DR. BRR GOVERNMENT DEGREE COLLEGE,

JADCHERLA, MAHABUBNAGAR (Dist.).

DEPARTMENT OF CHEMISTRY

Title of the Project

Interpretation of Spectral data of

1. Picoline
2. 1-Phenyl butane
3. Diethyl terephthalate
4. 2- Butanone

By

Sl. No	Name of the student	H. T. No	Group
1	B. Nandini	20033006441007	M.P.C EM
2	G. Manasa	20033006441016	M.P.C EM
3	SK. Shainaaz	20033006441054	M.P.C EM
4	R. Aravind	20033006441050	M.P.C EM
5	M. Shivalingam	20033006441034	M.P.C EM
6	P. Lokesh	20033006441043	M.P.C EM

Supervision by

N. SAI KONDALU

Assistant Professor of Chemistry

HOD

Lecturer in Chemistry
Dr.B.R.R.Govt. Degree College
JADCHERLA

Principal
Dr BRR Govt. College
Jadcherla-509 301

CERTIFICATE

This is to certify that the student study project on Interpretation of Spectral data of 1. Picoline, 2. 1-Phenyl butane, 3. Diethyl terephthalate, 4. 2- Butanone is a bonafide project work done by B. Nandini, G. Manasa, Sk. Shainaaz, R. Aravind, M. Shivalingam and P. Lokesh under my supervision in the department of Chemistry, Dr. BRR. Government Degree college, Jadcherla, Telangana state.

Date: 25.05.2023

Place: JADCHERLA

(N. SAI KONDALU)

supervisor

DECLARATION

We are hereby declare that the study project on Interpretation of Spectral data of 1. Picoline, 2. 1-Phenyl butane, 3. Diethyl terephthalate, 4. 2- Butanone is a record work done by us under the supervision of N. SAI KONDALU, Assistant Professor of Chemistry , Dr. BRR. Government Degree college, Jadcherla, Telangana, and that the project has not been previously done by any others in this college and any other college/University.

Date: 25.05.2023

Place: JADCHERLA

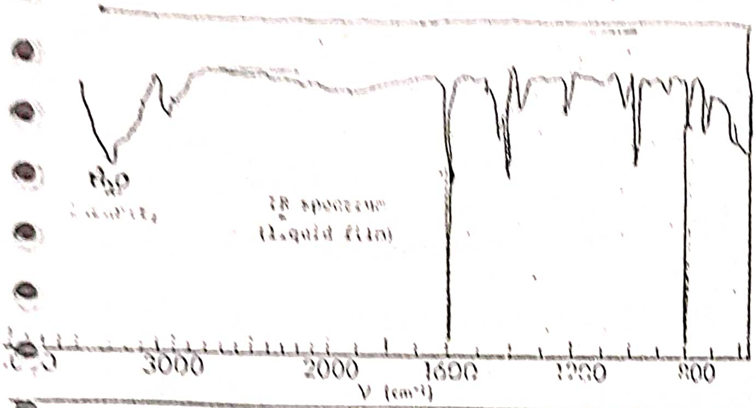
Sl. No	Name of the student	H. T. No	Group	Signature
1	B. Nandini	20033006441007	M.P.C EM	B. Nandini
2	G. Manasa	20033006441016	M.P.C EM	Manasa
3	SK. Shainaaz	20033006441054	M.P.C EM	SK. Shainaaz
4	R. Aravind	20033006441050	M.P.C EM	R. Aravind
5	M. Shivalingam	20033006441034	M.P.C EM	Shivalingam
6	P. Lokesh	20033006441043	M.P.C EM	P. Lokesh

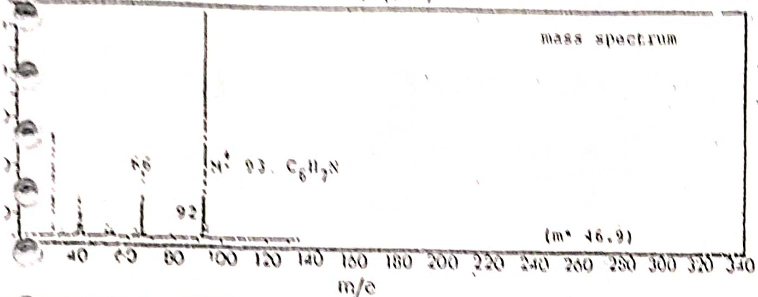
(12)

