Amine m/z = 30; ∴ 2° Amine m/z = 58; ∴ 3° Amine m/z = 86

Example

$R-CH_2-NH_2 \xrightarrow{-R} CH_2=\overset{\oplus}{N}H_2$ m/z = 30 Base peak

1° Amine

M-1 → $R-\underset{H}{CH}-NH_2 \leftrightarrow R-CH=\overset{\oplus}{N}H_2$ m/z = M-1=

2° Amine

Di-ethyl-Amine

$CH_3\{CH_2-NH-CH_2-CH_3 \xrightarrow{-CH_3} CH_2=\overset{\oplus}{N}H-CH_2-CH_3$ m/z = 58 (Stable) → Base peak

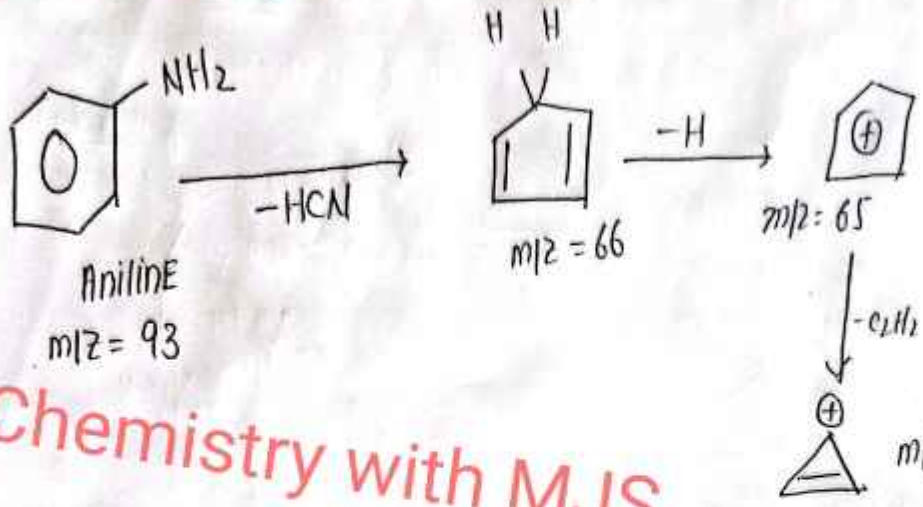
$CH_2=\overset{\oplus}{N}H-CH_2-\underset{H}{CH_2} \xrightarrow{-C_2H_4} CH_2=\overset{\oplus}{N}H_2$ m/z = 30 (Stable)

3° Amine

$CH_3\{CH_2-\underset{CH_2}{\overset{CH_3}{\underset{|}{\overset{|}{N}}}}-CH_2-CH_3 \xrightarrow{-CH_3} CH_2=\underset{\oplus}{\overset{C_2H_5}{\underset{|}{N}}}-CH_2-\underset{H}{CH_2}$ m/z = 86 (Base peak)

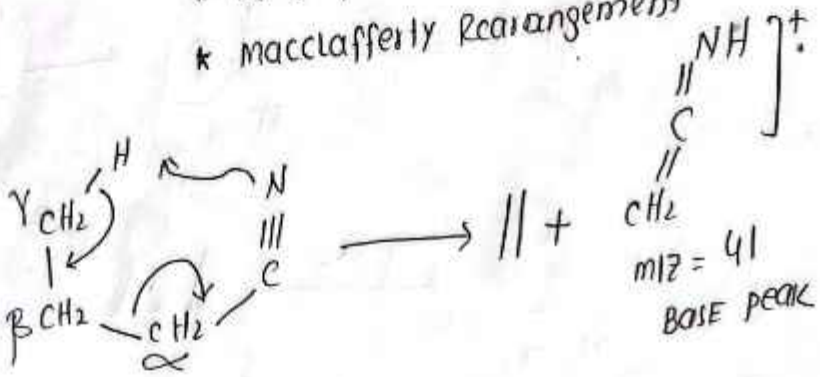
$\xrightarrow{-CH_2=CH_2} CH_2=\underset{H}{\overset{C_2H_5}{\underset{|}{\overset{|}{\oplus N}}}}$ m/z = 58 $\xrightarrow{CH_2=CH_2} CH_2=\overset{\oplus}{N}H_2$ m/z = 30

