

2(a) IR Analysis

(a) The fingerprint region of the IR spectrum is usually the region range $1400 - 500 \text{ cm}^{-1}$. From ~~the~~ IR spectrum usually the diagnostic peak for meta-substituted ring is the presence of C-H wagging peak from $10 - 750 \text{ cm}^{-1}$ and the bending peak at 690 cm^{-1}

- For ortho the C-H wagging peak is $770 - 735 \text{ cm}^{-1}$ and there's no ring bending peak at 690 cm^{-1}
- para-substituted have strong ring-mode peak at 1516 cm^{-1} and C-H wag at $660 - 790 \text{ cm}^{-1}$ and no ring bend.

- From our IR spectrum; we have a C-H wagging at 753.91 cm^{-1} and no ring bending at 690 cm^{-1} and hence we can conclude that this is an ortho-substitution.

(b) $^1\text{H NMR}$ and $^{13}\text{C NMR}$

(i) - To identify the phenolic hydrogen then we need to examine the aryl protons which occur a region of $6.5 - 8 \text{ ppm}$. It has four signals which means the phenol is;



Carbon chain of the ester considering the expanded upfield.

2. (ii)

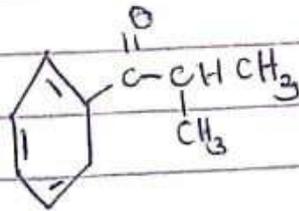
It has 3 signals at;

1.0 ppm \rightarrow R-CH₃

1.8-1.9 ppm \rightarrow CH

4.3-4.4 ppm \rightarrow CH₂

From this we can deduce the structure of the ester as



(iii) Expanded downfield Region (8.0-8.5 ppm)

From this spectrum we can observe

four signals. These are usually

These are usually the signal of aromatic protons.

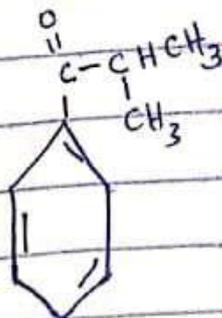
- Ortho protons show six signals in substituted

- Meta shows six signals

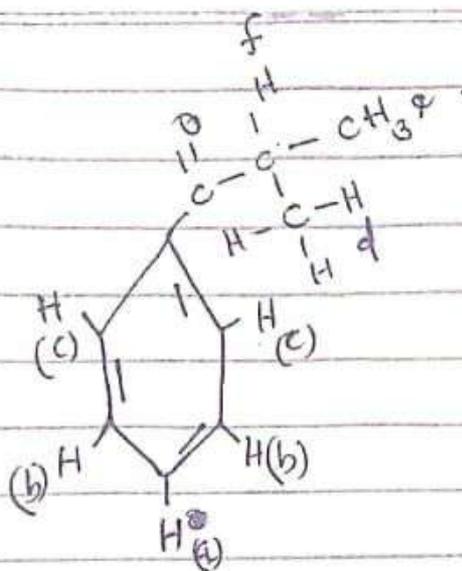
- Para shows four signals.

- We can conclude that the following is a para-substituted compound.

Therefore the structure of the ester is



3.



- a) 6.573
- b) 7.43
- c) 6.98
- d) 4.325
- e) 1.059
- f) 1.78

4 - The substitution by NMR differed with the substitution IR. ¹H NMR is more definitive since it explores all the factors including the electron donating and electron withdrawing which brings about the shielding and deshielding of protons. The magnetic power of NMR is important since the deshielded protons ^{are} usually ~~have~~ a downfield and therefore require a longer NMR to absorb.