



# KIBABII UNIVERSITY

UNIVERSITY EXAMINATIONS  
2020/2021 ACADEMIC YEAR

FOURTH YEAR FIRST SEMESTER  
SUPPLIMENTARY/SPECIAL EXAMINATIONS

FOR THE DEGREE OF BSC (CHEMISTRY)

**COURSE CODE:** SCH 420

**COURSE TITLE:** ORGANIC SPECTROSCOPY

**DATE:** 14/1/2022

**TIME:** 8-10AM

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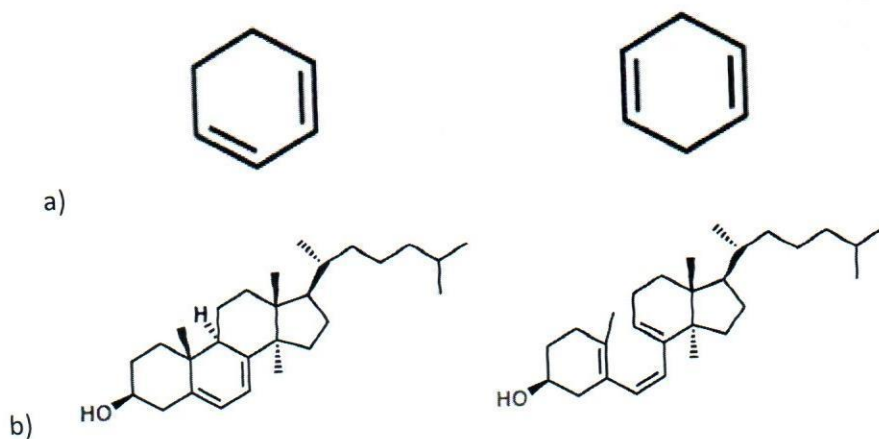
## INSTRUCTIONS TO CANDIDATES

Time: 2 Hours

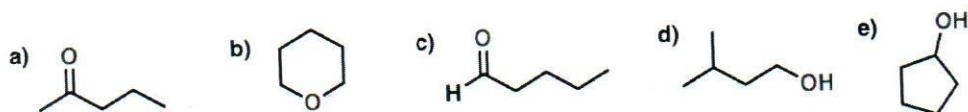
Answer question ONE and any other TWO of the remaining

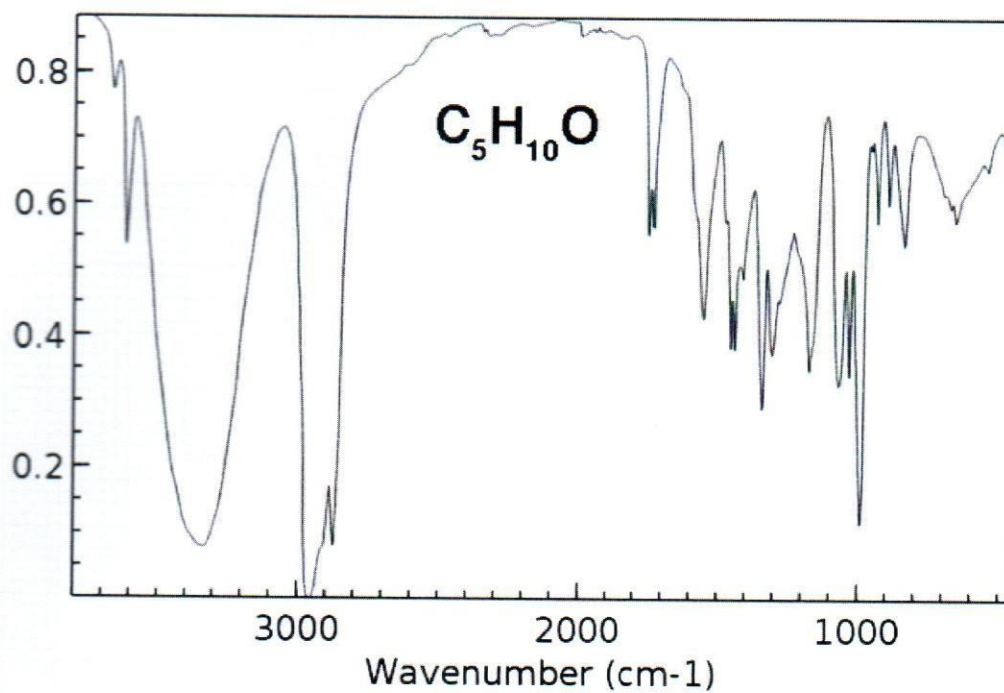
### QUESTION ONE (30 MARKS)