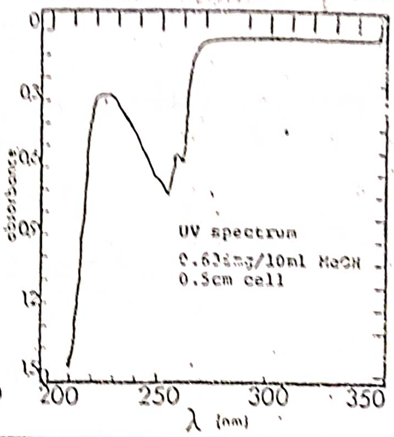
In the given mass spectrum M/z = 93, M/z 92, M/z 66, M/z 39 ... compound. (12)

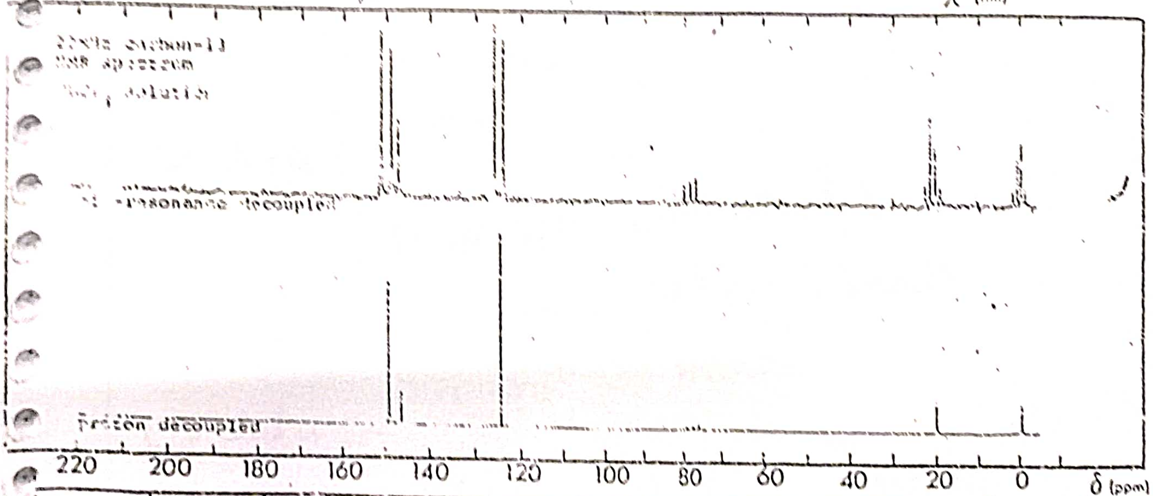
problem 36

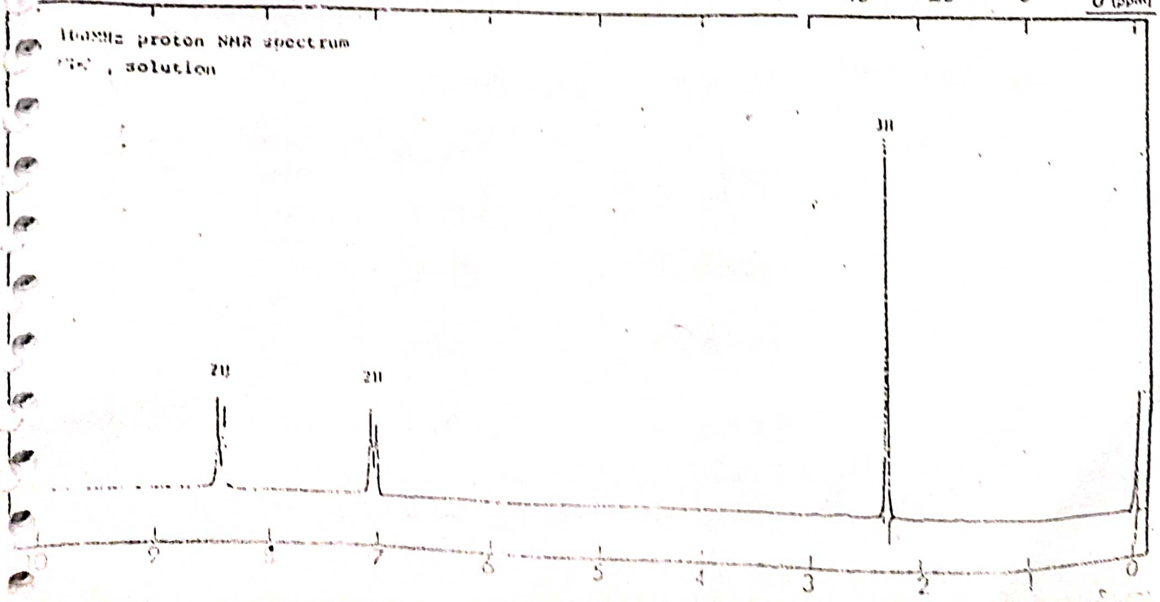
Molecular M/z is odd NO(93). So one 'N' is present. The mol. formula of compound is given as C_6H_7N











Spectral problem - XII

Mass spectral data :-

The mass spectrum shows,

⇒ m/z = 93, 92 and 66 containing peaks are observed

⇒ The molecular ion m/z is odd (i.e, 93)

So, the nitrogen is present.

