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

DEPARTMENT OF CHEMISTRY

Title of the Project

Interpretation of Spectral data of

1. 1 - Phenyl acetone

2. 4, 4 -Di methoxy 2 - butanone

3. 3 - Phenyl propyl bromide

4. 1 -Phenyl ethanol-1

By

Sl. No	Name of the student	H. T. No	Group
1	K. Naveen	20033006441028	M.P.C EM
2	Y. Anusha	20033006441059	M.P.C EM
3	S. Sandhya	20033006441053	M.P.C EM
4	M. Rajesh	20033006441033	M.P.C EM
5	P. Shireesha	20033006441048	M.P.C EM
6	M.D. Saleem	20033006441035	M.P.C EM

Supervision by

J. VIKRAM KUMAR

Assistant Professor of Chemistry

HOD
Lecturer in Chemistry
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Jadcherla-509 301

CERTIFICATE

This is to certify that the student study project on

Interpretation of Spectral data of 1. 1 - Phenyl acetone,2. 4,4 - Di methoxy 2 – butanone, 3. 3 - Phenyl propyl bromide, 4. 1 - Phenyl ethanol-1 is a bonafide project work done by K. Naveen , Y. Anusha, S. Sandhya, M. Rajesh, P. Shireesha and M.D. Saleem under my supervision in the department of Chemistry, Dr. BRR. Government Degree college, Jadcherla, Telangana state.

Date: 25.05.2023

Place: JADCHERLA

(J. VIKRAM KUMAR)

supervisor

DECLARATION

We are hereby declare that the study project on **Interpretation of Spectral data of 1. 1 - Phenyl acetone,2. 4,4 - Di methoxy 2 – butanone, 3. 3 - Phenyl propyl bromide, 4. 1 - Phenyl ethanol-1**is a record work done by us under the supervision of J. VIKRAM KUMAR, 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.

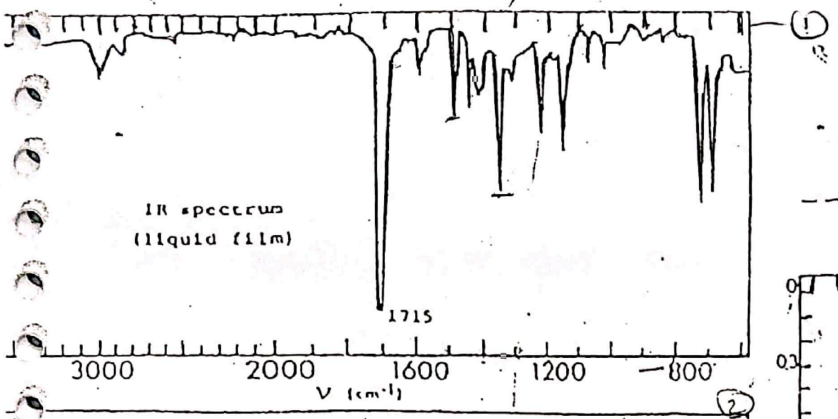
Date: 25.05.2023

Place: JADCHERLA

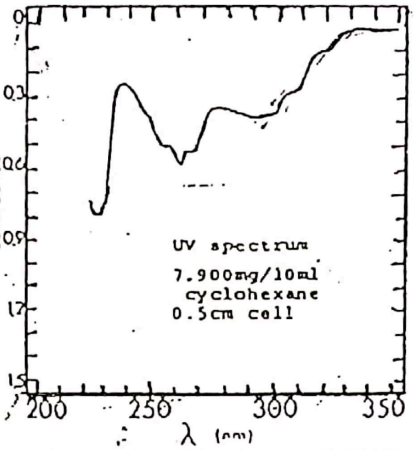
Sl. No	Name of the student	H. T. No	Group	Signature
1	K. Naveen	20033006441028	M.P.C EM	K. Naveen
2	Y. Anusha	20033006441059	M.P.C EM	Y. Anusha
3	S. Sandhya	20033006441053	M.P.C EM	S. Sandhya
4	M. Rajesh	20033006441033	M.P.C EM	M. RAJESH
5	P. Shireesha	20033006441048	M.P.C EM	P Shireesha
6	M.D. Saleem	20033006441035	M.P.C EM	MD. Saleem

