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

DEPARTMENT OF CHEMISTRY

Title of the Project

Interpretation of Spectral data of

1. p - Nitro benzaldehyde
2. p - Chloro acetophenone
3. Benzyl bromide
4. Diethyl phthalate

By

Sl. No	Name of the student	H. T. No	Group
1	C. Rajesweari	20033006441008	M.P.C EM
2	P. Chaitanya	20033006441045	M.P.C EM
3	C. Sangeetha	20033006441010	M.P.C EM
4	C. Naresh	20033006441009	M.P.C EM
5	C. Kalyani	20033006441005	M.P.C EM
6	K. Rambabu	20033006441021	M.P.C EM

Supervision by

CH. VENKATESWARLU

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. p - Nitro benzaldehyde, 2. p - Chloro acetophenone, 3. Benzyl bromide, 4. Diethyl phthalate is a bonafide project work done by C. Rajeswari, P. Chaitanya, C. Sangeetha, C. Naresh, C. Kalyani and K. Rambabu under my supervision in the department of Chemistry, Dr. BRR. Government Degree college, Jadcherla, Telangana state.

Date: 25.05.2023

Place: JADCHERLA

(CH. VENKATESWARLU)

supervisor

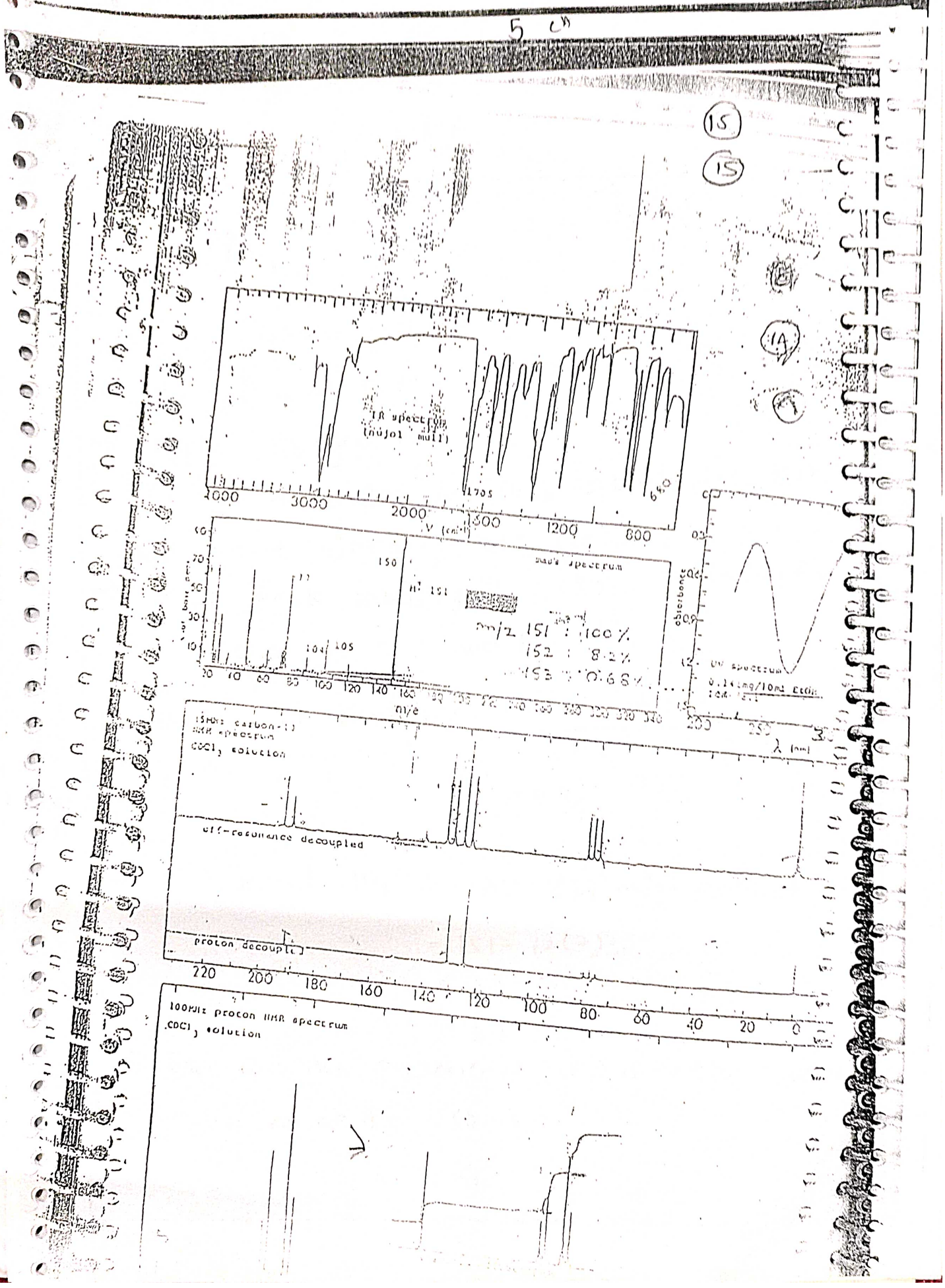
DECLARATION

We are hereby declare that the study project on Interpretation of Spectral data of 1. p - Nitro benzaldehyde, 2. p - Chloro acetophenone, 3. Benzyl bromide, 4. Diethyl phthalate is a record work done by us under the supervision of **CH. VENKATESWARLU**, 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	C. Rajesweari	20033006441008	M.P.C EM	C. Rajesw
2	P. Chaitanya	20033006441045	M.P.C EM	P. Chaitanya
3	C. Sangeetha	20033006441010	M.P.C EM	Sangeetha
4	C. Naresh	20033006441009	M.P.C EM	C. Naresh
5	C. Kalyani	20033006441005	M.P.C EM	C. Kalyani
6	K. Rambabu	20033006441021	M.P.C EM	K. Rambabu


IR spectrum (nujol mull)
3000
2000
1705
1300
1200
800
ν (cm⁻¹)
mass spectrum
m/z 151 : 100%
152 : 8.2%
153 : 0.6%
m/e
UV spectrum
0.1 mg/10ml EtOH
λ (nm)
15MHz carbon-13 NMR 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 - XV

mass spectral data :-