⇒ The molecular formula for the given compound is given as "C_6H_7N".

⇒ $DBE = \text{no. of C's} - \frac{\text{no. of H's}}{2} - \frac{\text{no. of X's}}{2} + \frac{\text{no. of N's}}{2} + 1$

$= 6 - 7/2 - 0/2 + 1/2 + 1$

$= 7 - 6/2$

$= 4$

IR data :-

$1600 cm^{-1}$	C=C stretch
$1380 cm^{-1}$	sp^3 C-H (bend)
$950 cm^{-1}$	HC=CH

UV data :-

225 nm	$n \rightarrow \pi^*$ transition
270 nm	$\pi \rightarrow \pi^*$ transition

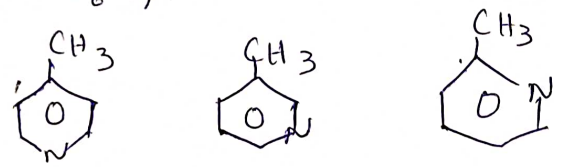
^{13}C - NMR data :-

20 δ	quartet
78 δ	Triplet
125 δ	doublet
150 δ	Triplet

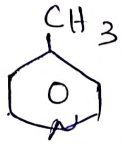
H^1-NMR data :-

S.NO	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	2.3	doublet	–	–	3H	CH_3
02.	7	doublet	–	–	2H	Aromatic H's
03.	8.4	doublet	–	–	2H	

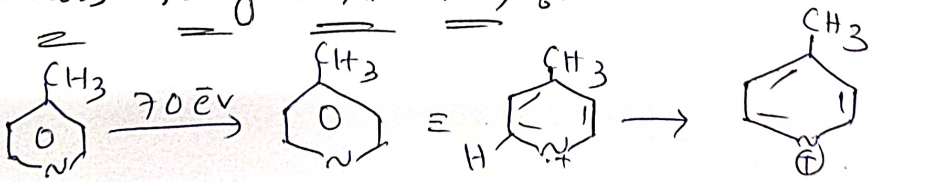
Based on the above data. The possible structure for "C_6H_7N". are



In the above structure's. structure (i) co-relates with the NMR data. ∴ The correct structure is,