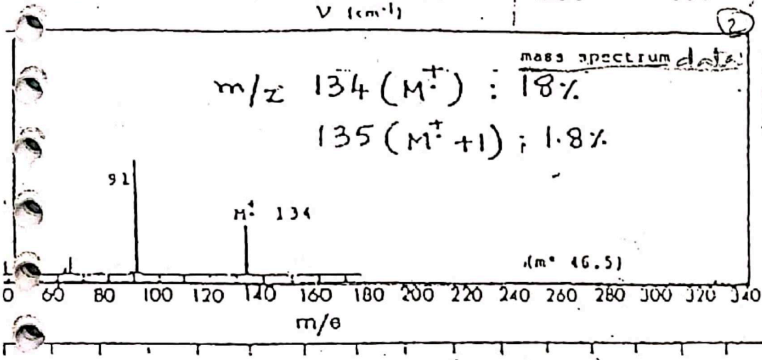
left side increase

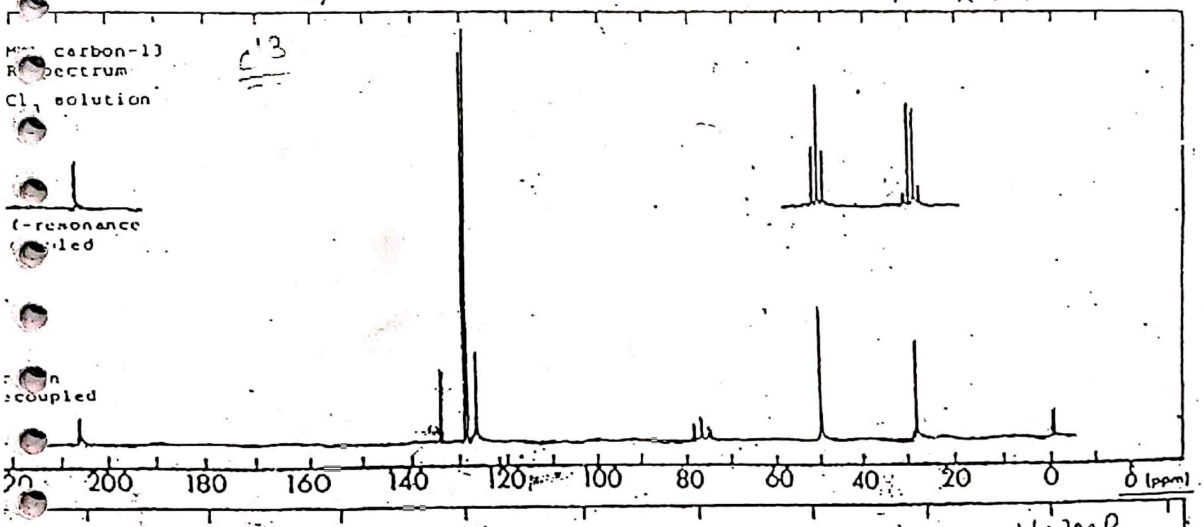
Right side decrease

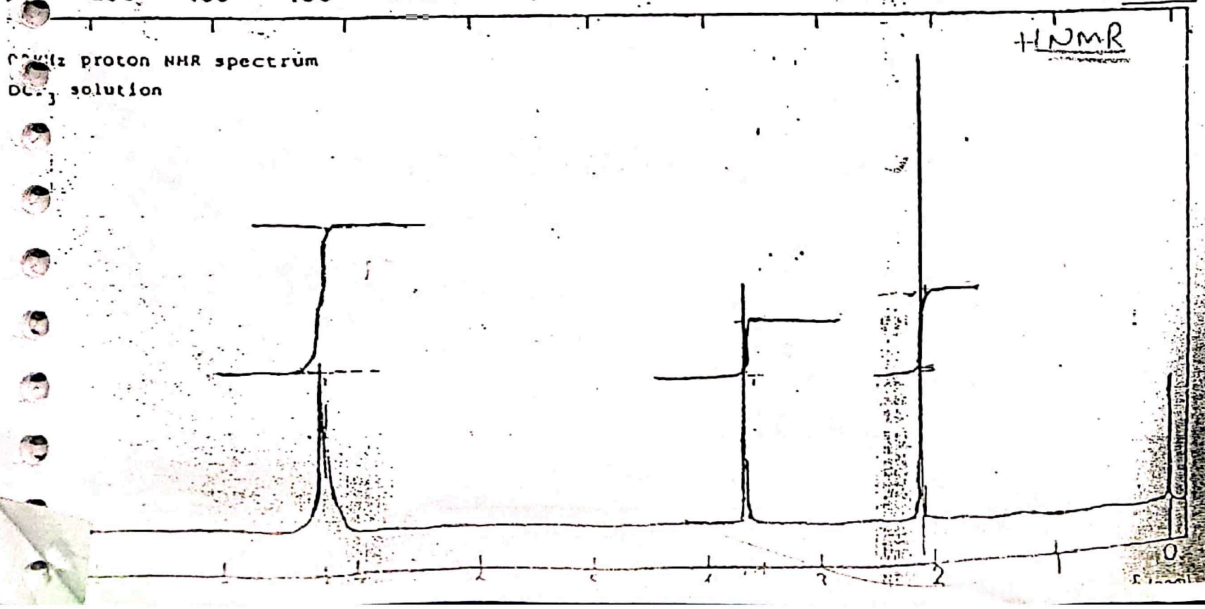


UV









Mass spectral data :-

M/z	% of R.A.	
134	18 %	$\frac{18}{18} \times 100 = 100\ \%$
$[m^+ + 1)$ 135	1.8 %	$1.8/18 \times 100 = 10\ \%$

⇒ The molecular ion % of R.A is used upto 100 %

⇒ Apply nitrogen rule,

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

M+2 peak intensity is absent, it indicates the absence of S, Cl, Br.

$$\text{Number of carbon's} = \frac{\dot{M}+1 \text{ intensity}}{^{13}C \text{ intensity}}$$

$$= \frac{10}{1.1}$$

$$= \sim 9$$

Number of Hydrogens = $\dot{m}$ m/z − mass of Carbon

$$= 134 - 12(9)$$

$$= 134 - 108$$

$$= 26$$

⇒ let us assume the presence of one oxygen atom

⇒ no of H's = 26 − 16

= 10

Therefore, The molecular formula is

"$C_9H_{10}O$"

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

$$= 9 - 10/2 - 0/2 + 0/2 + 1$$

$$= 10 - 5$$

$$= 5$$

It indicates that, aromatic benzene ring consisting side chain with one double bond.

UV data :-

λ_{max} = 235 nm indicates $\pi \rightarrow \pi^*$ transition

λ_{max} = 330 nm indicates $n \rightarrow \pi^*$ transition

IR data :

3000 cm^{-1}	sp^3, C-H (stretch)
1715 cm^{-1}	C=O stretch (aldehyde)
1450 cm^{-1}	C=C ring stretch
1350 cm^{-1}	sp^3, C-H (bend)
1200 cm^{-1}	sp^3, C-C (stretch)
690 cm^{-1}	mono substituted benzene

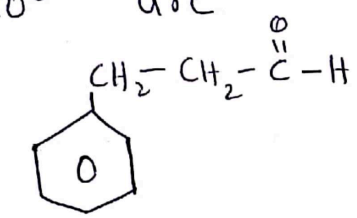
H^1 NMR data :-

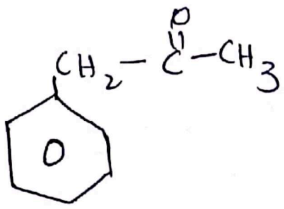
S.No	δ value	multiplicity	Integration	no of H's	Interference
01.	2.1	Singlet	12/4	3	H_3C
02.	3.7	Singlet	8/4	2	CH_2
03.	7.3	multiplet	20/4	5	

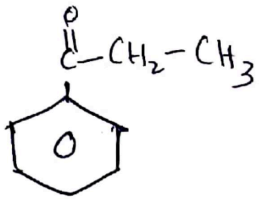
$^{13}_{c}$ data :-

δ value	Type of Carbon's
29 δ	quatet (CH_3)
50 δ	Triplet (CH_2)
128 δ	Singlet } Aromatic 'c'
129 δ	doublet } Aromatic 'c'
134 δ	singlet } Aromatic 'c'
207 δ	Singlet (carbonyl carbon)

