DR. BRR GOVERNMENT DEGREE COLLEGE, JADCHERLA, MAHABUBNAGAR (Dist.).

DEPARTMENT OF CHEMISTRY

Title of the Project

Interpretation of Spectral data of
1. 2 - Phenyl ethanol
2. Cinnamaldehyde
3. 2 - Chloro 2 - methyl butane
4. Ethyl iodide

By

Sl. No	Name of the student	H. T. No	Group
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2	T. Maheshwari	20033006441056	M.P.C EM
3	E. Nagalaxmi	20033006441012	M.P.C EM
4	J. Sowmya	20033006441019	M.P.C EM
5	P. Shireesha	20033006441044	M.P.C EM
6	K. Girija	20033006441026	M.P.C EM

Supervision by

A. RAJANI

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Jadcherla-509 301

CERTIFICATE

This is to certify that the student study project on Interpretation of Spectral data of 1. 2 - Pheny ethanol, 2. Cinnamaldehyde, 3. 2 - Chloro 2 - methyl butane, 4. Ethyl iodide is a bonafide project work done by N. Mahesh, T. Maheshwari, E. Nagalaxmi, J. Sowmya, P. Shireesha and K. Girija under my supervision in the department of Chemistry, Dr. BRR. Government Degree college, Jadcherla, Telangana state.

Date: 25.05.2023

Place: JADCHERLA

(A. RAJANI)

supervisor

DECLARATION

We are hereby declare that the study project on Interpretation of Spectral data of 1. 2 - Pheny ethanol, 2. Cinnamaldehyde, 3. 2 - Chloro 2 - methyl butane, 4. Ethyl iodide is a record work done by us under the supervision of A. RAJANI, 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	N. Mahesh	20033006441041	M.P.C EM	N. Mahesh
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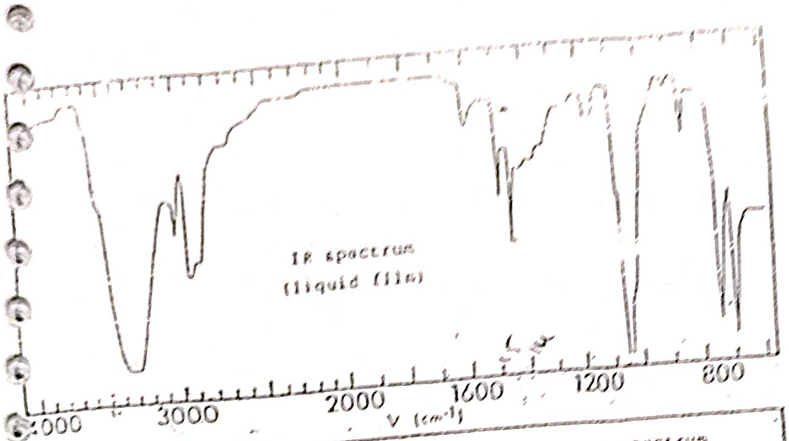
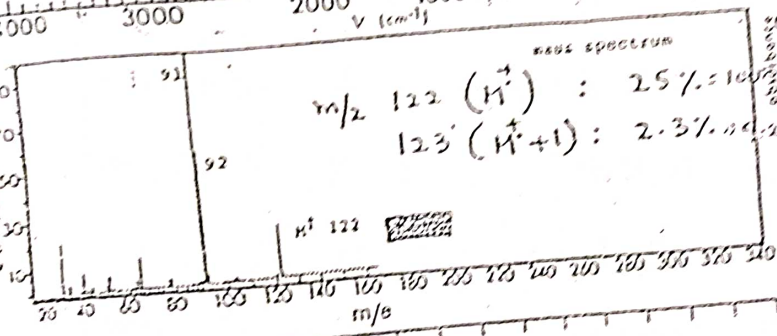
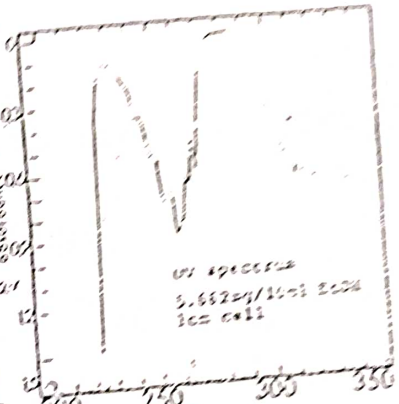
4	J. Sowmya	20033006441019	M.P.C EM	Sowmya
5	P. Shireesha	20033006441044	M.P.C EM	Shireesha
6	K. Girija	20033006441026	M.P.C EM	Girija