	m/z	% of R.A
M^+	151	100%
$[M^+ + 1)$	152	8.2%
$[M^+ + 2]$	153	0.68%

⇒ The M^+ % of R-A is 100%

⇒ Apply nitrogen rule,

"The molecular ion m/z is odd (i.e, 151)

∴ odd no. of nitrogens are present.

⇒ $M^+ + 2$ peak intensity is 0.68%. It indicates the absence of S, Cl and Br.

⇒ Number of Carbon's $= \frac{M^+ + 1 \text{ intensity}}{1.1}$

$= 8.2 / 1.1$

$= \sim 7$

⇒ Number of Hydrogen's $= M^+ \text{ m/z} - \text{mass of carbon}$

$= 151 - 12(7)$

$= 151 - 84$

$= 67$

⇒ Due to the presence of one nitrogen atom,

no. of H's $= 67 - 14$

$= 53$

⇒ Let us assume the presence of 3 oxygen atom,

⇒ no. of H's = 53 − 16(3)

= 53 − 48

= 15

⇒ D_{BE} = 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

$= 7 - 5/2 - 0/2 + 1/2 + 1$

$= 8\left[\frac{-5+1}{2}\right]$

$= 8 - 4/2$

$= 6$

IR data :-

2910 cm^{-1} sp^3 C–H (stretch)

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

1550 cm^{-1} C=C ring stretch

1350 cm^{-1} O=N stretch

880 cm^{-1} 

UV data :-

230 nm $\pi \rightsquigarrow \pi^*$

310 nm $n \rightsquigarrow \pi^*$

^{13}C-NMR data :-

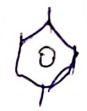
78 δ singlet C–N

125 δ doublet

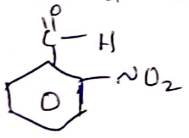
132 δ doublet 

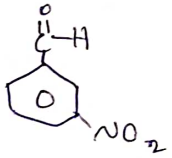
190 δ doublet

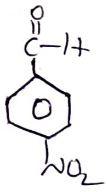
H^1-NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	8.1	doublet	8	8/4=2	2	
02.	8.4	doublet	8	8/4=2	2	
03.	9.9	Singlet	4	4/4=1	1	=C-H

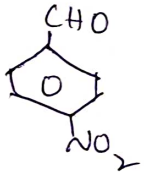
Based on the above data, The possible structures for "$C_7H_5NO_4$" are

i) 

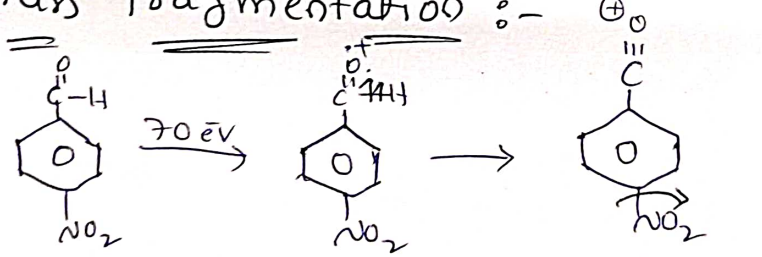
ii) 

(iii) 

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

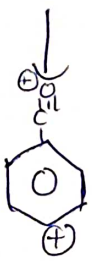


mass fragmentation :-



m/z=151

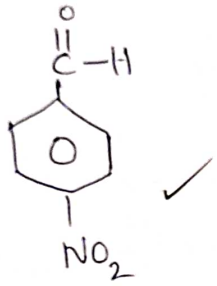
m/z=150



105

Result:-

Based on the above four spectral data given spectral sheeth belongs to p-nitro benzalde-hyde.