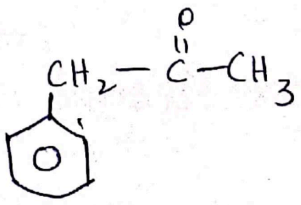
Based on above data. The possible structures for "$C_9H_{10}O$" are



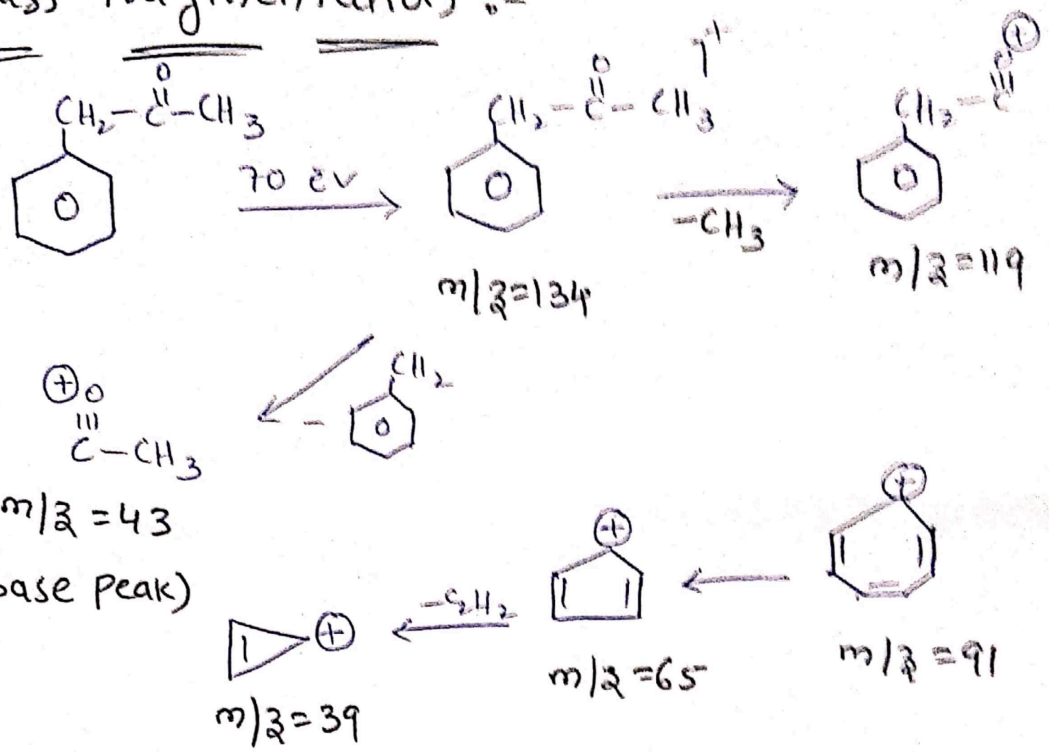




In the above structures. structure (ii) co-relates with the NMR data ∴ The connect structure is,

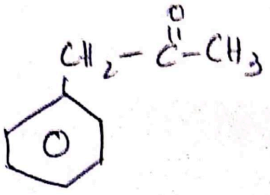


mass fragmentation :-



Result :-

Based on the above four spectral data's. The given spectral sheelh belongs to give the following structure consisting compound.

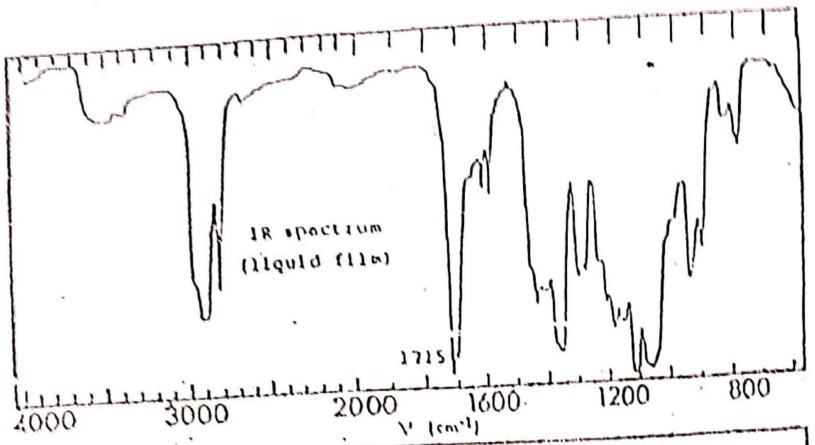


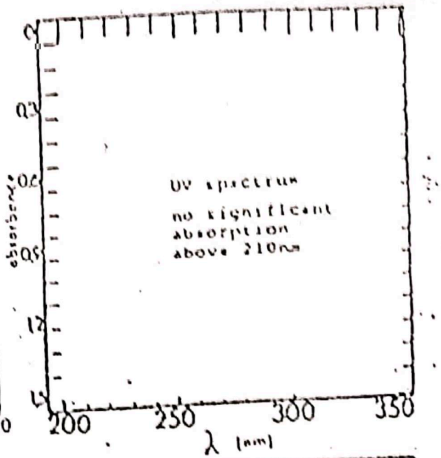
1-phenyl 2-propanone

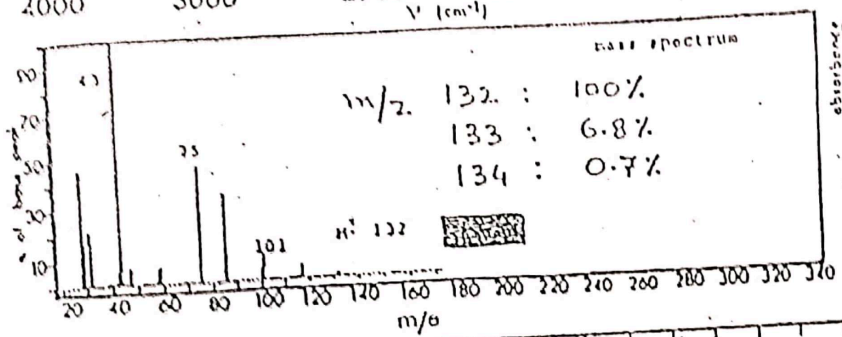
(or)