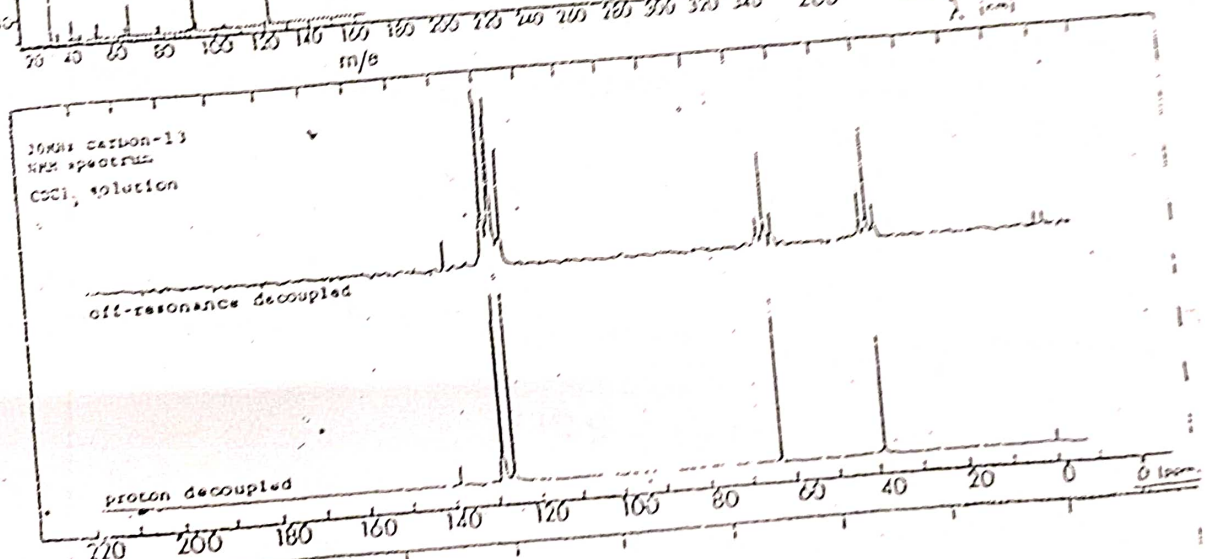
(7)

(10)


IR spectrum
(liquid film)
4000
3000
2000
1600
1200
800
ν (cm⁻¹)


mass spectrum
m/z 122 (M⁺) : 25% = 100
123 (M⁺+1) : 2.3% = 9.2
M⁺ 122
92
m/e


UV spectrum
0.662 mg/10ml EtOH
1cm cell
λ (nm)


100MHz carbon-13
NMR spectrum
CDCl₃ solution
off-resonance decoupled
proton decoupled
220
200
180
160
140
120
100
80
60
40
20
0
δ (ppm)


100MHz proton NMR spectrum
CDCl₃ solution
exchanges with D₂O

Spectral Problem - VII

mass Spectral data :-

	m/z	% of R.A
m^+	122	25 100%
$m^+ + 1$	123	2.3 9.2%

⇒ The molecular ion % of R.A is 100%.

⇒ Apply nitrogen rule,

The molecular ion m/z is even ∴ zero/even number of nitrogens are present

⇒ m+2 peak is absent. It indicates the absence of S, Cl and Br.

⇒ Number of Carbon's = $\frac{m^+ + 1 \text{ intensity}}{^{13}C \text{ intensity}}$

$= 92/1.1$

$= \sim 8$

⇒ No. of H's $= m^+$ m/z − mass of caron

$= 122 - 12(8)$

$= 122 - 96$

$= 26.$

Assume the presence of one oxygen atom

⇒ no. of H's $= 26 -$ mass of 'O'

$= 26 - 16 = 10$

∴ The molecular formula is given as "$C_8H_{10}O$".

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

$$= 8 - \frac{10}{2} - \frac{0}{2} + \frac{0}{2} + 1$$

$$= 9 - 5$$

$$= 4.$$

IR data :-

$3300\ cm^{-1}$	OH stretch
$1450\ cm^{-1}$	$HC=CH$ stretch
$1050\ cm^{-1}$	C–O (stretch)
$1450\ cm^{-1}$	mono substituted benzene

UV data :-

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

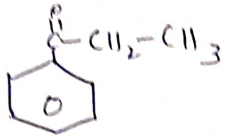
^{13}C- NMR data :-

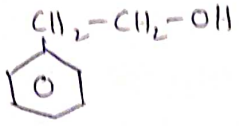
39δ	Triplet
63δ	Triplet
128δ	Triplet

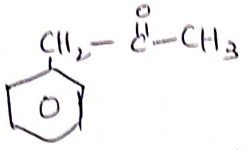
^1H-NMR data :-

S.No	δ value	multiplicity	Integration	no. of H's	Interference
01.	2.2	Singlet	3/3	1	OH
02.	2.8	Triplet	6/3	2	CH_2
03.	3.8	Triplet	6/3	2	CH_2
04.	7.2	Singlet	15/3	5	

Based on the above data the possible structure for $C_8H_{10}O$ are,

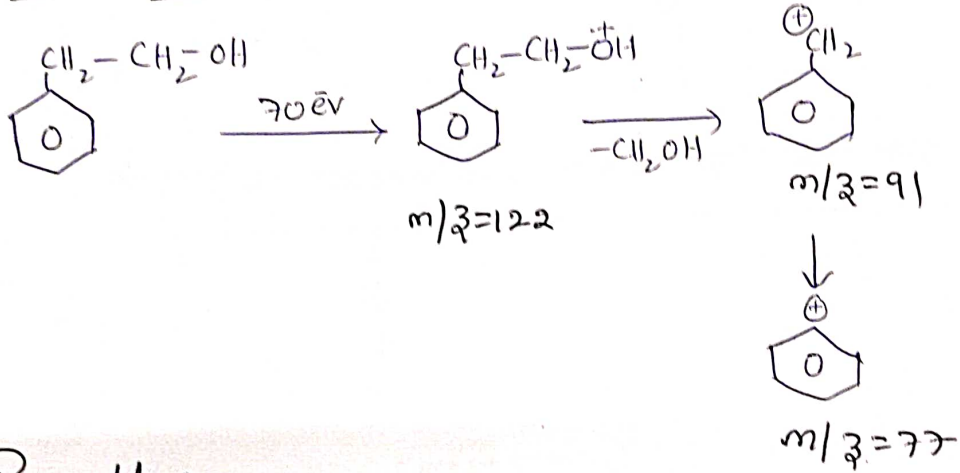
i) 

ii) 

iii) 