15

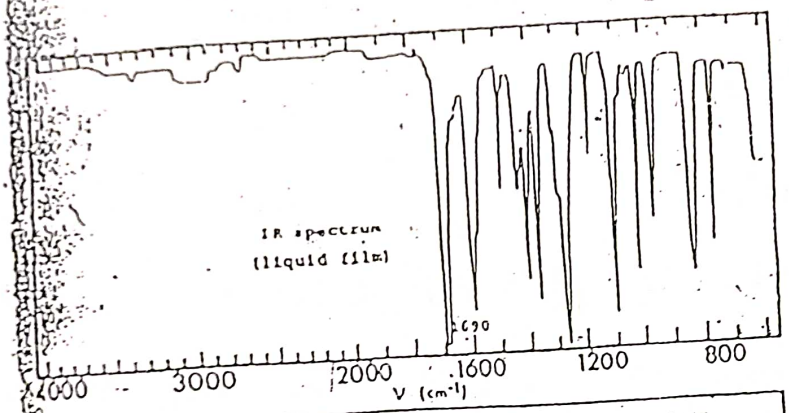
(5)

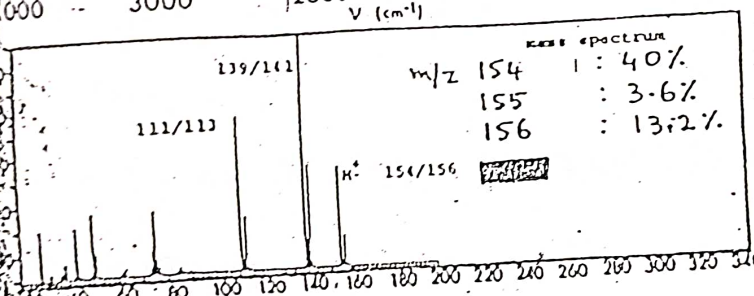
(17)