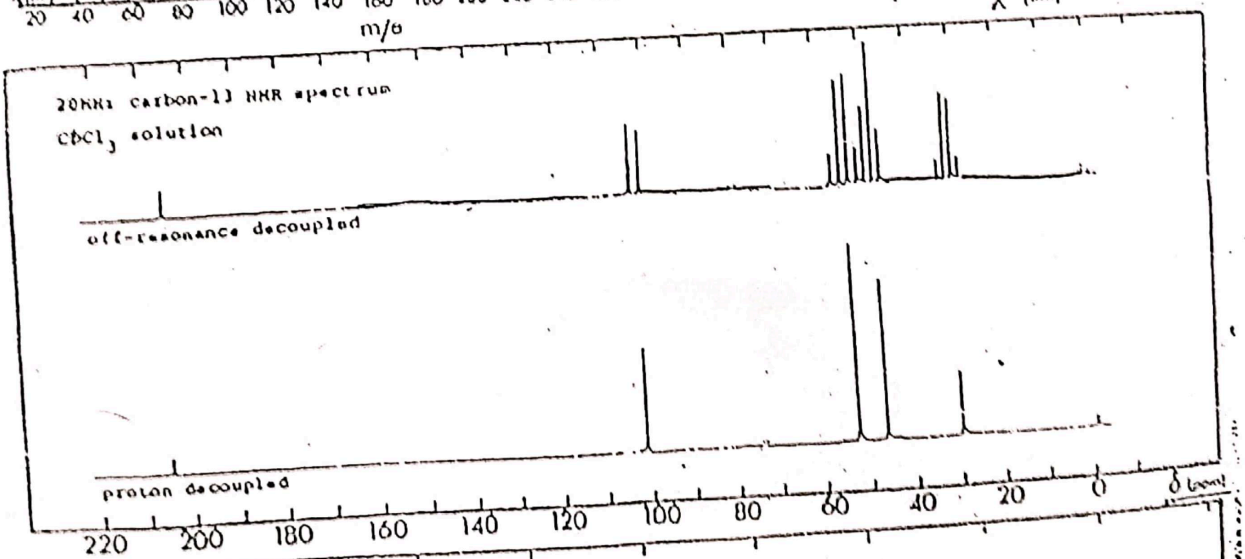
methyl benzyl lactone

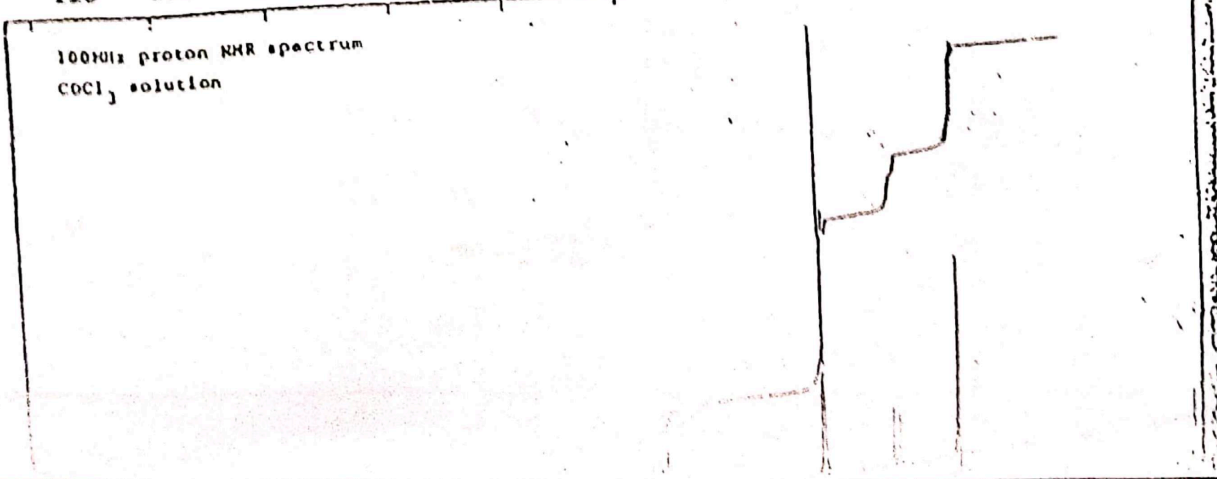
(17)











Spectral Problem – XVII

mass spectral data :-

	m/z	% of R.A
M^+	132	100%
$[m^+ + 1]$	133	6.8%
$[m^+ + 2]$	134	0.7%

⇒ The molecular ion % of R.A is 100%.

⇒ Apply nitrogen rule

The m^+ m/g is even ∴ zero/even no. of nitrogen are present

⇒ $m^+ + 2$ peak intensity is 0.7%. It indicates the absence of S, Cl and Br.

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

$= 6.8 / 1.1$

$= \sim 6$

⇒ Number of hydrogens = m^+ m/g – mass of 'C'

$= 132 - 12(6)$

$= 132 - 72$

$= 60$

⇒ Let us assume the presence of '3' oxygen atoms.

⇒ no. of H's $= 60 - 3(16)$

$= 60 - 48$

$= 12$

∴ The molecular formula is "$C_6H_{12}O_3$".

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

$$= 6 - 12/2 - 0/2 + 0/2 + 1$$

$$= 1$$

IR data :-

2980 cm^{-1}	sp^3 C-H (stretch)
2850 cm^{-1}	=C-H (aldehyde)
1715 cm^{-1}	C=O
1370 cm^{-1}	sp^3 C-H (bend)
1210 cm^{-1}	sp^3 C-C (stretch)

UV data :-

No significant absorption above 210 nm

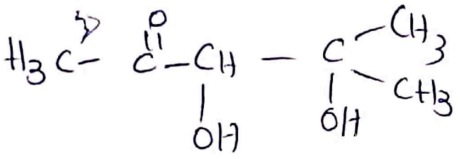
^{13}C-NMR data :-

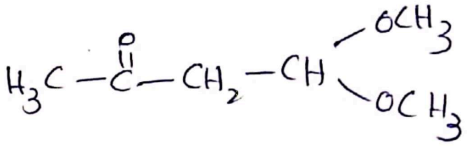
30 δ	quatet
46 δ	Triplet
53 δ	quatet
101 δ	doublet
206 δ	singlet