- a) Name three functions of mass spectrometer (3 marks)
- b) Explain the following observations in IR spectrum (3 marks)
- Units in the x axis of IR spectrum is measured in wavenumbers rather than wavelength
  - Lighter atoms have faster oscillation
  - Weaker bonds have lower energy oscillations
- c) The UV radiation region extends from about 200 nm to 400 nm and the visible radiation region extends from 400 nm to 800 nm. Answer the following question based on UV-VIS Spectroscopy
- Briefly explain working principle of UV-VIS Spectroscopy (3 marks)
  - List the allowed electronic transitions (4 marks)
  - Explain which molecule absorbs at the longest wavelength (4 marks)

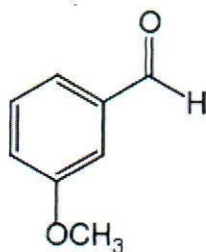


- iv. Unknown molecule has a molecular formula  $C_5H_{10}O$ . Based on IR spectrum below and citing reasons which of these five molecules is it most likely to be? (3 marks)



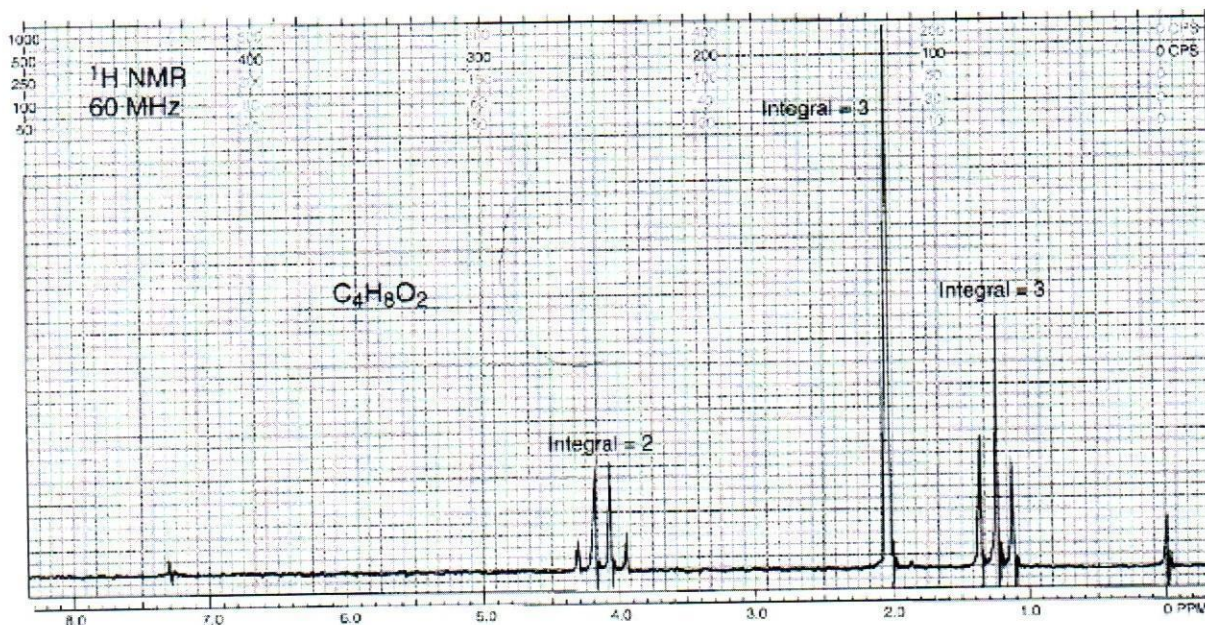


- d) Draw what you would expect to see in the  $^1H$  NMR of this compound. Your drawing should clearly show the number of signals, their approximate chemical shift (within 1 ppm) and the expected splitting pattern **(5 marks)**



- e) The following compound, with the formula  $C_4H_8O_2$  is an ester. Deduce its structure and assign its chemical shift value **(5 marks)**