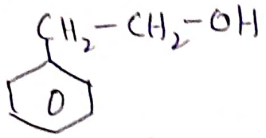
Based on H^1-NMR and ^{13}C-NMR spectral data structure (ii) is correct.

Mass fragmentation



Result :-

Based on the above four spectral data's. The given spectral sheeth belongs to 2-phenyl ethanol

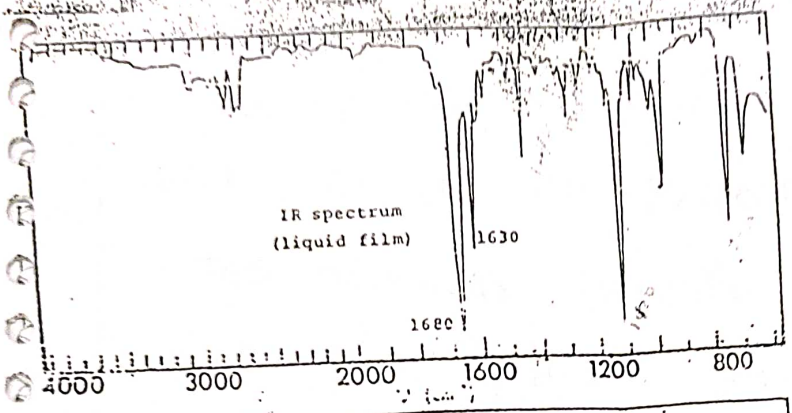


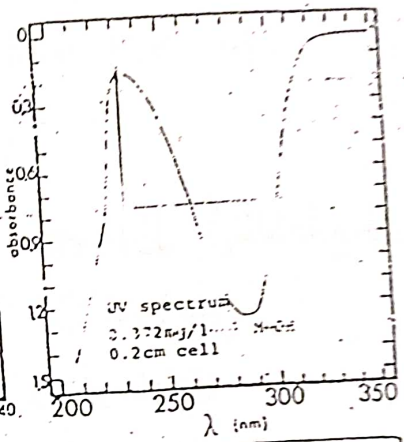
(13)

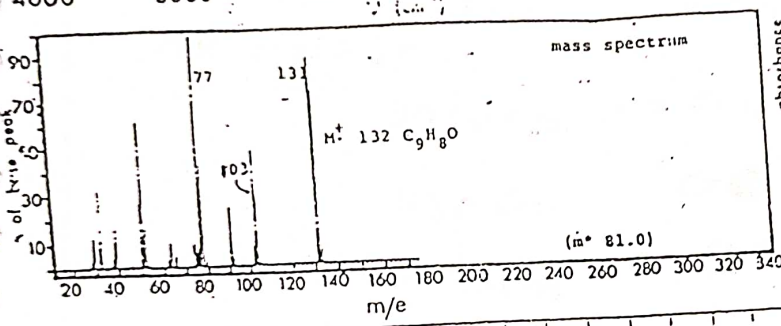
17

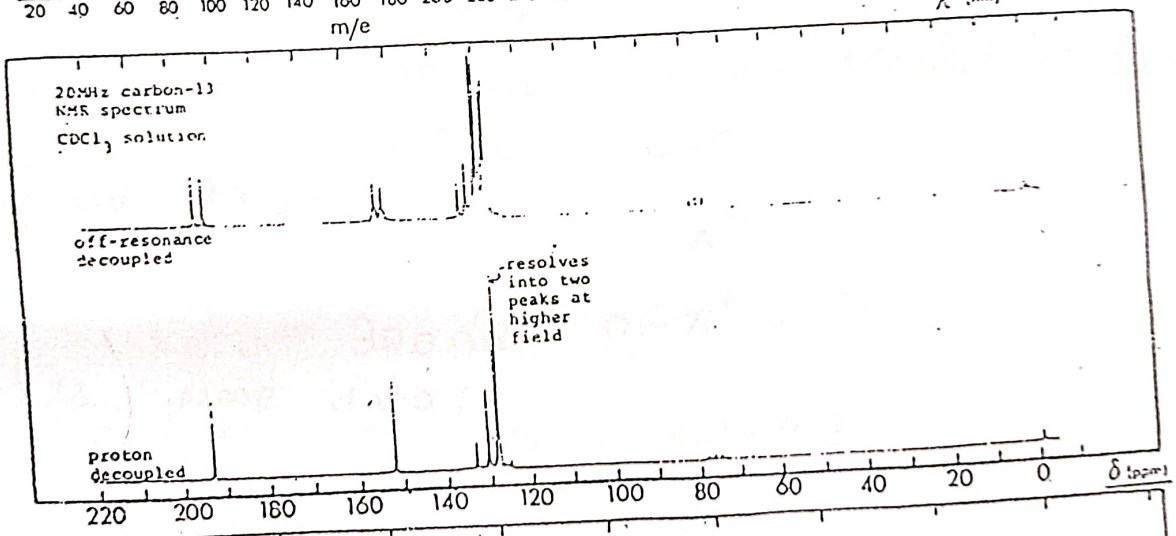
(13)