^1H-NMR data :-

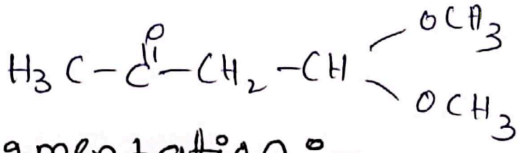
S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Inter ference
01.	2.1	singlet	12	12/4	3	CH_3
02.	2.6	doublet	8	8/4	2	CH_2
03.	3.3	Singlet	24	24/4	6	OCH_3 OCH_3
04.	4.7	Triplet	4	4/4	1	CH

∴ The possible structure for $C_6H_{12}O_3$ are

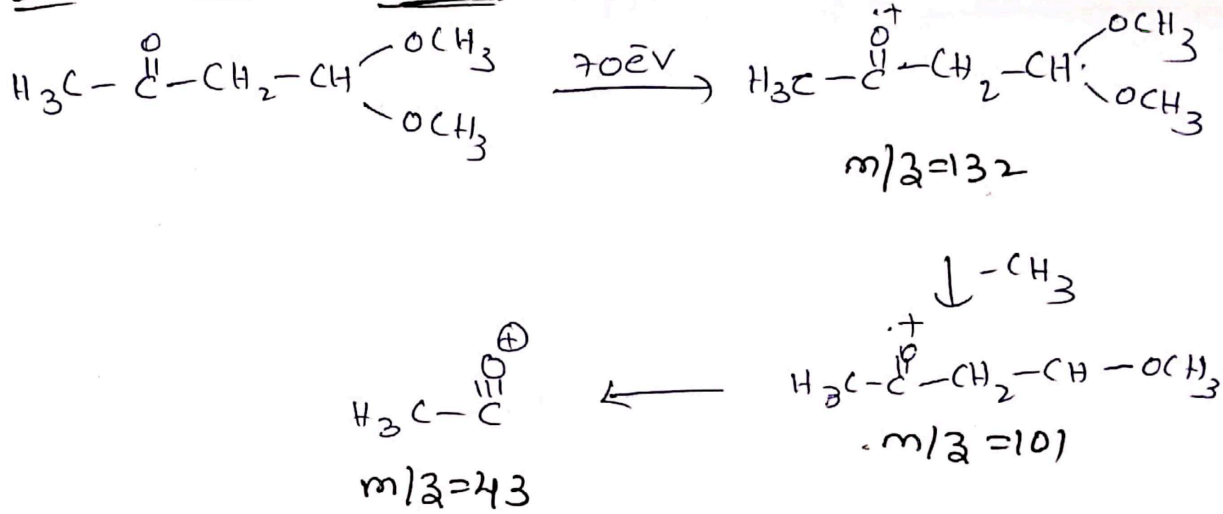
i) 

(ii) 

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

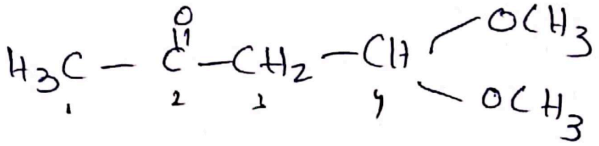


mass fragmentation :-

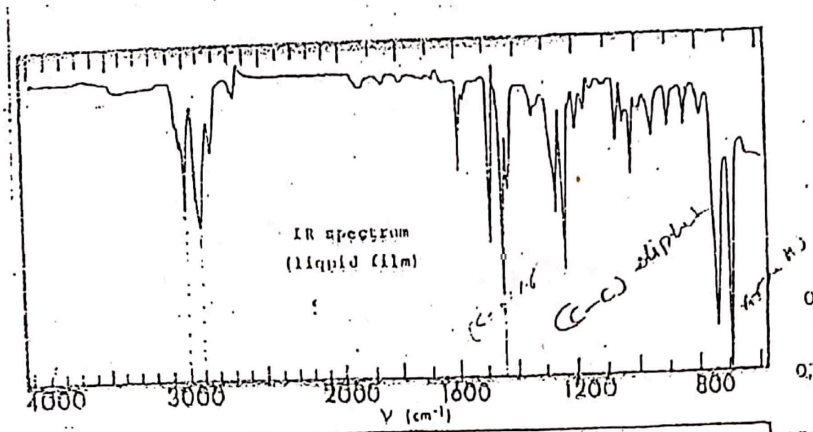


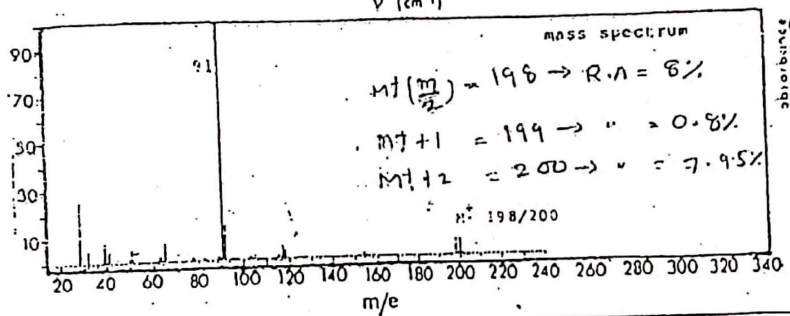
Result :-

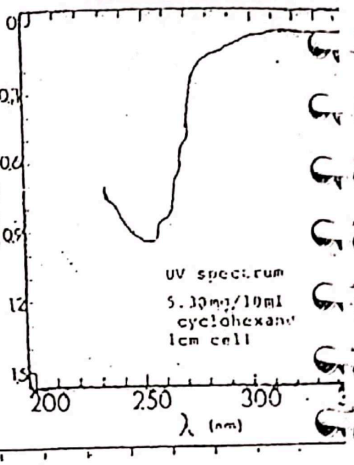
Based on the above four spectral data the given spectral sheeth belongs to the following structure containing compound.