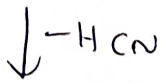


mass fragmentation :-



m/z = 93

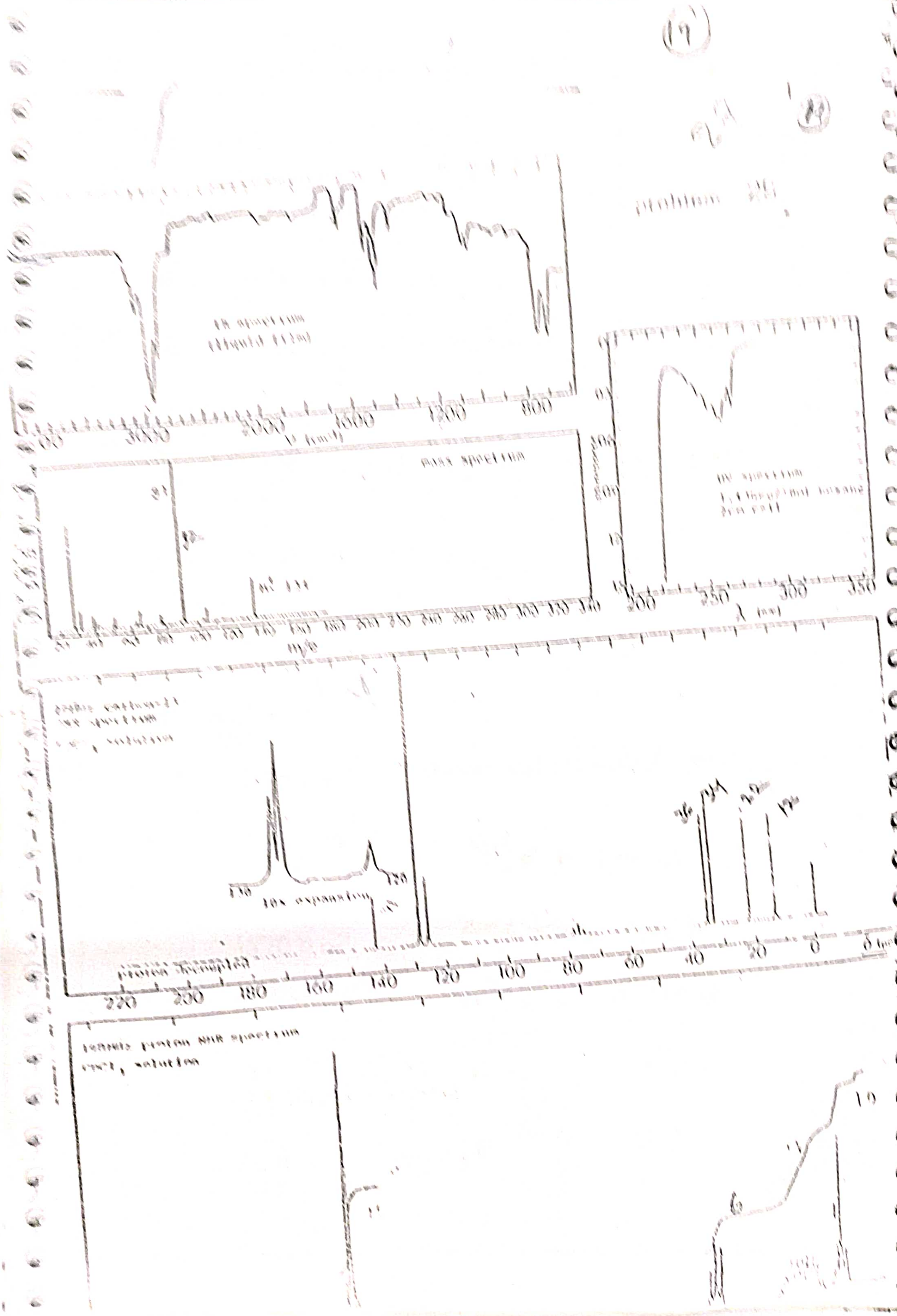
m/z = 92



m/z = 66

Result :-

Based on the above four spectral data the given spectral sheath belongs to Pyridine


IR spectrum
(liquid film)
3000
2000
1600
1200
800
mass spectrum
m/e
UV spectrum
200
250
300
350
10x expansion
proton decoupled
220
200
180
160
140
120
100
80
60
40
20
0

Spectral Problem - XIX

mass spectral data :-

In the given mass spectrum,

→ m/z = 134, 92, 91 containing peaks are present.

→ The molecular ion m/z is even, ∴ zero/even no. of nitrogens are present.

→ The molecular formula for the given spectral sheeth is, "$C_{10}H_{14}$".

→ $D_{BE} = \text{no. of C's} - \frac{\text{no. of H's}}{2} - \frac{\text{no. of X's}}{2} + \frac{\text{no. of N's}}{2} + 1$

$= 10 - \frac{14}{2} - 0/2 + 0/2 + 1$

$= 11 - 7$

$= 4$

IR data :-

690 cm^{-1}	mono substituted benzene
750 cm^{-1}	sp^3, C-H (bend)
1450 cm^{-1}		
1510 cm^{-1}	C=C ring stretch
2930 cm^{-1}	sp^3, C-H (stretch)

UV data :-

230 nm	$n \sim \pi^*$
280 nm	$\pi \sim \pi^*$

^{13}C-NMR data :-

12δ Singlet

22δ Singlet

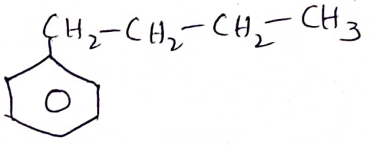
34δ Singlet

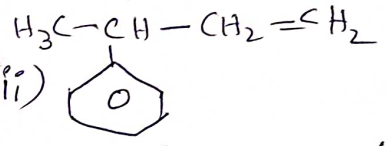
36δ Singlet

H^1-NMR data :-

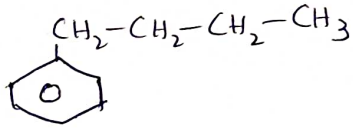
S.No	δ values	multiplicity	Integration	Ratio	no. of H's	Interference
01.	0.9	quatet	9	9/3 = 3	3	CH_3
02.	1.5	multiplet	12	12/3 = 4	4	CH_2-CH_2
03.	2.7	Triplet	6	6/3 = 2	2	CH_2
04.	7.2	singlet	15	15/3 = 5	5	

The Possible structures for "$C_{10}H_{14}$" are.