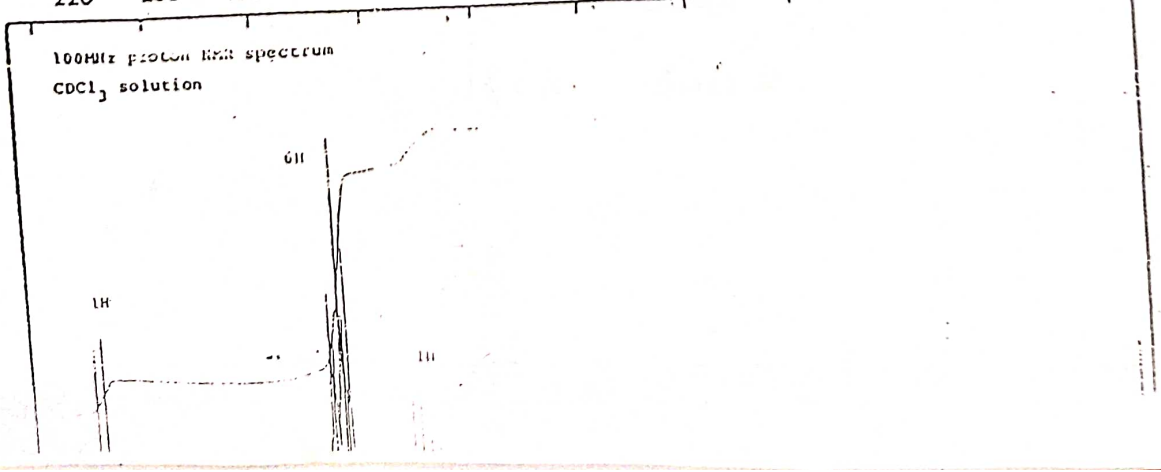
problem 52











Spectral Problem- XIII

mass spectral data :-

In the mass spectral m/z = 132, 103, 77 containing peaks are observed

The nt m/z is even (i.e, 132) ∴ even/zero no. of nitrogen are present.

The molecular formula for the given spectral sheeth is. "C_9H_8O".

IR data :-

2780 cm^{-1}	=C-H stretch (aldehyde)
1680 cm^{-1}	C=C (stretch)
1470 cm^{-1}	C=C (stretch)
690 cm^{-1}	mono substituted benzene
1630 cm^{-1}	C=O

UV data :-

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

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

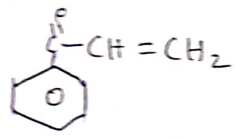
^{13}C- NMR data :-

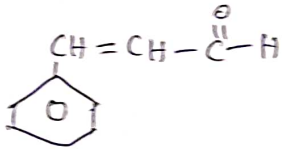
129 δ	multiplet
151 δ	doublet
192 δ	doublet

· H^1 NMR data :-

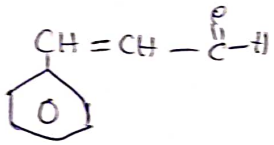
S.No	δ value	multiplicity	Integration	Ratio	no of H's	Interference
01.	6.1	doublet of	–	–	1H	=CH–
02.	7.2	doublet septate	–	–	6H	
03.	9.8	doublet	–	–	1H	aldehydic 'H'

Based on the above data the possible structures for "C_9H_8O". are

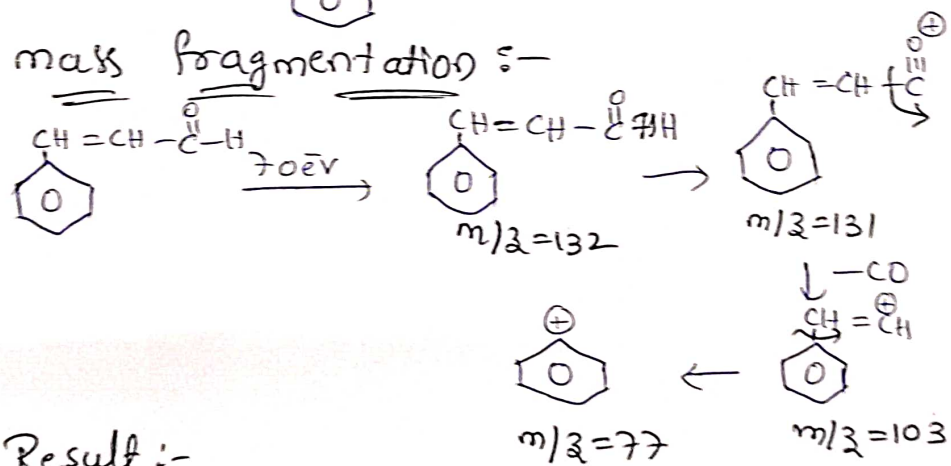
i) 

ii) 