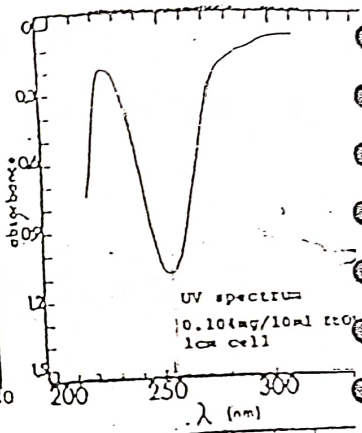
$CH_3.CH_2.C=O$

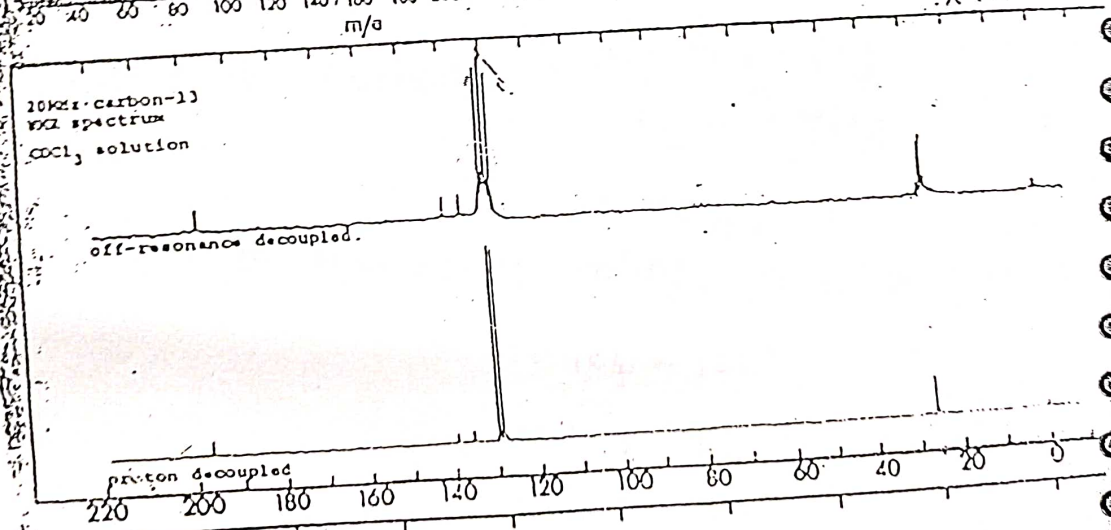
Aromatic

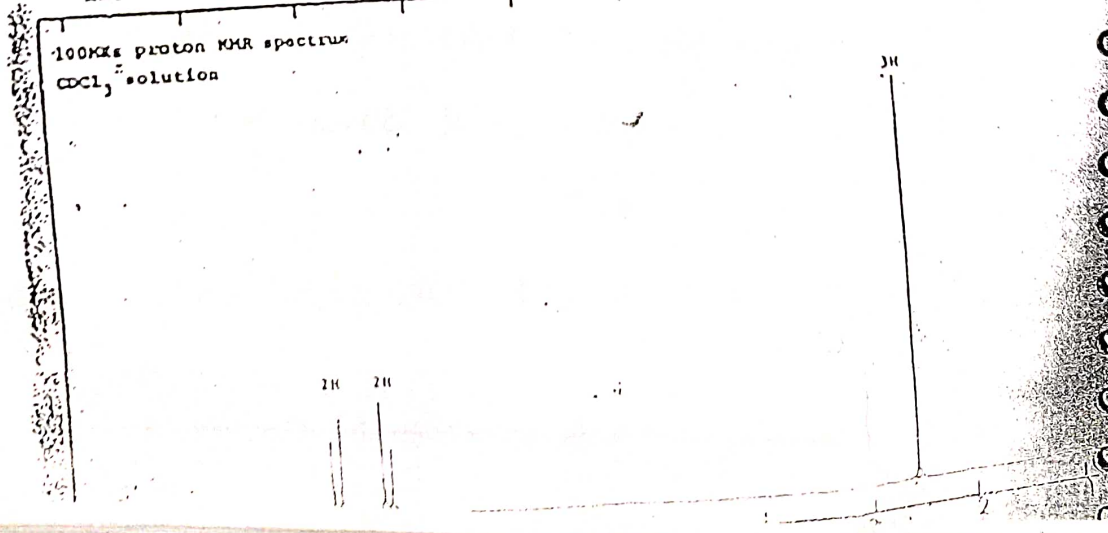
C=O Stretching











Spectral Problem-V

Mass spectral data :-

	m/z	% of R.A	
m^+	154	40%	$40/40 \times 100 = 100\%$
$[m^+ + 1]$	155	3.6%	$3.6/40 \times 100 = 90\%$
$[m^+ + 2]$	156	13.2%	$13.2/40 \times 100 = 33\%$

⇒ The molecular ion m/z is even. According to nitrogen rule. zero/even number of nitrogens are present.

⇒ $[m^+ + 2]$ Peak intensity is 33%. it indicates. The presence of "Cl" atom.

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

$= 90/1.1$

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

$= 154 - 12(8)$

$= 154 - 96$

$= 58$

Due to the presence of one oxygen atom.

⇒ no. of H's $= 23 - 16$

$= 7$

∴ The molecular formula is "C_9H_7OCl".

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

$$= 8 - 7/2 - 1/2 + 0/2 + 1$$

$$= 9 - \left[\frac{7+1}{2}\right]$$

$$= 9 - 8/2$$

$$= 5$$

UV data :-

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

330 nm $n \sim \pi^*$

IR data :-

1705 cm^{-1} C=O stretch

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

1200 cm^{-1} C-C stretch

1025 cm^{-1} C-O

730 cm^{-1} C-Cl

810 cm^{-1} disubstituted benzene

H^1 NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	1.5	Singlet	-	-	3H	CH_3
02.	7.4	doublet	-	-	2H	
03.	7.9	doublet	-	-	2H	

^{13}C - NMR data :-

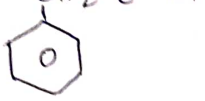
25 δ singlet

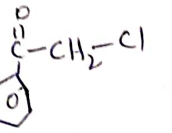
130 δ Triplet

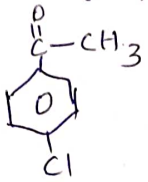
2.58 δ · singlet

1.41 δ singlet

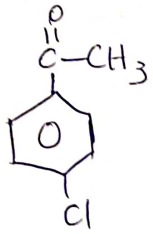
The possible structure is for 'C_8H_7OCl' are

i) 

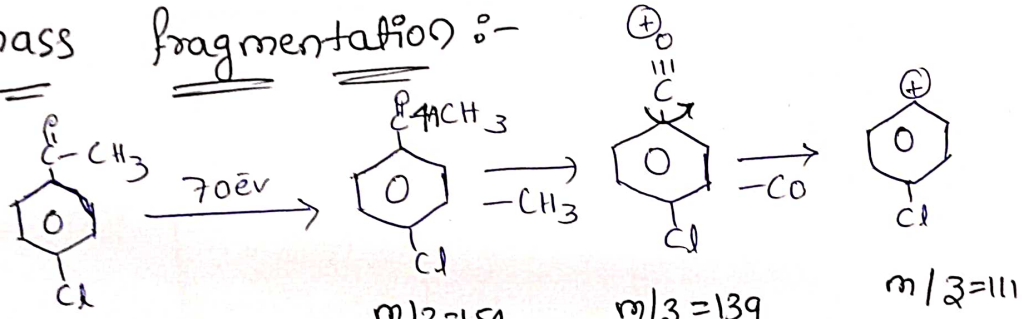
ii) 

(iii) 

Based on the above NMR spectral data's. structure (iii) is correct, therefore. The correct structure is,