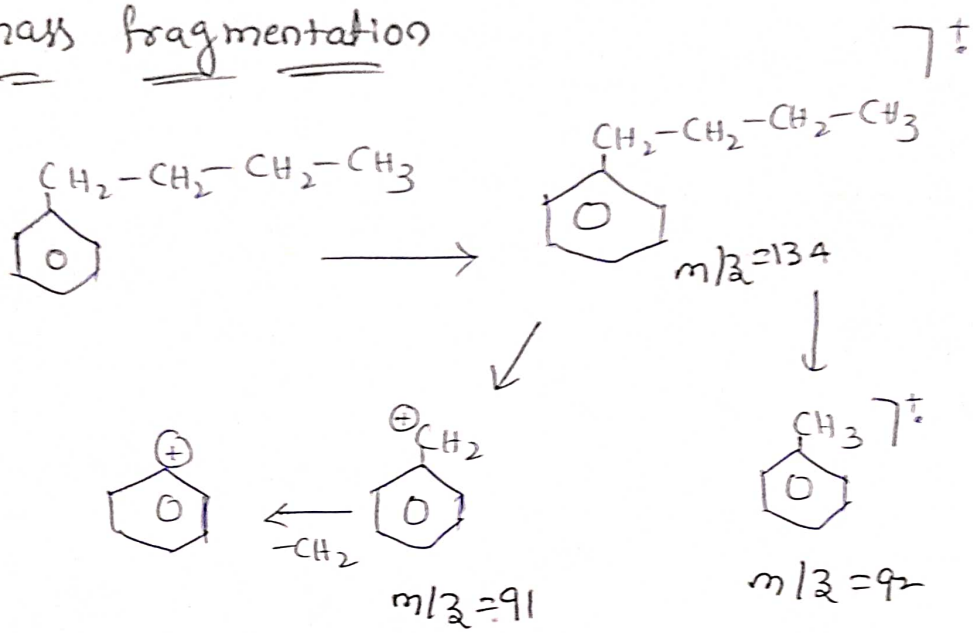
i) 

ii) 

In the above structures . structure (i) co-relating with the NMR data . ∴ The correct structure is

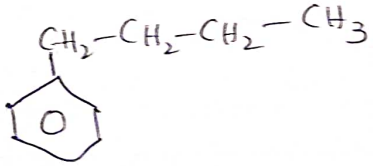


mass fragmentation



Result :-

Based on the above four spectral data's the given spectral sheeth belongs to 1-Phenyl butane.



(14)

(19)

(25)

(6)

IR spectrum
(major multi)

4000 3000 2000 1600 1200 800

ν (cm⁻¹)

mass spectrum

m/z 222 : 100%
223 : 13·5%
224 : 1·0%

m/e

UV spectrum

200 250 300

70MHz carbon-13
NMR spectrum
$CDCl_3$ solution

off-resonance decoupled

proton decoupled

220 200 180 160 140 120 100 80 60 40 20 0

200MHz proton NMR spectrum
$CDCl_3$ solution

Spectral Problem – XIV

mass spectral data:-

	m/z	% of R.A
m^+	222	100%
$[m^+ + 1]$	223	13.5%
$[m^+ + 2]$	224	1.0%

⇒ The molecular ion % of R.A is 100%

⇒ Apply nitrogen rule,

"The molecular ion m/z is even ∴ zero/even no. of nitrogen are present.

⇒ $(m^+ + 2)$ peak intensity is 1.0%. It indicates the absence of S, Cl and Br.

⇒ No. of carbon's $= \dfrac{m^+ + 1 \text{ intensity}}{1.1}$

$= \dfrac{13.5}{1.1}$

$= \sim 12$

⇒ No. of hydrogen's $= m^+ m/z - \text{mass of carbon}$

$= 222 - 12(12)$

$= 222 - 144$

$= 78$

⇒ Let us assume the presence of 4 oxygen atoms

⇒ no. of H's $= 78 - 64$

$= 14$

∴ The molecular formula can be given/calculated as "$C_{12}H_{14}O_4$".

$$\Rightarrow DBE = \frac{\text{no. of C's}}{} - \frac{\text{no. of H's}}{2} - \frac{\text{no. of X's}}{2} + \frac{\text{no. of N's}}{2} + 1$$

$$= 12 - \frac{14}{2} - 0/2 + 0/2 + 1$$

$$= 13 - 7$$

$$= 6$$

IR data :-

3010 cm^{-1}	=C-H stretch
1720 cm^{-1}	C=O (Ketone)
1470 cm^{-1}	C=C ring stretch
1380 cm^{-1}	sp^3 C-H stretch
1205 cm^{-1}	sp^3 C-H stretch
880 cm^{-1}	P-disubstituted benzene

