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OFFICE OF THE DEPUTY PRINCIPAL
ACADEMICS, STUDENT AFFAIRS AND RESEARCH

UNIVERSITY EXAMINATIONS

2019/2020 ACADEMIC YEAR

SECOND YEAR FIRST SEMESTER REGULAR MAIN EXAMINATION

FOR THE DEGREE OF BACHELOR OF EDUCATION SCIENCE

COURSE CODE: **CHE 201**

COURSE TITLE: **CHEMICAL ANALYSIS AND STRUCTURAL DETERMINATION**

DATE: 6TH DECEMBER, 2019 **TIME: 9.00AM – 12.00 PM**

INSTRUCTION TO CANDIDATES

- **SEE INSIDE**

THIS PAPER CONSISTS OF 8 PRINTED PAGES **PLEASE TURN OVER**

CHE 201: CHEMICAL ANALYSIS AND STRUCTURAL DETERMINATION

STREAM: BED (Science) **DURATION: 3 Hours**

INSTRUCTIONS TO CANDIDATES

*Answer **ALL** questions.*

Question One

a) Give the applications of the following structural analytical techniques

i) Elemental microanalysis (2 Marks)

ii) Mass spectrometry (3 Marks)

iii) Infra-red spectroscopy (3 Marks)

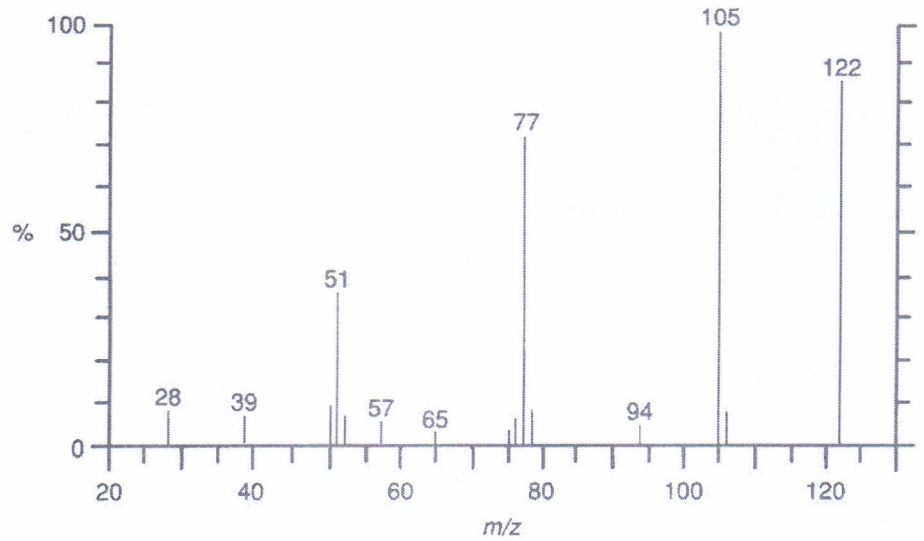
iv) Nuclear magnetic resonance spectroscopy (3 Marks)

v) X-ray crystallography (2 Marks)

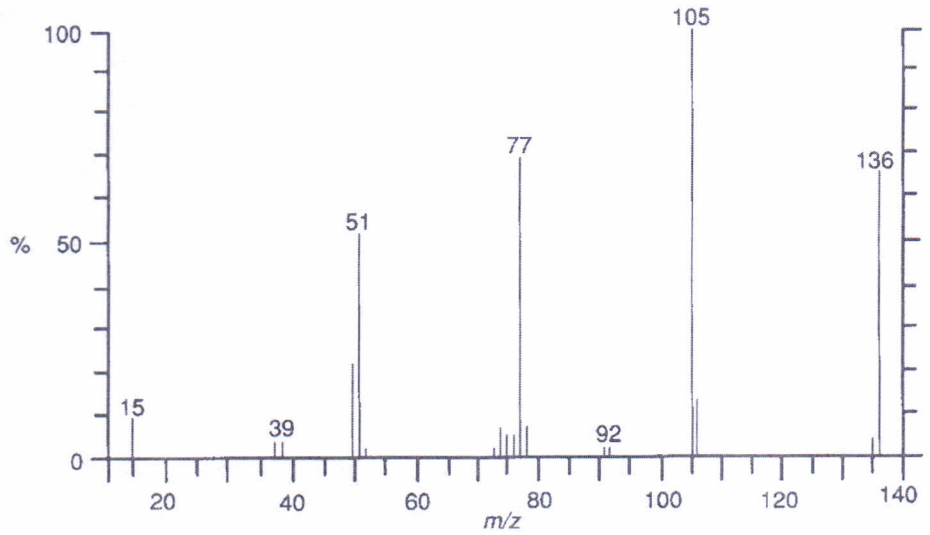
b) A sample of an organic compound with a mass of 1.224 g was completely burned in oxygen and found to produce 2.340 g of carbon dioxide and 1.433 g of water only. Calculate the empirical formula of the organic compound. (7 Marks)