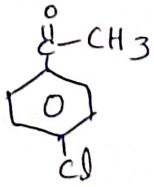


mass fragmentation :-



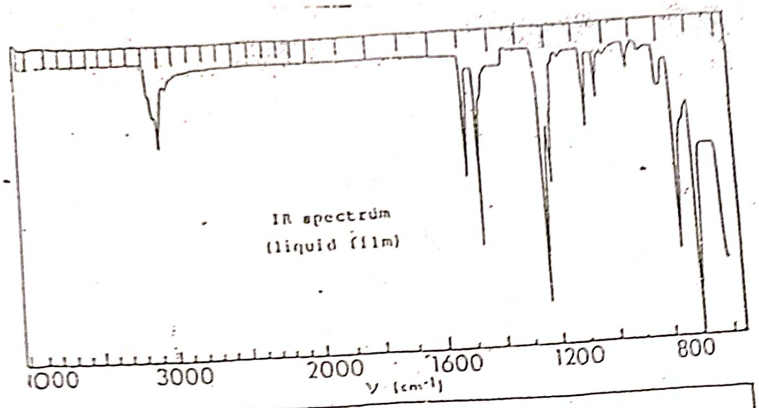
Result :-

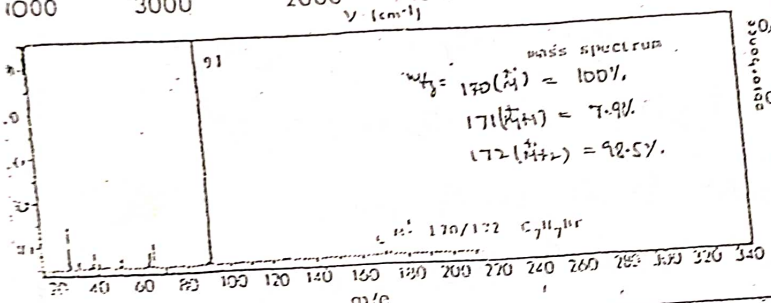
Based on the above four spectral data; The given spectral sheeth belongs to the following structure containing compound.

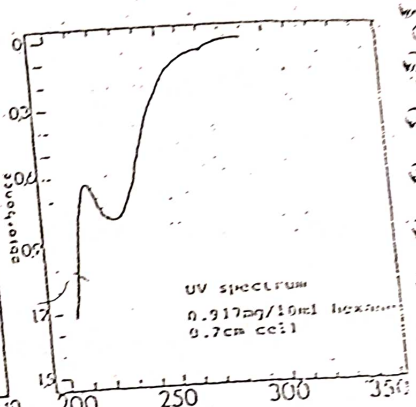


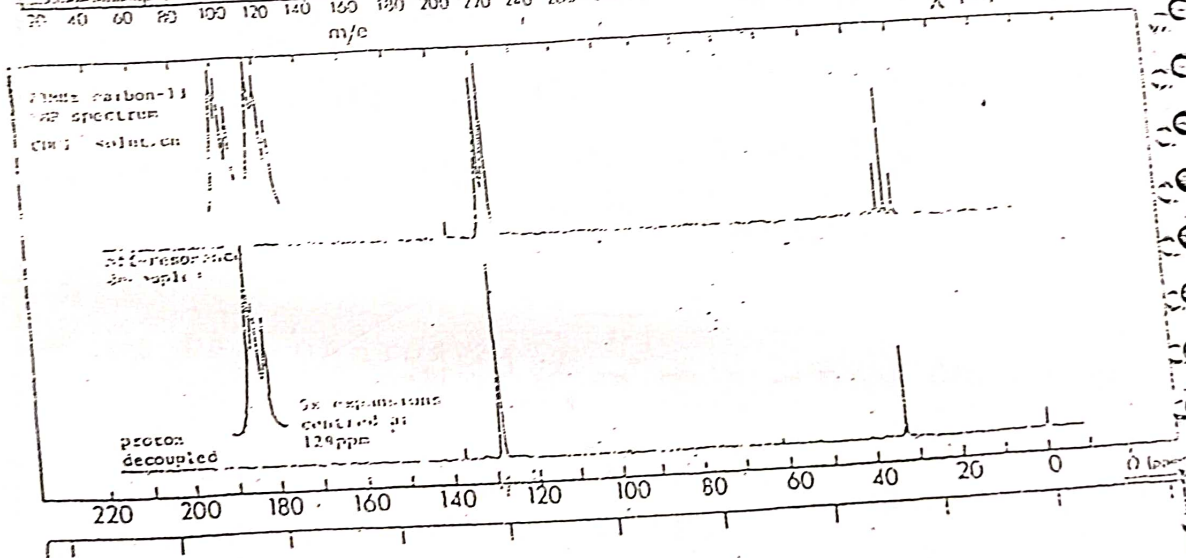
P-chloro acetophenone ✓

problem









100MHz proton NMR spectrum
$CDCl_3$ solution

Spectral Problem – XI

mass spectral data :-

	m/z	% of R.A
M^+	170	100 %
$m^+ + 1$	171	7.9 %
$m^+ + 2$	172	98.5 %

⇒ The molecular ions % of R.A is 100 %.