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

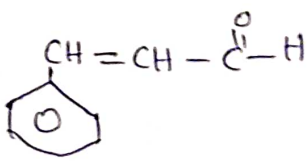


mass fragmentation :-



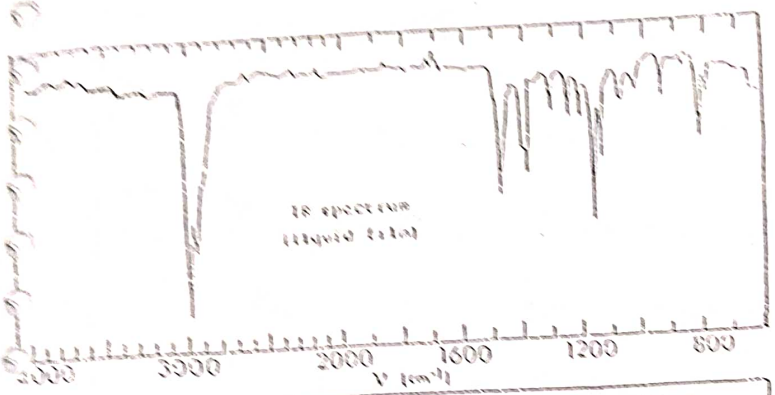
Result :-

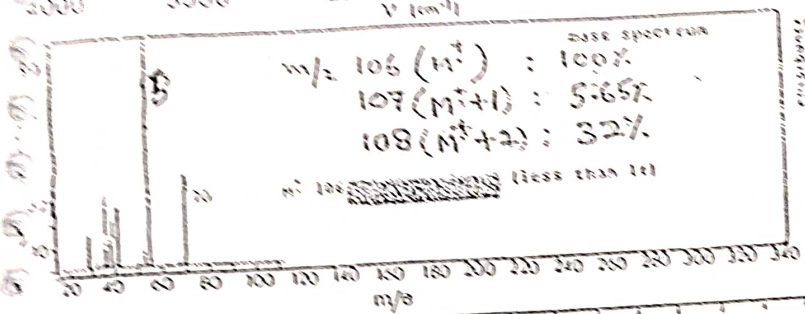
Based on the above four spectral data the given spectral sheath belongs to the following structure containing compound.

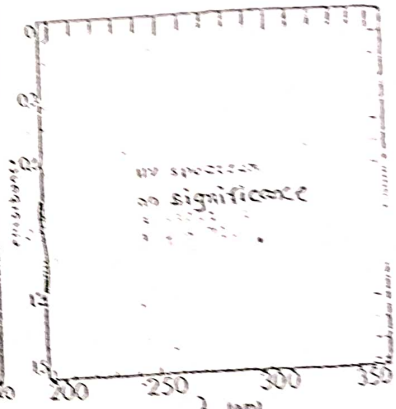


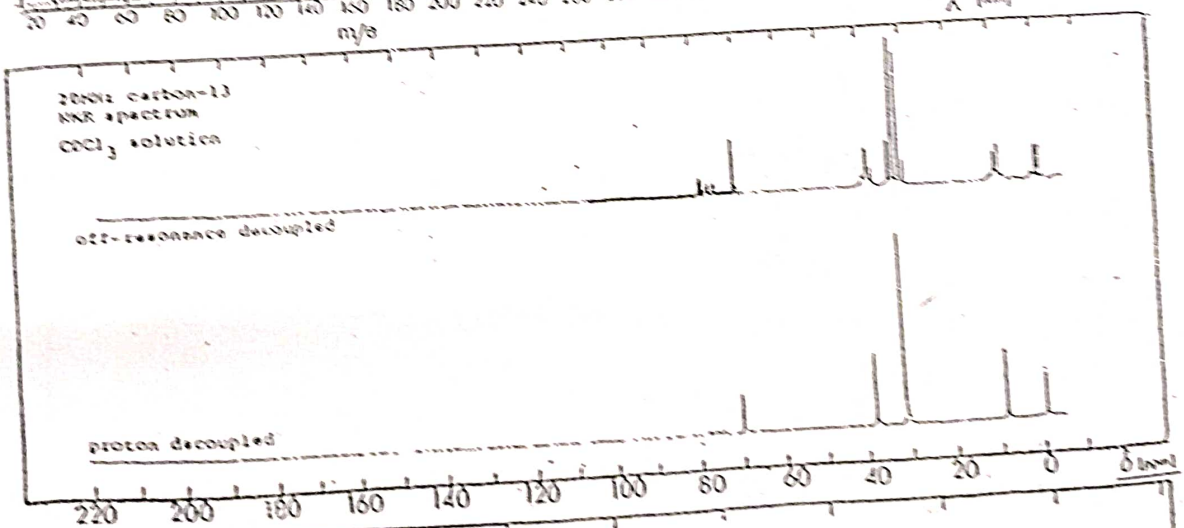
(16)