QuestionTwo

Look at the figure below showing the mass spectra of benzoic acid and methyl benzoate and identify the ions responsible for the major peaks in each case. (11 Marks)



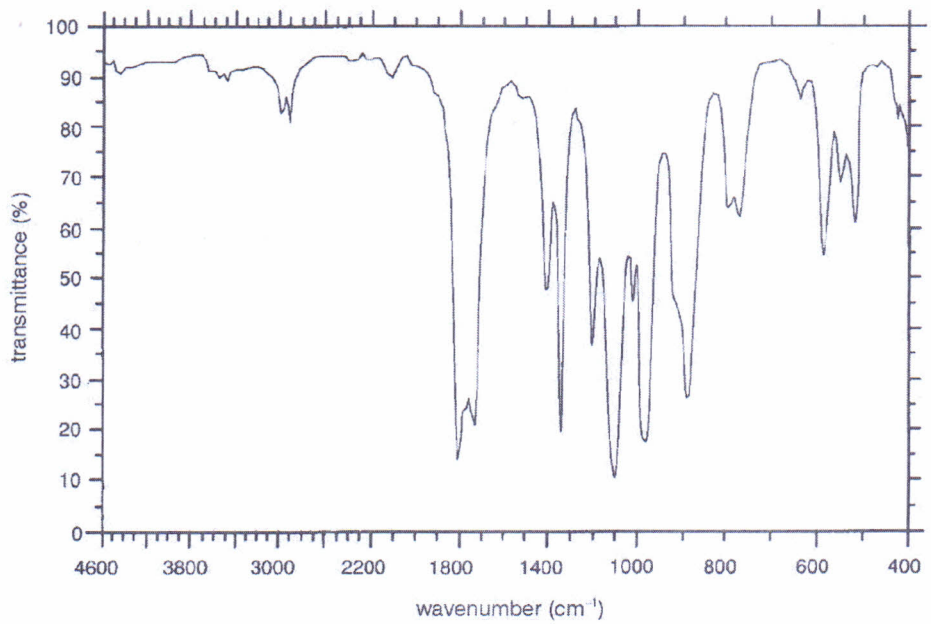
Mass Spectra of benzoic acid



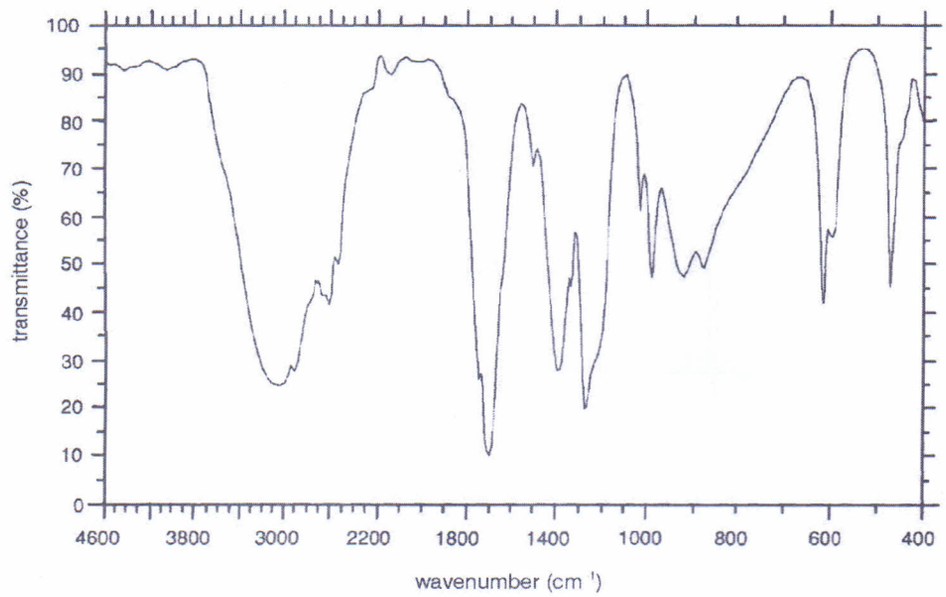
Mass spectra of methyl benzoate

Question Three

The spectra below are of ethanoic acid, CH_3COOH, and ethanoic anhydride, $(CH_3CO)_2O$. Draw the full structural formulas