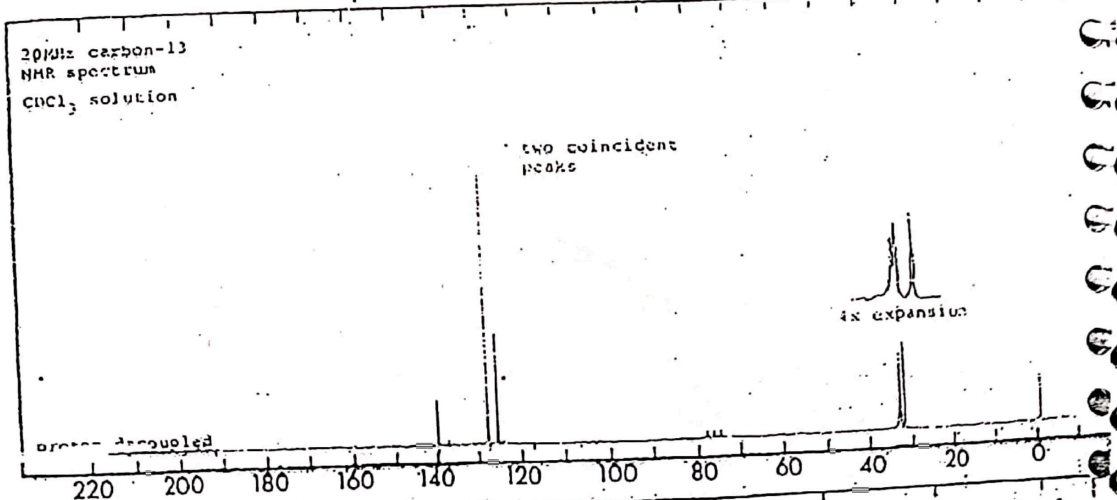


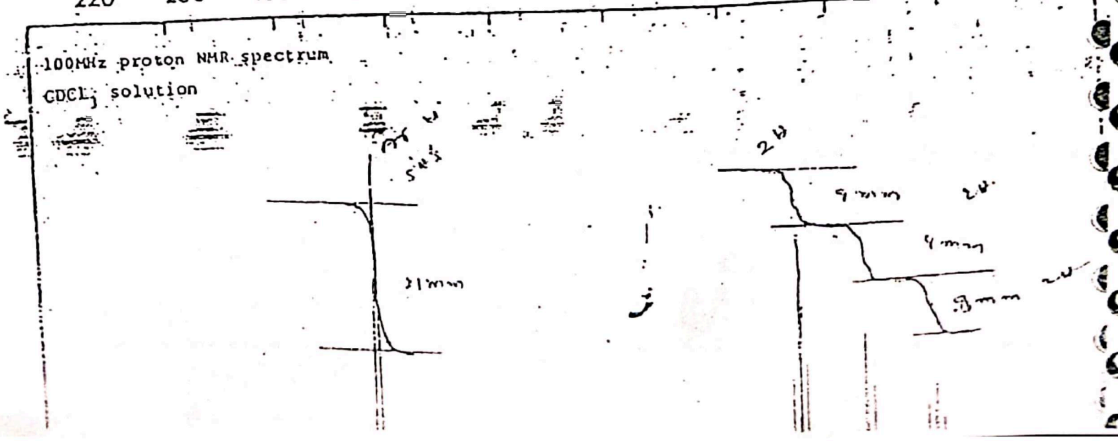
problem 13











Spectral Problem - XX

mass Spectral data :-

	m/z	% of R.A
M^+	198	8% $8/8 \times 100 = 100\%$
$[m^+ + 1]$	199	0.8% $0.8/8 \times 100 = 10\%$
$[m^+ + 2]$	200	7.95% $7.95/8 \times 100 = 99.37\%$

⇒ The molecular ion % of R.A is used upto 100%.

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

⇒ $[m^+ + 2]$ peak rule even zero no. of nitrogens are Presente of 'Br' atom

⇒ No. of carbons $= \dfrac{[m^+ + 1] \text{ intensity}}{^{13}C \text{ intensity}}$

$= 10/1.1$

$= \sim 9$

⇒ no. of hydrogens $= m^+ m/z$ - mass of carbon

$= 198 - 12(9)$

$= 198 - 108$

$= 90.$

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

⇒ no. of H's $= 90 - 79$

$= 11$

∴ The molecular formula is "$C_9H_{11}Br$"

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

$$= 9 - 11/2 - 1/2 + 0/2 + 1$$

$$= 9 - 12/2 + 1 = 4$$

IR data :-

3000 cm^{-1}	=C-H (stretch)
2900 cm^{-1}	sp^3, C-H (stretch)
1600 cm^{-1}	C=C ring stretch
1400 cm^{-1}	sp^3, C-H (bend)
1225 ~850 cm^{-1}	HC=CH stretch
750 cm^{-1}	C-Br
690 cm^{-1}	mono substituted benzene

UV data :-

300 nm $\pi \rightarrow \pi^*$ transition

^{13}C-NMR data :-

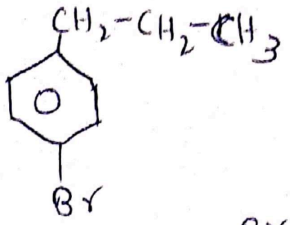
32 δ doublet

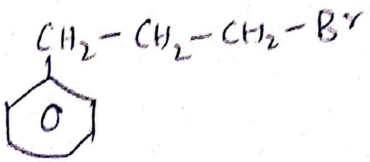
128 δ doublet

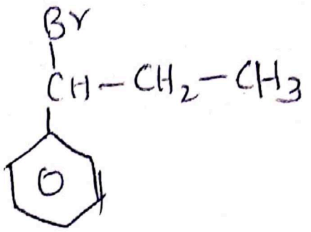
^1H-NMR data :-

S.NO	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	1	pentet	8	8/4=2	2	CH_2
02.	1.5	Triplet	8	8/4=2	2	CH_2
03.	2.2	Triplet	8	8/4=2	2	CH_2
04.	6.1	Singlet	20	20/4=5	5	

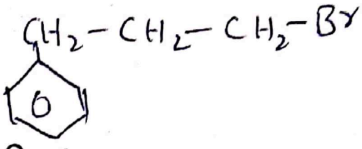
The possible structure's for "$C_9H_{11}Br$" are,

i) 

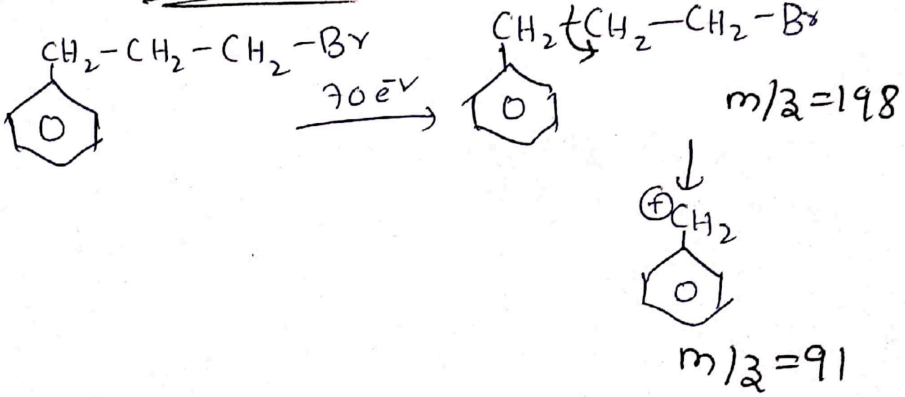
(ii) 