### QUESTION TWO (20 MARKS)

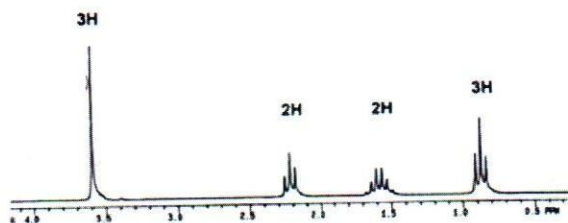
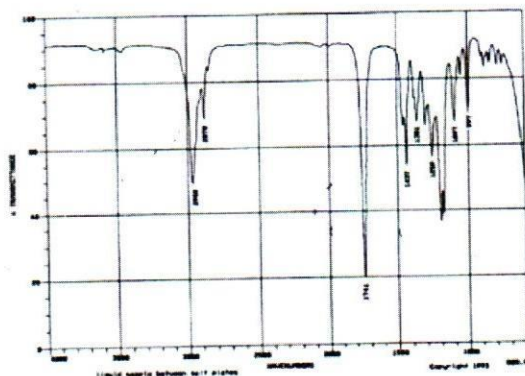
- a) Briefly explain working principle of mass spectrometer (4 marks)
- b) Calculate the molecular formulas for the possible compounds with the molecular mass of 136, using Rule of Thirteen and calculate index of hydrogen deficiency for each molecular formula. You may assume that the only other atoms present in each molecule are carbon and hydrogen (4 marks)
- A compound with two oxygen atoms (4 marks)
  - A compound with two nitrogen atoms (4 marks)
  - A compound with two nitrogen atoms and one oxygen atom (4 marks)
  - A compound with five carbon atoms and four oxygen atoms (4 marks)

### QUESTION THREE (20 MARKS)

- a) By definition, differentiate the following (2 marks)
- Chromophore and auxochrome (2 marks)
  - Bathochromic shift and Hypsochromic shift (2 marks)
  - Hyperchromic effect and Hypochromic effect (2 marks)
- b) Provide a structure of a compound having molecular formula  $C_5H_{10}O_2$  that is consistent with the following spectra.

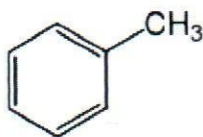
Show your work by assigning all the relevant peaks in IR and NMR spectra

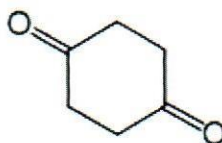
(12 marks)

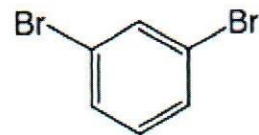


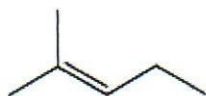
**QUESTION FOUR (20 MARKS)**

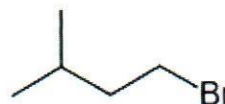
a) Predict how many signals you would see in the  $^{13}\text{C}$  NMR spectrum of each of these molecules. (5 marks)