UV data :-

220 nm	$\pi \sim \pi^*$
300 nm	$n \sim \pi^*$

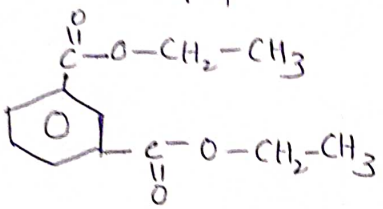
^{13}C-NMR data :-

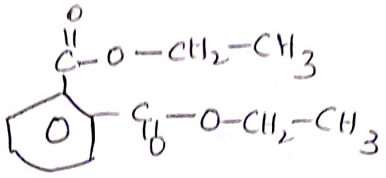
8 δ	quatet
61 δ	Triplet
130 δ	doublet

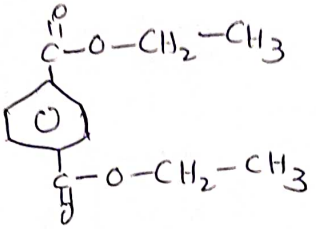
H^1-NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	1.2 δ	Triplet	18	18/3 = 6	6	CH_3 , CH_3
02.	4.4 δ	Singlet	12	12/3 = 4	4	H_2C . CH_2
03.	7.2 δ	Singlet	12	12/3 = 4	4	

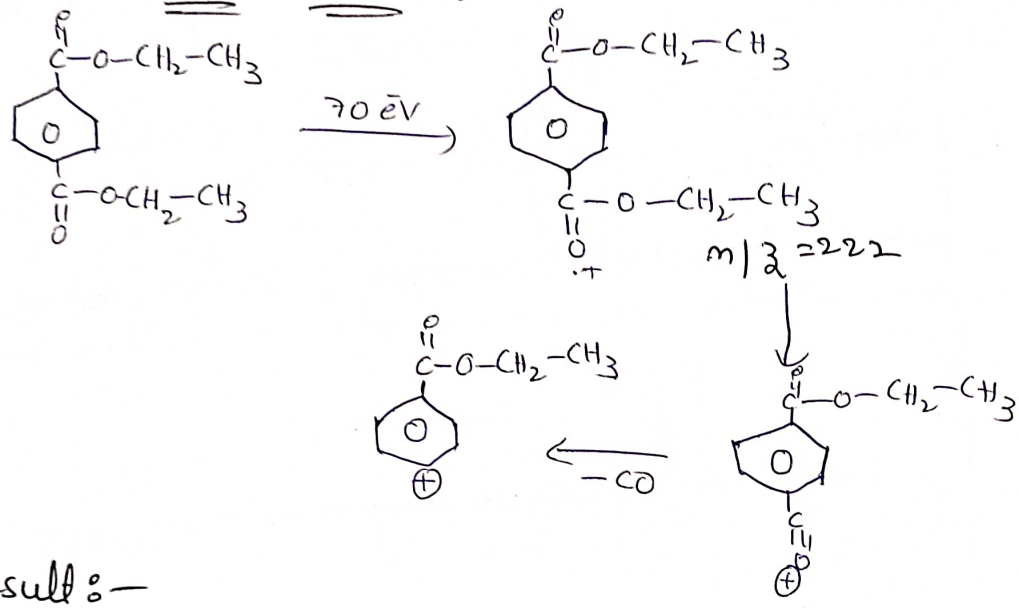
Based on the above data. The possible structure for "$C_{12}H_{14}O_4$". are

i) 

(ii) 

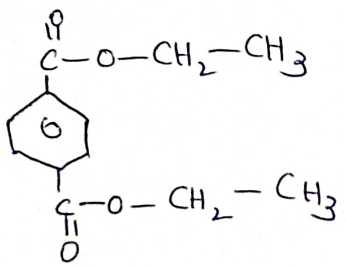
(iii) 

mass fragmentation :-



Result :-

Based on the above four spectral data's the given spectral sheeth belongs to the following structure containing compound.