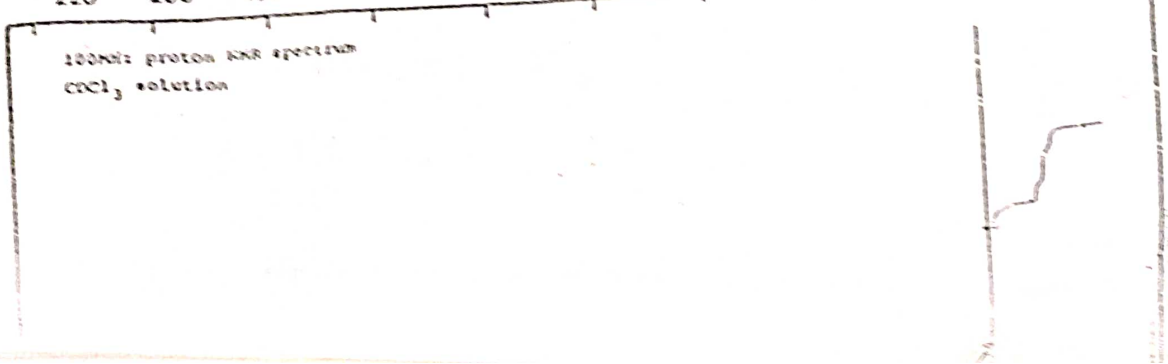
(17)


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


mass spectrum
m/z 106 (M⁺) : 100%
107 (M⁺+1) : 5·65%
108 (M⁺+2) : 32%
m/e


UV spectrum
no significance
200
250
300
350
λ (nm)


100Hz carbon-13
NMR spectrum
CDCl3 solution
off-resonance decoupled
proton decoupled
220
200
180
160
140
120
100
80
60
40
20
0
δ (ppm)


100MHz proton NMR spectrum
CDCl3 solution

Spectral Problem – XVI

mass spectral data :-

	m/z	% of R.A
M^+	106	100%
$[m^+ + 1]$	107	5.65%
$[m^+ + 2]$	108	32%

⇒ 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 32%, It indicates. The presence of "Cl" atom.

⇒ Number of carbons = $\frac{m^+ + 1 \text{ intensity}}{^{13}C \text{ intensity}}$

$= 5.65/1.1$

$= \sim 5$

⇒ Number of hydrogens = m^+ m/z – mass of carbon

$= 106 - 12(5)$

$= 106 - 60$

$= 46$

⇒ Let us assume the presence of one 'Cl' atom

⇒ no. of H's $= 46 - 35 = 11$

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

$$= 5 - 11/2 - 1/2 + 0/2 + 1$$

$$= 6 - 12/2$$

$$= 0$$

IR data :-

2990 cm^{-1} sp^3, C-H (stretch)

1470 cm^{-1} sp^3, C-H (bend)

1210 cm^{-1} C-C (stretch)

780 cm^{-1} C-Cl

UV data :-

Not significant

^{13}C-NMR data :-

198 doublet (CH_2)

30δ quatlet (CH_3)

39δ Triplet (CH_2)

70δ Singlet (C-Cl)

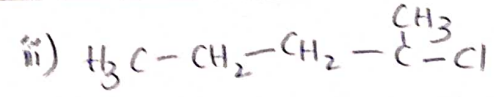
^1H-NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no.of H's	Interference
01.	1	Triplet	9	9/3 = 3	3	CH_3
02.	1.6	singlet	18	18/3 = 6	6	CH_3 / CH_3
03.	1.8	Quatet	6	6/3 = 2	2	CH_2

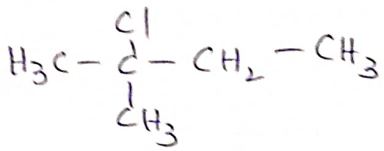
The possible structures for "$C_5H_{11}Cl$" are

(i) $H_3C-\underset{Cl}{\overset{CH_3}{\underset{|}{\overset{|}{C}}}}-CH_2-CH_3$

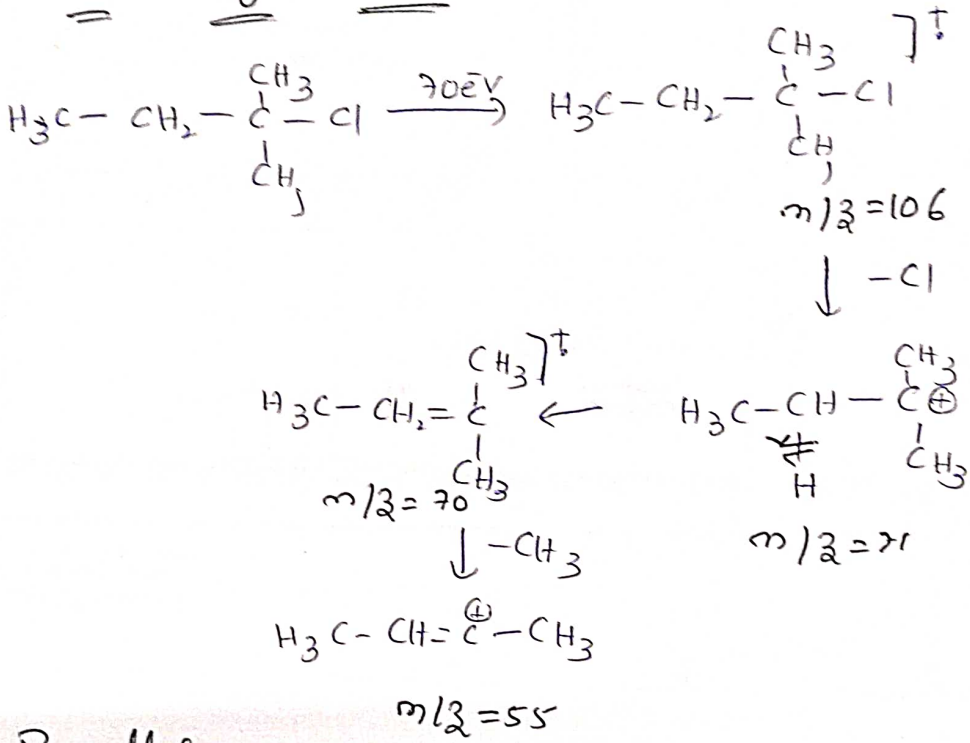
(ii) $H_3C-\underset{Cl}{\overset{CH_3}{\underset{|}{\overset{|}{C}}}}-CH-CH_3$