for both compounds and then determine, giving reasons, which spectrum is due to which compound (14 Marks)



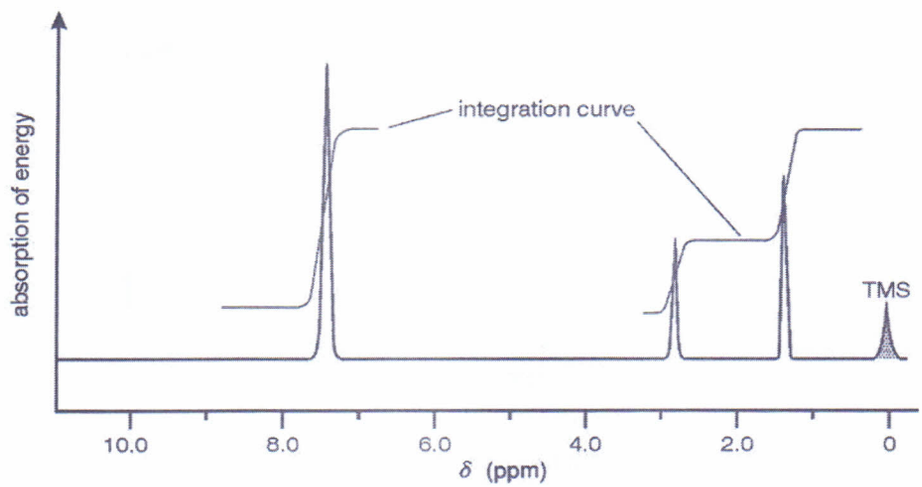
Spectra of ethanoic acid



Spectra of ethanoic anhydride

Question Four

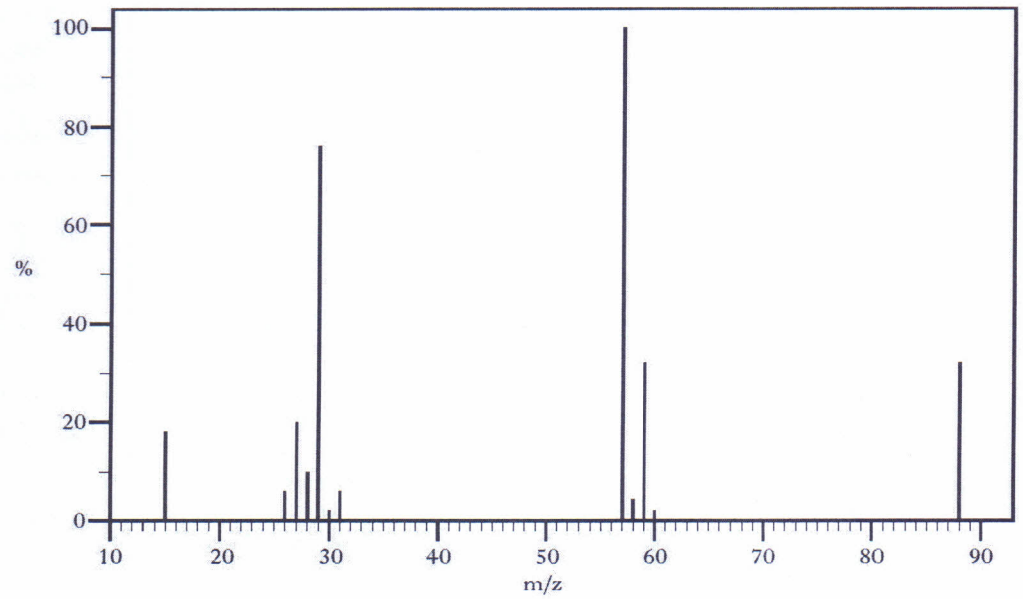
From the following low-resolution NMR spectra and other information given, suggest a possible structure for each substance. The Figure below shows the 1H NMR spectrum of a hydrocarbon (14 Marks)