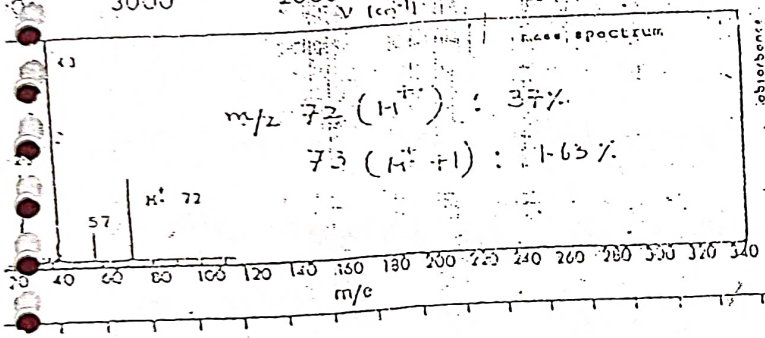
Diethyl Terephthalate

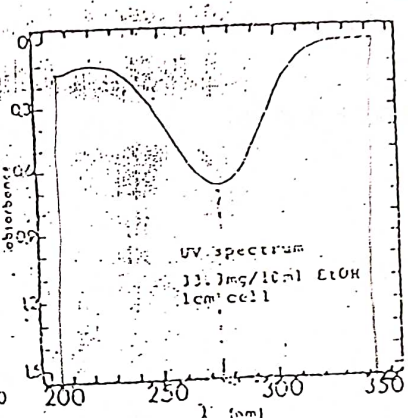
10

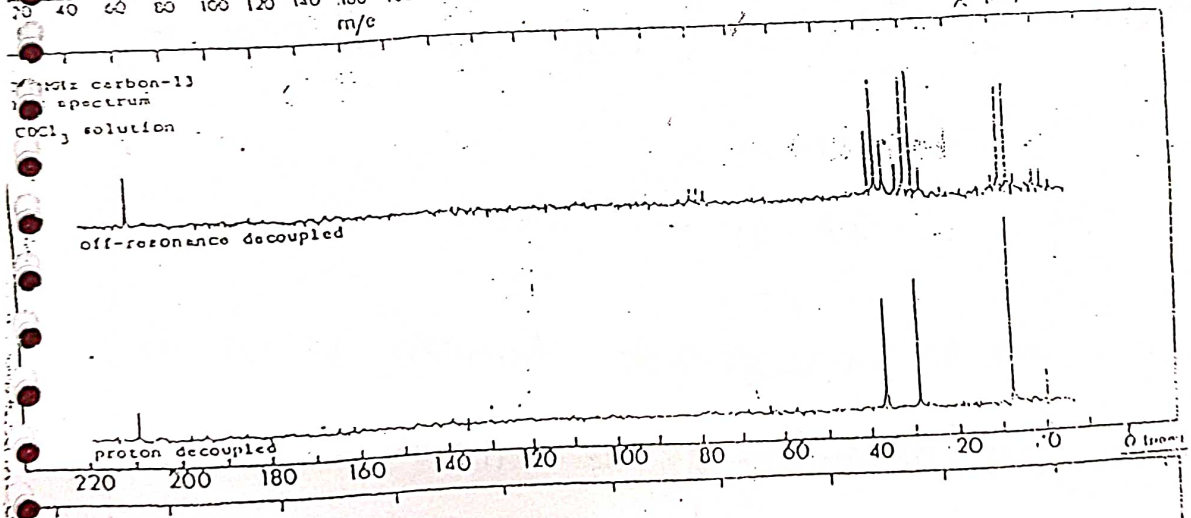
(1)

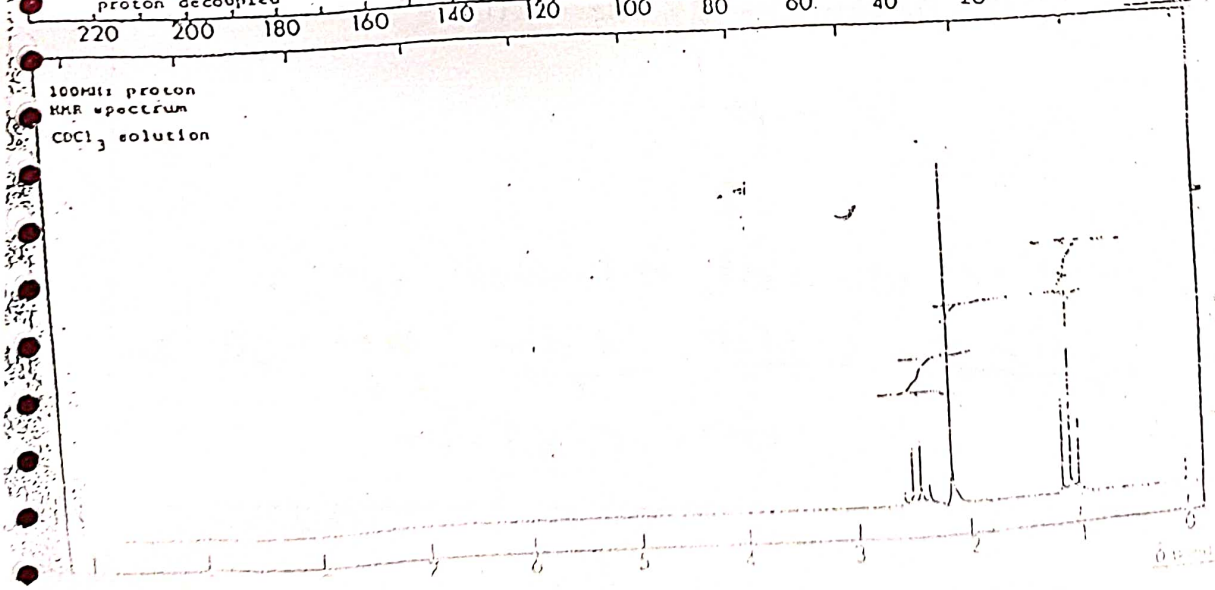
(4)