ii) 

Based on the above data structure (i) co-relates perfectly with NMR data. ∴ The correct structure is

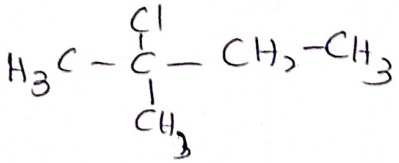


mass fragmentation :-



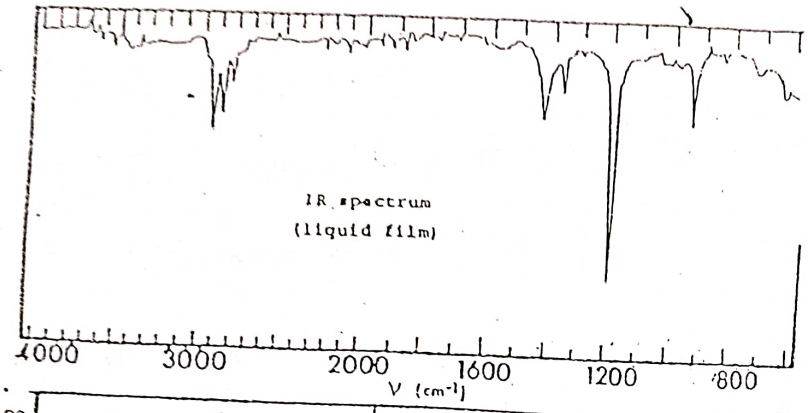
Result :-

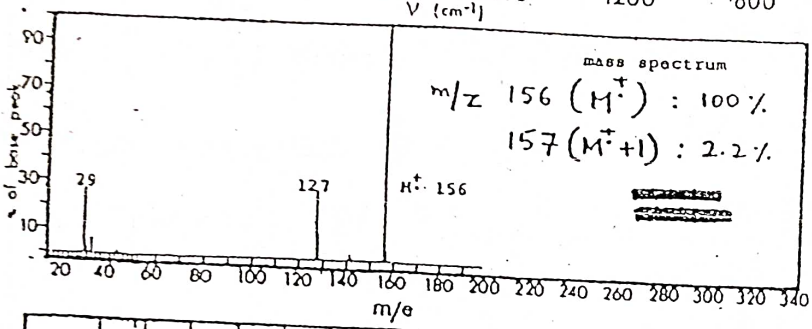
Based on the above the four spectral data. the given spectral sheeth belongs to 2 chloro 2-methyl butane

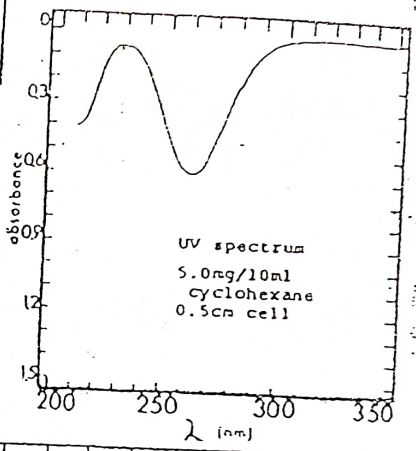


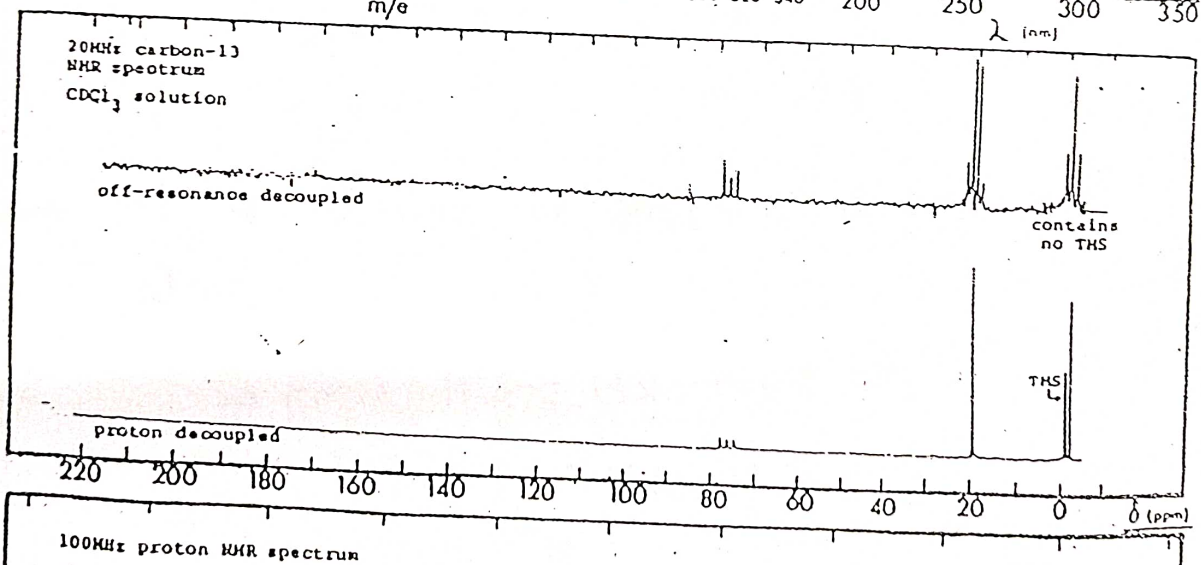
(6)