⇒ Apply nitrogen rule.

The molecular ion m/z is even (i.e, 170)

Therefore, even /zero no. of nitrogens are present.

⇒ $m^+ + 2$ peak is % of R-A is 98.5 %. It indicates the presence of "Br".

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

$= \frac{7.9}{1.1} = \sim 7$

⇒ No. of hydrogens = m^+ m/z − mass of carbon

$= 170 - 12(7)$

$= 170 - 84$

$= 86$

Due to the presence of 'Br' atom of hydrogens

$= 86 -$ mass of 'Br'

$= 86 - 79$

$= 7$

∴ The molecular formula is given as, "C_7H_7Br".

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

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

$$= 4$$

IR data :-

690 cm^{-1}	mono substituted benzene
770 cm^{-1}	C-Br
1215 cm^{-1}	C-C (stretch)
1470 cm^{-1}	sp^3, C-H (bend)

UV data :-

215nm	$n \sim \pi^*$
285nm	$\pi \sim \pi^*$

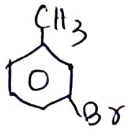
^{13}C-NMR data :-

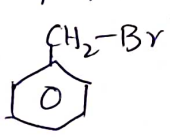
32 δ	Triplet (CH_2)
129 δ	doublet (aromatic compound)

H^1-NMR data :-

S.No	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	4.2	Singlet	8	8/4=2	2	CH_2
02.	7.3	Singlet	20	20/4=5	5	

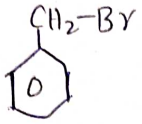
Based on the above spectral data the possible structures for "C_7H_7Br" are,

i) 

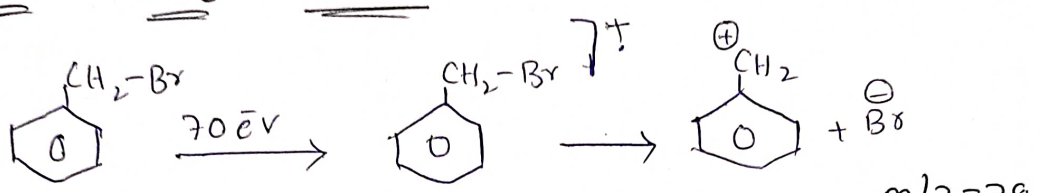
(ii) 

iii) 

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



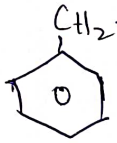
mass fragmentation :-



m/z=170 m/z=91 m/z=79

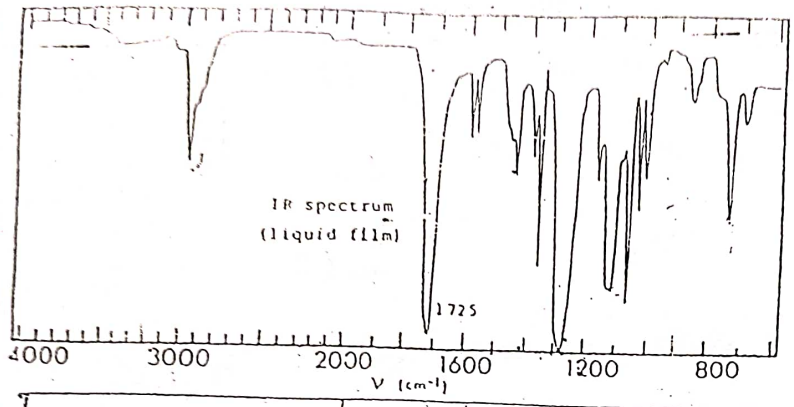
Result :-

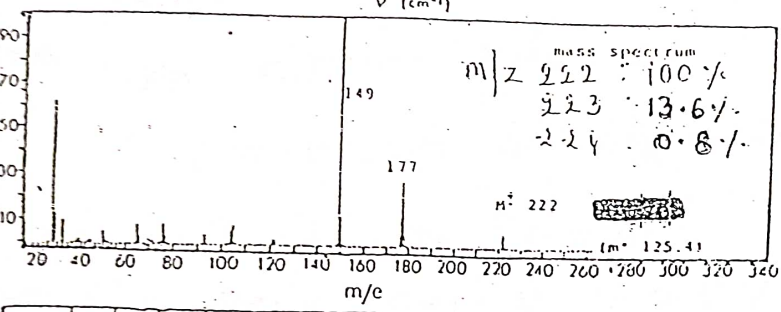
Based on the above four spectral data's The given spectral sheeth belongs to the following structure containing compound.