IR spectrum
(liquid film)
1705
3000
2000
1600
1200
800
ν (cm⁻¹)


(1)
mass spectrum
m/z 72 (M⁺) : 37%
73 (M⁺+1) : 1·63%
M⁺ 72
57
m/e


UV spectrum
absorbance
λ (nm)


spectrum
CDCl3 solution
off-resonance decoupled
proton decoupled
220
200
180
160
140
120
100
80
60
40
20
0


100MHz proton
NMR spectrum
CDCl3 solution

Spectral Problem - IV

Mass spectral data :-

	m/z	% of R.A	
M^+	72	37	$37/37 \times 100 = 100\%$
$[m^+ + 1)$	73	1.67%	$1.63/37 \times 100 = 4.5\%$

⇒ The molecular ion m/z is even. According to nitrogen rule "even/zero no. of nitrogens are present.

⇒ $m^+ + 2$ peak intensity is absent, it indicates the absence of S, Cl, and Br.

⇒ Number of hydrogens = M^+ m/z − mass of 'c'

$= 72 - 12\,(4)$

$= 72 - 48$

$= 24$

⇒ Let us assume the presence of one oxygen atom,

⇒ no. of H's = 24 − mass of oxygen

$= 24 - 16$

$= 8$

∴ The molecular formula is "C_4H_8O"

⇒ $D_{BE} = \text{no of C's} - \frac{\text{no. of H's}}{2} - \frac{\text{no. of X's}}{2} + \frac{\text{no. of N's}}{2} + 1$

$= 4 - 8/2 - 0/2 + 0/2 + 1$

$= 1$

UV data :-

225 nm $\pi \sim \pi^*$ transition

320 nm $n \sim \pi^*$ Transition

IR data :-

2900 cm^{-1} sp^3, C-H (stretch)

1705 cm^{-1} C=O (Stretch)

1370 cm^{-1} sp^3, C-H (bend)

1200 cm^{-1} sp^3, C-C (stretch)

1050 cm^{-1} C-O (stretch)

H^1 NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	1.1δ	Triplet	9	9/3=3	3	CH_3
02.	2.2δ	Singlet	9	9/3=3	3	CH_3
03.	2.5δ	Quatet	6	6/3=2	2	CH_2

^{13}C -NMR data :-

14δ quatet (CH_3)

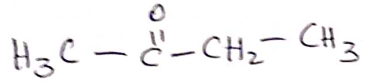
29δ quatet (CH_3)

37δ Triplet (CH_2)

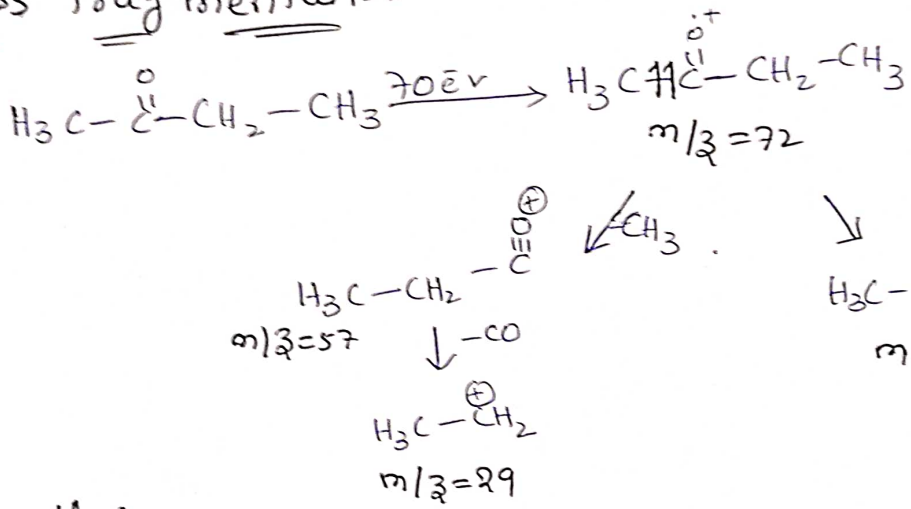
Based on the above data's, The possible structure for "C_4H_8O" are

i) $H_3C-CH_2-\overset{O}{\overset{\|}{C}}-CH_3$ ii) $H_3C-CH_2-CH_2-\overset{O}{\overset{\|}{C}}-H$

In the above structure's. structure (i) co-relates with H^1-NMR and ^{13}C-NMR spectral data ∴ The correct structure is,

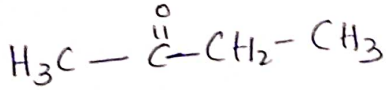


Mass fragmentation :-



Result :-

Based on the above four spectral data's. The given spectral sheeth belongs to the following structure containing compound.



2-butanone