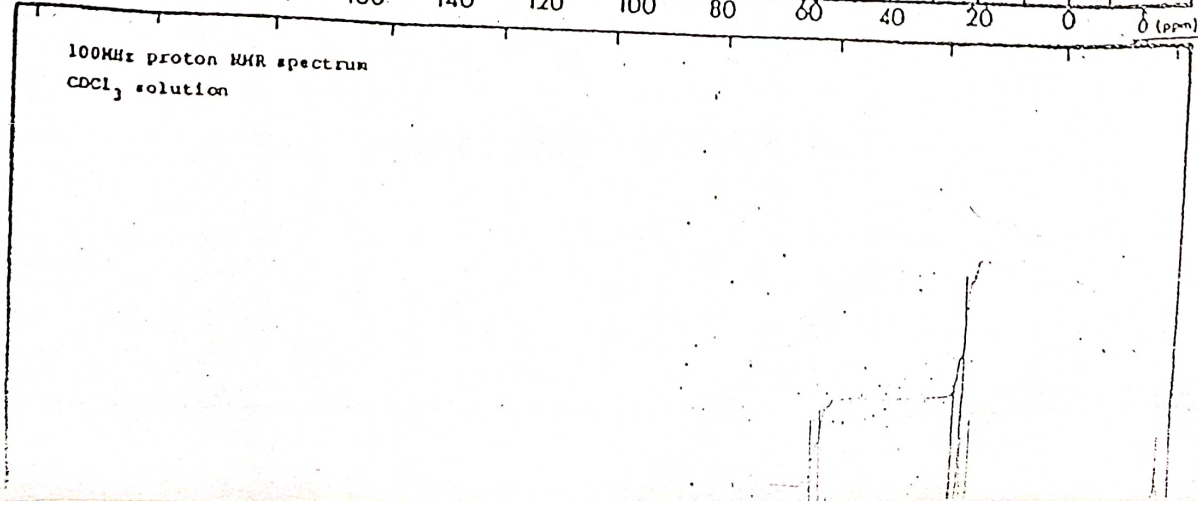
(6)


IR spectrum
(liquid film)
4000
3000
2000
1600
1200
800
ν (cm⁻¹)


mass spectrum
m/z 156 (M⁺) : 100 %
157 (M⁺+1) : 2.2 %
29
127
M⁺ 156
% of base peak
m/e


UV spectrum
5.0mg/10ml
cyclohexane
0.5cm cell
absorbance
λ (nm)


20MHz carbon-13
NMR spectrum
CDCl3 solution
off-resonance decoupled
contains
no TMS
TMS
proton decoupled
δ (ppm)


100MHz proton NMR spectrum
CDCl3 solution

Spectral Problem - VI

Mass spectral data :-

	m/z	% of R.A
M^+	156	100%
$(m^+ + 1)$	157	2.2%

⇒ The molecular ion m/z is even(156). According to nitrogen rule even/zero number 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 Carbon

$= 156 - 12(2)$

$= 156 - 24$

$= 132$

⇒ Let us assume The presence of one iodine atom,

⇒ no. of H's = 132 − mass of 'I'

$= 132 - 127$

$= 5$

∴ The molecular formula is "C_2H_5I".

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

$$= 2 - \frac{5}{2} - \frac{1}{2} + \frac{0}{2} + 1$$

$$= 3\left[\frac{-5-1}{2}\right]$$

$$= 3 - 6/2$$

$$= 0$$

UV data :-

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

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

IR data :-

2980 cm^{-1} sp^3, C-H (stretch)

1420 cm^{-1} sp^3, C-H (bend)

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

H^1 NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Inter ference
01.	1.9δ	Triplet	18	18/6	3	CH_3
02.	3.3δ	quatet	12	12/6	2	CH_2

^{13}C data :-

δ value	type of carbon
0δ	Triplet (CH_2)
19δ	quatet (CH_3)

Based on the above data the possible structure is,

H_3C-CH_2-I

mass fragmentation

$$H_3C-CH_2-I \xrightarrow{70eV} H_3C-CH_2-I^{+\cdot}$$

$$\downarrow$$

$$H_3C-\overset{\oplus}{C}H_2 + I^{\oplus}$$

$m/z = 29$ $\quad$ $m/z = 127$

Result :-

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

H_3C-CH_2-I