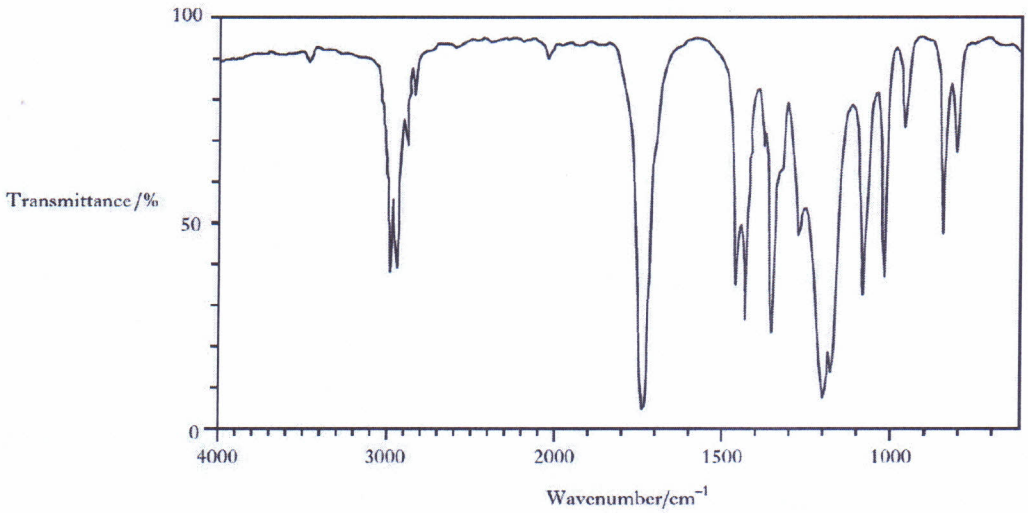
Spectrum of a Hydrocarbon

Question Five

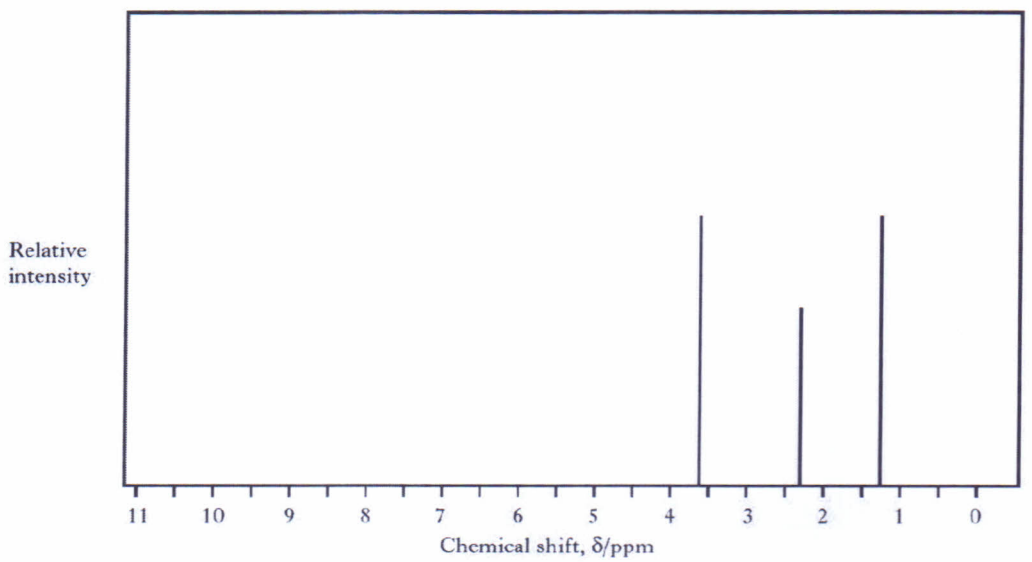
Spectra of an organic compound A are shown below