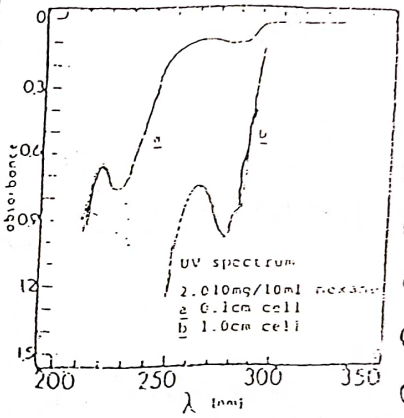


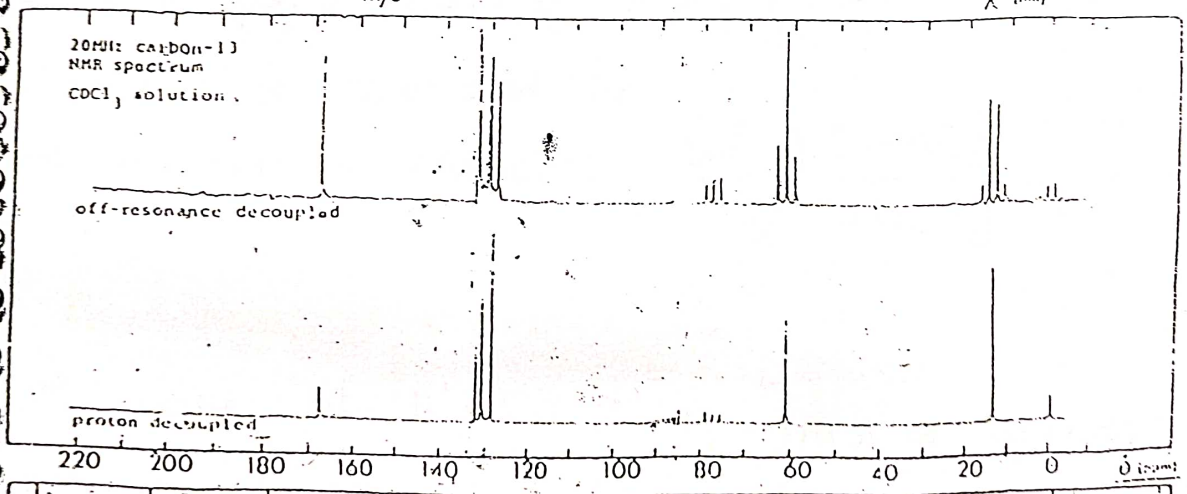
benzyl bromide

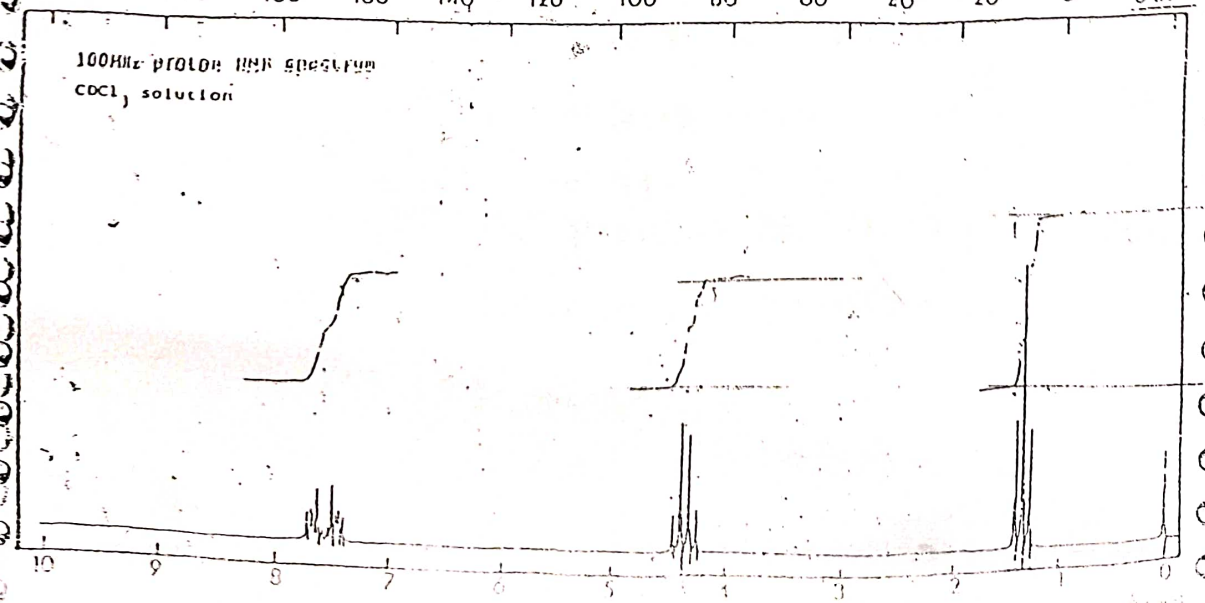
(10)


IR spectrum
(liquid film)
1725
4000
3000
2000
1600
1200
800
ν (cm⁻¹)


mass spectrum
m/z 222 : 100 %
223 : 13·6 %
224 : 0·8 %
149
177
M⁺ 222
(m* 125.4)
m/e


UV spectrum
2.010mg/10ml hexane
a 0.1cm cell
b 1.0cm cell
absorbance
λ (nm)


20MHz carbon-13
NMR spectrum
CDCl₃ solution
off-resonance decoupled
proton decoupled
δ (ppm)


100MHz proton NMR spectrum
CDCl₃ solution

Spectral Problem - X

mass spectral data :-

	m/z	% of R.A
m^+	222	100%
$[m^+ + 1]$	223	13.6%
$[m^+ + 2]$	224	0.8%

⇒ The m^+ % of R.A is 100%

⇒ Apply nitrogen rule,

"The molecular ion m/z is even ∴ zero/even no. of nitrogens are Present.