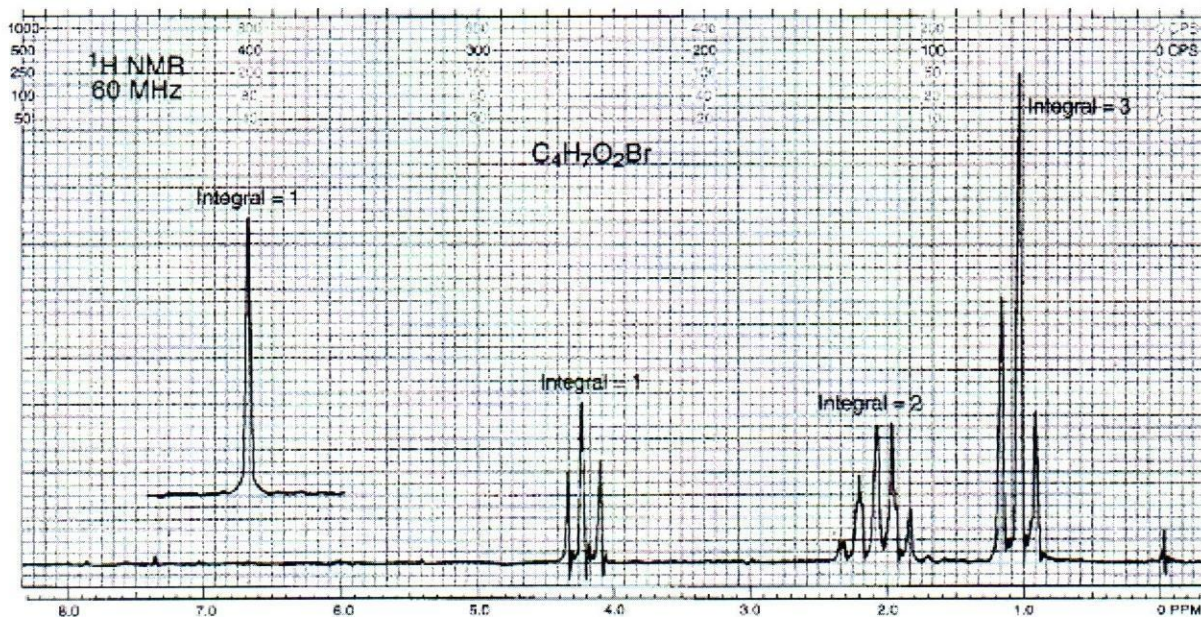






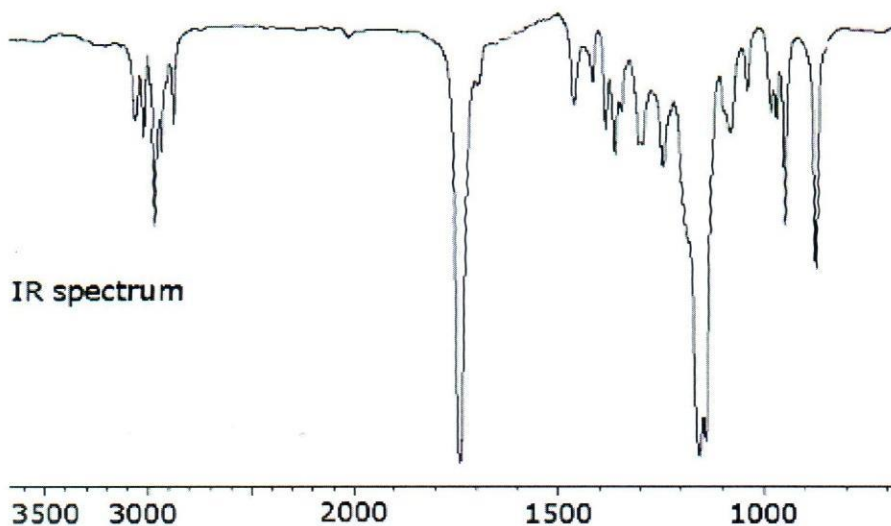


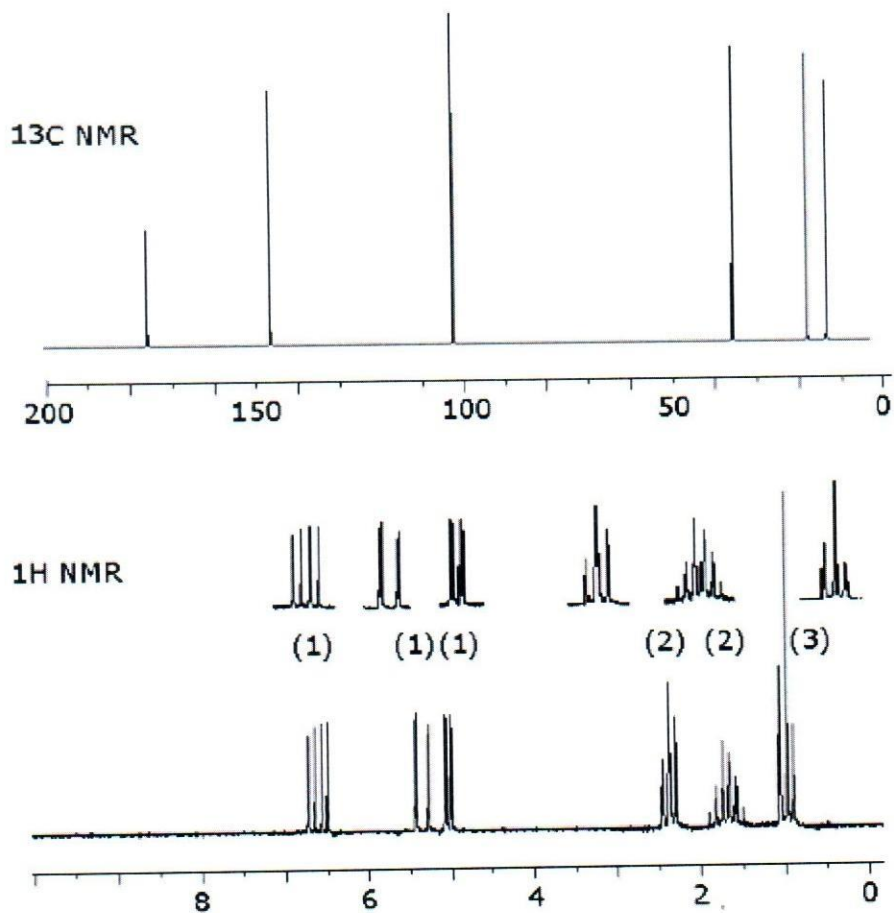
- b) Calculate the chemical shift in parts per million ( $\delta$ ) for a proton that has resonance 128 Hz downfield from TMS on the spectrometer that operates at 60 MHz (4 marks)
- c) The following compound is a carboxylic acid that contain a bromine atom:  $C_4H_7O_2Br$ . The peak at 10.97 ppm was moved onto the chart (which runs only from 0 to 8 ppm) for clarity. Deduce the structure of the compound