Mass spectrum of compound A



Infra-red spectrum of compound A



Proton nmr spectrum of compound A

a) Compound A has empirical formula C_2H_4O.

   i) Using this information and the mass spectrum, deduce the molecular formula of A. (3 Marks)

b) The absorption peak at 1745 cm^{-1} in the infra-red spectrum can be used to help identify A.

   i) Which bond is responsible for this absorption? (2 Marks)

   ii) Which type of compound is A? (2 Marks)

c) Draw the structure of the ion fragment responsible for the peak at m/z 57 in the mass spectrum. (2 Marks)

d) Considering all the evidence, including the proton NMR spectrum, name compound A. (2 Marks)

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Table of chemical shifts of NMR

Type of proton	Approximate chemical shift (ppm)	Type of proton	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0		6.5–8
$-CH_3$	0.9		
$-CH_2-$	1.3		9.0–10
	1.4		2.5–4
	1.7		
	2.1		2.5–4
	2.3		3–4
$-C\equiv C-H$	2.4		4–4.5
$R-O-CH_3$	3.3	RNH_2	Variable, 1.5–4
	4.7	ROH	Variable, 2–5
		ArOH	Variable, 4–7
	5.3		Variable, 10–12
			Variable, 5–8

*The values are approximate because they are affected by neighboring substituents.

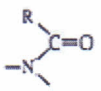
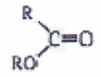
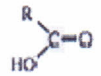
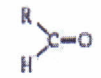
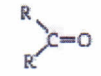
Type of carbon	Approximate chemical shift (ppm)	Type of carbon	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0	C—I	0–40
$R-CH_3$	8–35	C—Br	25–65
$R-CH_2-R$	15–50	C—Cl C—N C—O	35–80 40–60 50–80
	20–60		165–175
	30–40		165–175
$\equiv C$	65–85		175–185
$=C$	100–150		190–200
	110–170		205–220

Table of absorption bands

Major Functional Group	Absorption Frequency Region			
O-H	3650-3590			
N-H	3500-3300	1650-1590	900-650	
=CH-H	3100-3070	1420-1410	900-880	
=C-H	3100-3000	2000-1600		
C-H	2900-2700	1440-1320		
=-CH3	2880-2860	2970-2950	1380-1370	1470-1430
O-H	2700-2500	1320-1210	950-900	
C≡C	2140-2100			
C=O	1750-1700			
C=C	1600-1500			
C-N	1340-1250			
C-O-C	1200-1180			
-C-H	770-730			

Absorption frequency (cm^{-1})	Functional groups	Compounds
3500–3700	N—H stretching	Amines
3300–3400	O—H stretching	Aliphatic primary amine
3000–3100	C—H stretching	Alkene
2840–3000	C—H stretching	Alkane
1715–1730	C=O stretching	α,β-unsaturated ester
1600–1650	C=C stretching	conjugated alkane
1626–1662	C=C stretching	Alkane
1566–1650	C=C stretching	Cyclic alkene
1500–1550	N—O stretching	Nitro compound
1465	C—H bending	Methylene group
1450–1375	C—H bending	Methyl group
1380–1385	C—H bending	Alkane
1200–1275	C—O stretching	Alkyl aryl Ester
1163–1210	C—O stretching	Ester
1020–1075	C—O stretching	Vinyl Ether
665–730	C=C bending	Alkene