⇒ $m^+ + 2$ peak intensity is 0.8 %, It indicates the absence of S, Cl and Br.

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

$= 13.6 / 1.1$

$= \sim 12$

⇒ Number of H's $= m^+$ m/z − mass of carbon

$= 222 - 12\,(12)$

$= 222 - 144$

$= 78$

let us assume the presence of 4 oxygen atoms,

⇒ no. of H's $= 78 - 4$ (mass of nitrogen)

$= 78 - 4(16)$

$= 78 - 64$

$= 14$

∴ The molecular formula is given as, "$C_{12}H_{14}O_4$".

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

$$= 12 - 14/2 - 0/2 + 0/2 + 1$$

$$= 13 - 7$$

$$= 6$$

IR data :-

750 cm^{-1}	o-disubstituted benzene
1080 cm^{-1}	C-O, stretch
1120 cm^{-1}	HC=CH (stretch)
1290 cm^{-1}	sp^3, C-C (stretch)
1380 cm^{-1}	sp3, C-H (bend)
1725 cm^{-1}	C=O (stretch)

UV data :-

220 nm	$n \sim \pi^*$ transition
290 nm	$\pi \sim \pi^*$ transition

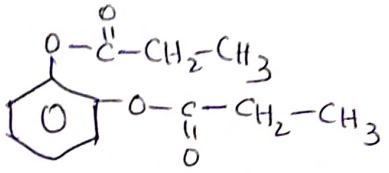
^{13}C - NMR data :-

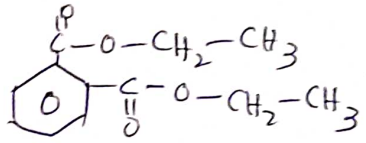
13 δ	s	CH_3
61 δ	Triplet	CH_2
130 δ	Triplet	CH_2
169 δ	Singlet	Aromatic 'C'

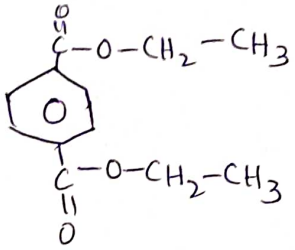
H^1 NMR data :-

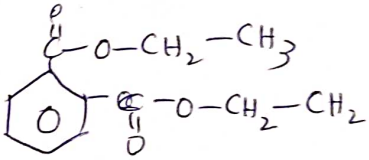
S.NO	δ value	multiplicity	Integration	Ratio	no. of H's	Interference
01.	1.4	Triplet	24	24/4	24/4 = 6	
02.	4.4	quatet	16	16	16/4 = 4	
03.	7.6	multiplet	16	16	16/4 = 4	

The possible structure's for molecular formula "$C_{12}H_{14}O_4$" are

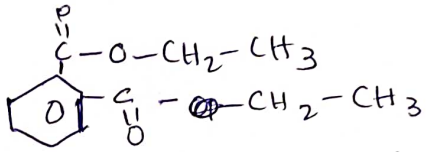
i) 

ii) 

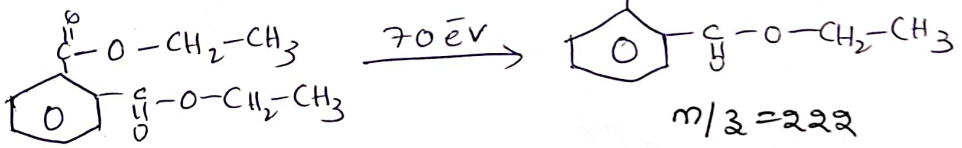
iii) 

iv) 

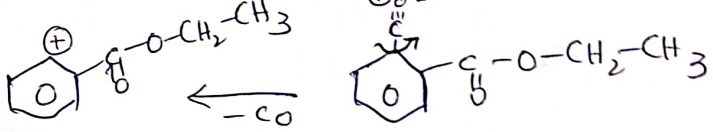
In the above structure's, structure (ii) co-relates with the NMR data ∴ The correct structure is,



mass fragmentation :-



m/z = 222

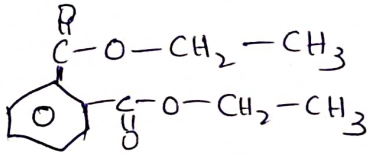


m/z = 149

m/z = 177

Result :-

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



Diethyl phthalate