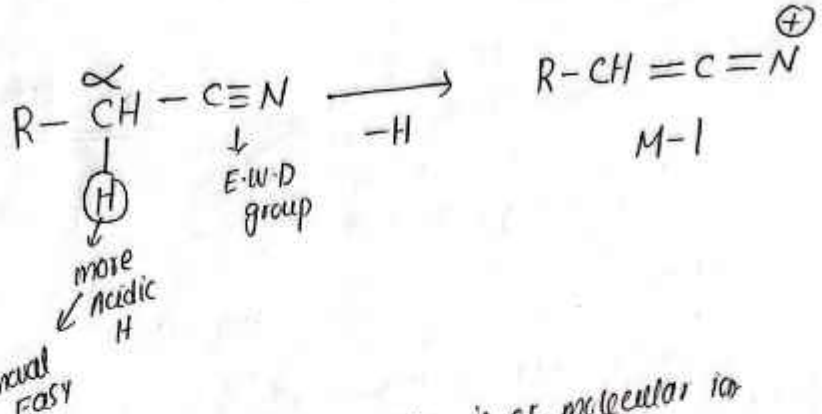
Aromatic Amines



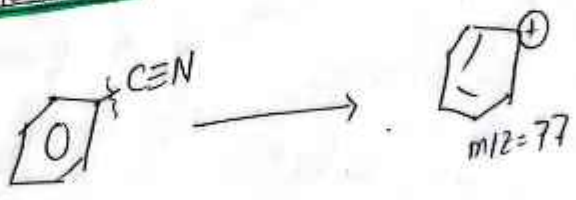
(6) ✓**Nitriles:-** → M^+ of Alephatic → too weak to be observed

* M-1 peak observed
* Macclafferty Rearangement





Aromatic Nitriles → Base peak is of molecular ion



✓ Nitro-Compounds → M^+ → peak of Aleptatic is usually weak ↓ undetectable

confirming peaks

$m/z = 46 \rightarrow NO_2^+$

$m/z = 30 \rightarrow NO^+$ ↓ intense peak

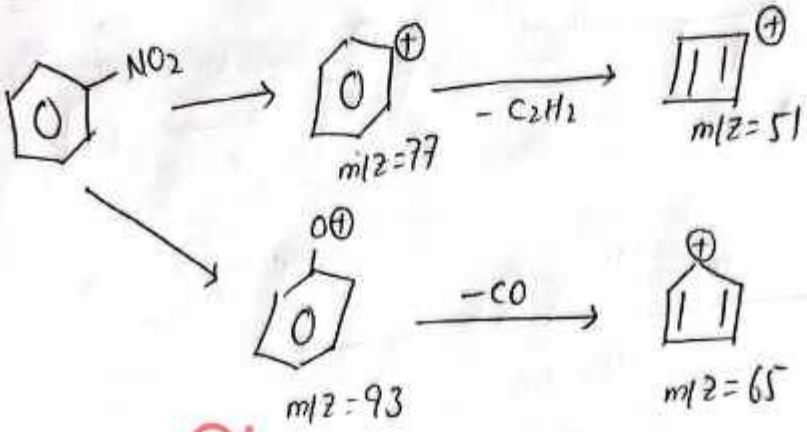
weak peak

$CH_3-CH_2-CH_2-NO_2$ → NO_2^+

→ NO^+

→ $CH_3-\overset{+}{C}H-CH_2$, $m/z = 43$

★ Aromatic → Give M^+ → intense



(18) ✓ Halides:

M^+ peak order

R-I > R-Br > R-Cl > R-F

↓ strongest ↓ (weakest)

