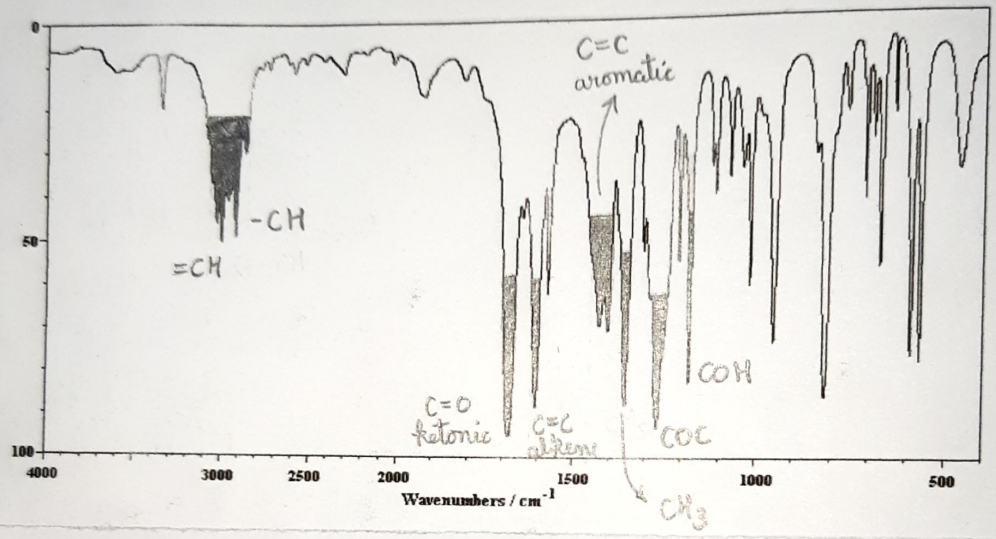
Observations:

IR Spectrum Analysis:

IR Spectrum of the Unknown Compound A



S.no.	Wave no. (cm^{-1})	Possible group	Explaination	Group present
01.	3100 - 3000	=C-H stretch	Sharp & broad	=C-H stretch
02.	2950 - 2840	-C-H stretch	Sharp & broad	-C-H stretch
03.	1745 - 1715	C=O ketone	Sharp & strong	C=O (ketone)
04.	1680 - 1600	C=C alkene	Sharp & strong	C=C alkene
05.	1600 - 1400	C=C aromatic	Sharp & broad	C=C aromatic
06.	1465 - 1440, 1390 - 1365	CH_3 bend	Sharp & strong	CH_3 bend
07.	1250 - 1050	C-O-C stretch	Sharp & strong	—
08.	1200 - 1020	C-OH stretch	Sharp & strong	—

Date 11/03/2021

Expt. No./ Name : ----------

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Experiment 7&8

Aim:

To determine the structure of an unknown compound A using the given spectroscopic data.

Theory:

1. Spectroscopy is the study of the interaction of the electromagnetic radiation with the matter.
2. Spectroscopy is an important tool for the qualitative & quantitative analysis of unknown compounds.
3. In the modern structure analysis, the powerful spectroscopic methods of IR and NMR play a major role.
4. In order to determine the structure of an unknown compound, it may be required to combine a variety of spectroscopic data.

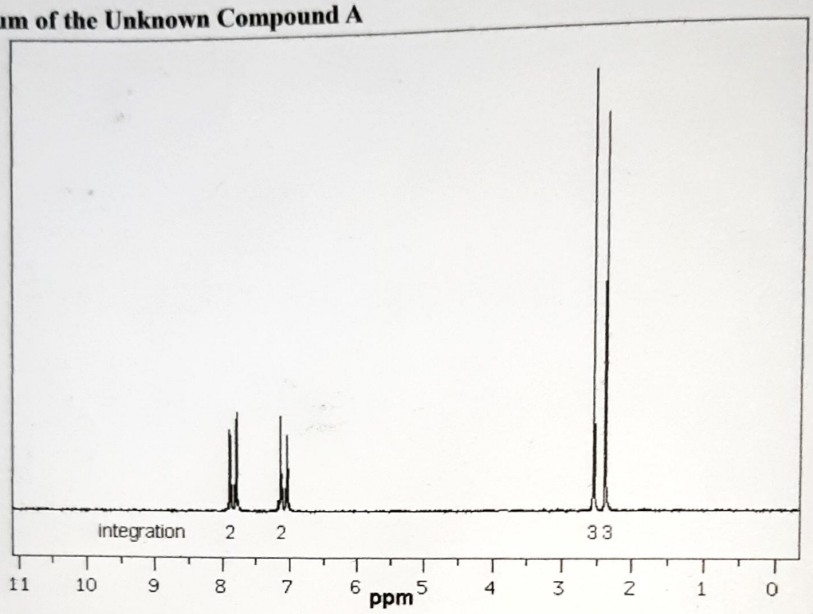
Infrared (IR) Spectroscopy:

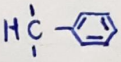
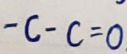
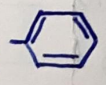
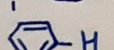
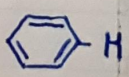
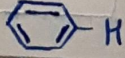
1. Infrared spectroscopy is especially useful in identifying the functional groups in unknown compounds. Thus, infrared spectroscopy is a type of functional group spectroscopy.
2. Conventionally, the IR spectrum is a plot of Transmittance (%T) v/s wave numbers (cm^{-1})
3. The peaks/signals observed in the spectrum can be used for the detection of various important functional groups, such as -OH, $-NH_2$ etc in samples
4. The IR spectrum is interpreted by referring to the reference tables containing the info. regarding the functional groups & their corresponding wave no., & the presence or absence of func. groups is analysed accordingly.

Teacher's Signature : ----------

NMR Spectrum Analysis:

NMR Spectrum of the Unknown Compound A



S.no.	Integration	Number of peaks	No. of neighbours	Chemical shift (δ)	Possible groups	Group present
1.	3	1	0	2.3 - 2.5	-OH, -NH, HCN, HCS, ≡C-CH H-C-C=O, 	H-C-C=O
2.	3	1	0	2.5 - 2.7	-OH, -NH, HCN, HCS, ≡C-CH H-C-C=O, 	
3.	2	2	1	6.8 - 7.2	 H	 H
4.	2	2	1	7.8 - 8.0	 H	 H

^{1}H - NMR Spectroscopy:

1. Proton Nuclear Magnetic Resonance (proton NMR or ^{1}H NMR) is a very important and widely used analytical technique.
2. It is primarily used in the characterisation of organic molecules.
3. ^{1}H NMR spectrum is a plot of signal intensity v/s the chemical shift (δ).
4. The information from the ^{1}H NMR spectrum is extracted, and is often combined with the information from other spectroscopic techniques such as IR for the characterization of unknown compounds.

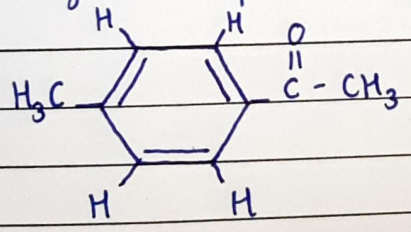
Interpretation of ^{1}H - NMR Spectrum:

Important information obtained from ^{1}H NMR spectrum includes

1. No. of signals / peaks (No. of H environments)
2. Types of Hs (Aliphatic / Aromatic / Func. groups), based on chemical shift (δ)
3. No. of Hs of each type (Integration)
4. No. of adjacent Hs (Splitting / multiplicity of each signal).

Results:

The given compound A after analysing IR & ^{1}H NMR may be



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