(iii) 

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

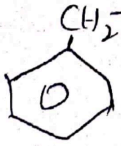


mass fragmentation :-



Result :-

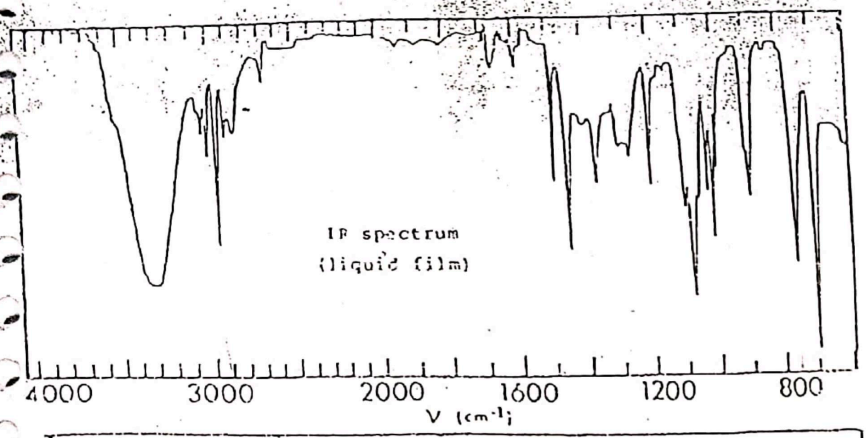
Based on the above four spectral data. The given spectral sheeth belongs to

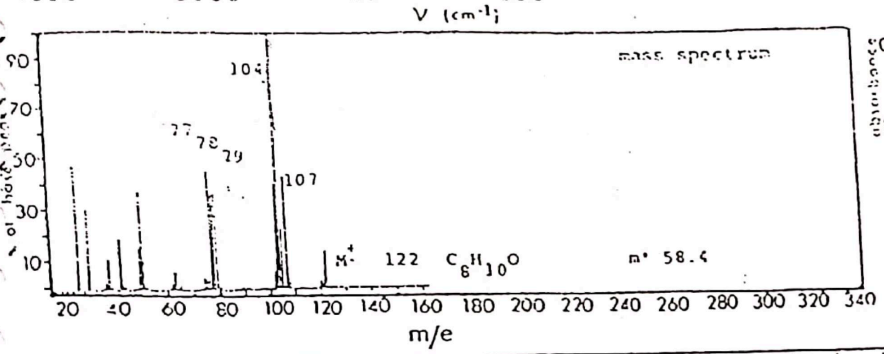


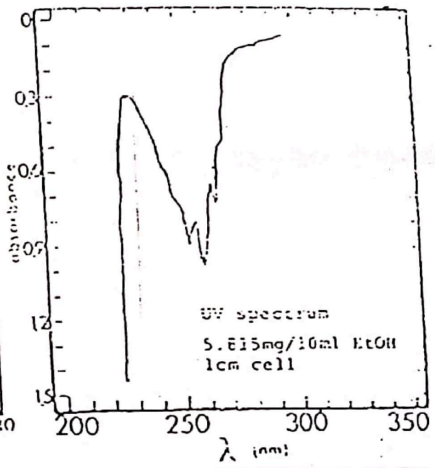
(18) 14

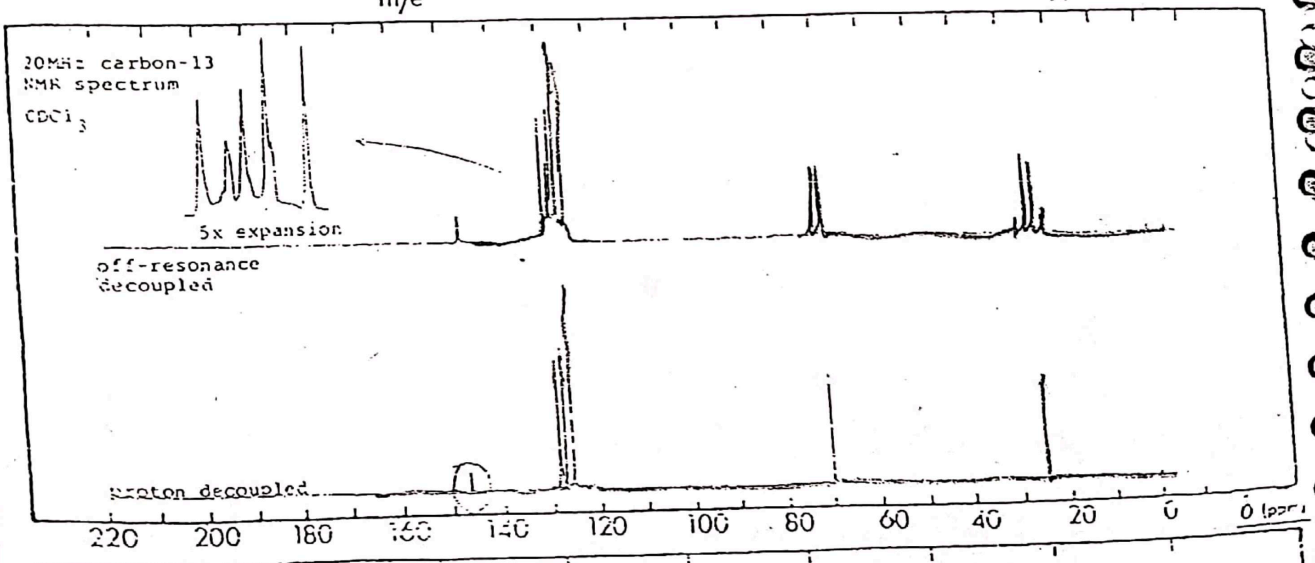
(11) (18)