★ R-Br & R-Br → show M+2 peak due to two isotopic form

★ ^{35}Cl, ^{37}Cl

★ ^{79}Br, ^{81}Br

↳ 7981 Almost equal intensity

Major Fragmentations

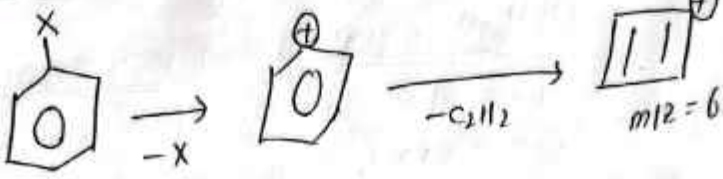
① loss of Halogen Atom (most significant for Br & I)

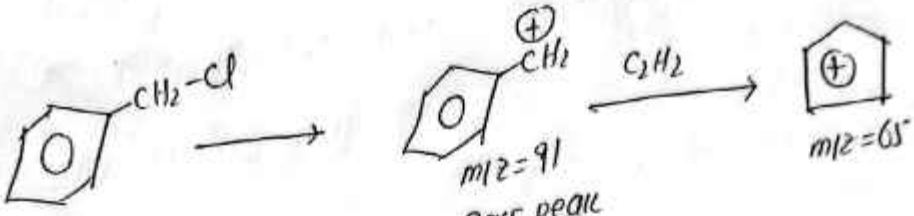
② Elimination of HX (most significant for Cl & F)

$\Rightarrow$ $R-CH_2-CH_2-X \xrightarrow{-X} R-CH_2-\overset{\oplus}{C}H_2$ m/z = ?

$\Rightarrow$ $R-\underset{\beta}{CH}-\overset{\alpha}{CH_2}-X \xrightarrow{-HX} [R-CH=CH_2]^{+\cdot} + HX$ m/z

AROMATIC HALIDES





Example

$\star$ CH_3-CH_2-Cl

M.wt = 64

- m/z = 35 → ^{35}Cl
- m/z = 36 → $[HCl]^{+\cdot}$
- m/z = 37 → ^{37}Cl
- m/z = 49 → $CH_2=\overset{\oplus}{C}l$
- m/z = 29 → $CH_3-\overset{\oplus}{C}H_2$
- m/z = 15 → $\overset{\oplus}{C}H_3$

$\star$ CH_3-CH_2-Br

M.wt = 108

- M-79 → $CH_3-\overset{\oplus}{C}H_2$ → m/z = 29
- $CH_2=\overset{\oplus}{B}r$ m/z = 93
- $[HBr]^{+\cdot}$ m/z = 80
- $Br^{\oplus}$ 79 (isotope)
- $Br^{\oplus}$ 81 (isotope)

Applications

① Qualitative applications:

- ① Determination of Molecular weight
- ② Determination of Molecular formula.
- ③ Determination of Structure of compounds.

② Differentiation of Geometrical isomers:

Both isomers cis & trans → have ~~different~~ Similar spectra But intentensity of M^+-peak of Both is different

trans $M^{\oplus}$-peak > cis-$M^{\oplus}$-peak

③ Determination of ionization potential:

Ionization potential of each compound is determined. By estimating the Amount of Energy of bombarded ē to generate ~~the~~ Molecular cations.

④ Detection of impurity:

↳ impurities can be detected by the Additional peaks.

⑤ identification of unknown compound:

↳ By comparing with the standards

⑥ Identification of proteins:

Most Efficient technique For the study of structure and Function of protein.

* ESI & MALDI-MS widely used ionization sources to study proteins.

* ~~sequenc~~ sequence of peptides Also determined by the MS-

⑦ Pharmaceutical Applications:

Structure determination of Drugs & medicine is very important. We can determine the structure of many drugs by identifying the ~~drug~~ Fragments.

⑧ Clinical studies:

↳ Blood samples, tissues composition, urine samples composition is checked.

⑨ Forensic Applications:

↳ Sample in forensic in minute quantity. So, high sensitivity is required which is achieved by MS.

* LC-MS is used for the identification & Separations.

⑩ Quality Control Analysis:

↳ Food Analysis → proteins, Lipids, Nucleic Acids etc.