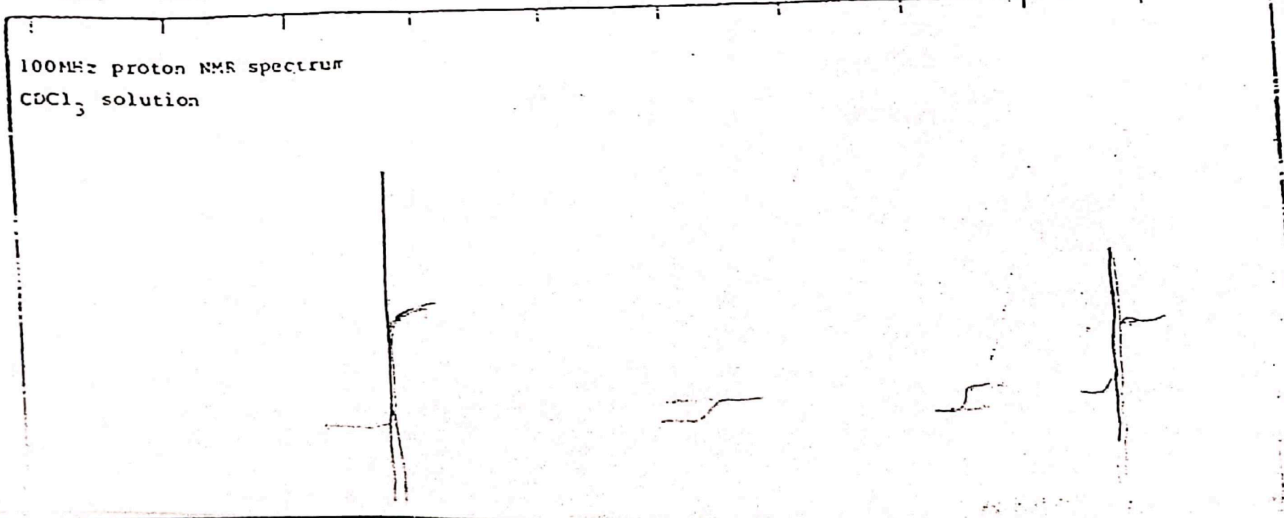
problem 12











Spectral problem - XVIII

Mass spectral data :-

In the given mass spectrum,

⇒ m/z = 122, 107, 104, 78, 77 containing peaks are observed

⇒ The m+ m/z is even (i.e. 122) ∴ even/zero no. of nitrogens are present.

⇒ The molecular formula for the given spectral sheeth is "$C_8H_{10}O$".

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

$= 8 - 10/2 - 0/2 + 0/2 + 1$

$= 9 - 5$

$= 4.$

IR data :-

3300 cm^{-1}	O-H (stretch)
2980 cm^{-1}	sp^3, C-H (stretch)
1450 cm^{-1}	C=C, ring stretch
1380 cm^{-1}	sp^3, C-H (bend)
1200 cm^{-1}	sp^3, C-C (stretch)
690 cm^{-1}	monosubstituted benzene

UV data :-

230 nm	$n \rightarrow \pi^*$ transition
290 nm	$\pi \rightarrow \pi^*$ transition

^{13}C - NMR data :-

25 δ quatet CH_3

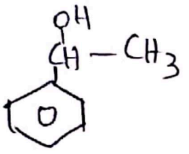
50 δ doublet CH

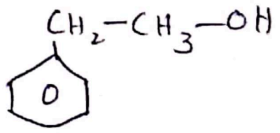
128 δ doublet (aryl 'c')

H^1 - NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	1.5	Singlet	9	9/3=3	3	CH_3
02.	2.8	singlet	3	3/3=1	1	CH
03.	4.7	doublet	3	3/3=1	1	CH
04.	7.3	singlet	15	15/3=5	5	

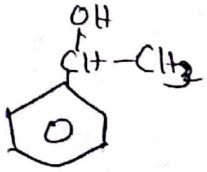
The possible structure's for "$C_8H_{10}O$" are

i) 

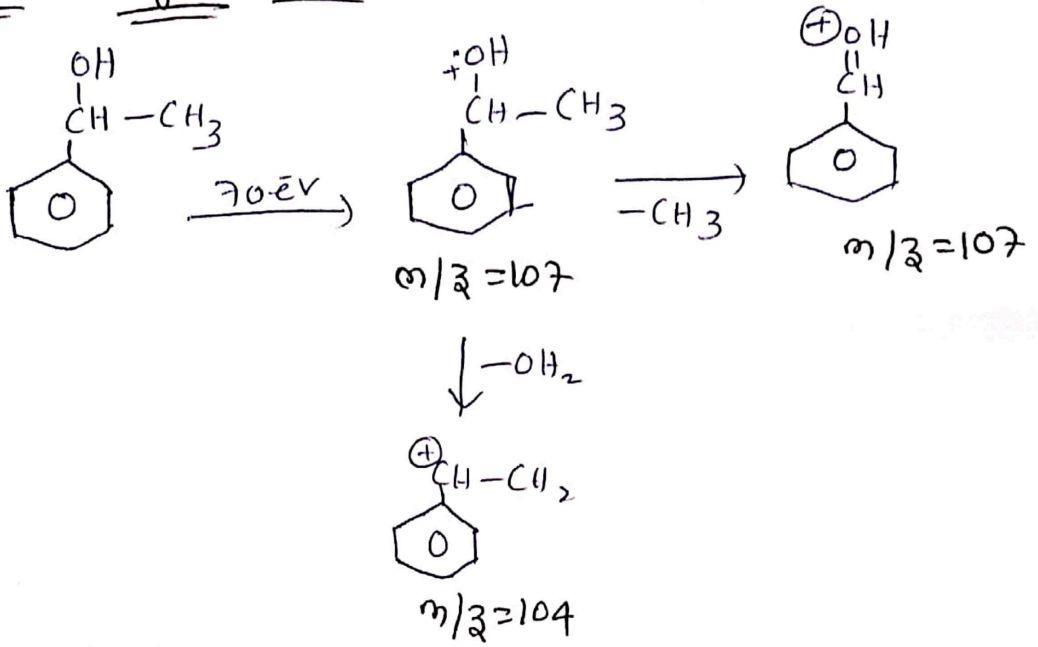
ii) 

In the above structure's . structure (i) co-relates with the NMR data perfectly

∴ The correct structure is,



mass fragmentation :-



Result :-

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