### QUESTION FIVE (20 MARKS)

Study the IR,  $^{13}C$  NMR and  $^1H$  NMR spectra for an unknown compound with the formula  $C_6H_{10}O_2$ , then answer the question on the next page.





- Determine degrees of unsaturation in this compound **(4 marks)**
- In the IR, what does the signal at about 1740 suggest? **(1 marks)**
- In the <sup>13</sup>C NMR, what does the chemical shift of the signal at about 105 suggest? **(1 marks)**
- In the <sup>1</sup>H NMR, what does the chemical shift of the signal at about 5.2 suggest? **(1 marks)**
- In the <sup>1</sup>H NMR, what does the integration of the signal at about 2.3 suggest? **(1 marks)**
- In the <sup>1</sup>H NMR, what does the splitting pattern of the signal at about 1.0 suggest? **(2 marks)**
- Deduce the structure of this unknown compound **(10 marks)**



## APPENDICES

### Approximate IR Absorption Frequencies

Bond	Frequency (cm <sup>-1</sup> )	Intensity
O-H (alcohol)	3650-3200	Strong, broad
O-H (carboxylic acid)	3300-2500	Strong, very broad
N-H	3500-3300	Medium, broad
C-H	3300-2700	Medium
C≡N	2260-2220	Medium
C=C	2260-2100	Medium to weak
C=O	1780-1650	Strong
C-O	1250-1050	Strong

### Approximate <sup>1</sup>H NMR Chemical Shifts

Hydrogen	δ (ppm)
CH <sub>3</sub>	0.8-1.0
CH <sub>2</sub>	1.2-1.5
CH	1.4-1.7
C=C-CH <sub>x</sub>	1.7-2.3
O=C-CH <sub>x</sub>	2.0-2.7
Ph-CH <sub>x</sub>	2.3-3.0
≡C-H	2.5
R <sub>2</sub> N-CH <sub>x</sub>	2.0-2.7
I-CH <sub>x</sub>	3.2
Br-CH <sub>x</sub>	3.4
Cl-CH <sub>x</sub>	3.5
F-CH <sub>x</sub>	4.4
O-CH <sub>x</sub>	3.2-3.8
C=CH	4.5-7.5
Ar-H	6.8-8.5
O=CH	9.0-10.0
ROH	1.0-5.5
ArOH	4.0-12.0
RNH <sub>x</sub>	0.5-5.0
CONH <sub>x</sub>	5.0-10.0
RCOOH	10-13

### Approximate <sup>13</sup>C NMR Chemical Shifts

Carbon	δ (ppm)
<i>Alkanes</i>	
Methyl	0-30
Methylene	15-55
Methine	25-55
Quaternary	30-40
<i>Alkenes</i>	
C=C	80-145
<i>Alkynes</i>	
C≡C	70-90
<i>Aromatics</i>	110-170
Benzene	128.7
<i>Alcohols, Ethers</i>	
C-O	50-90
<i>Amines</i>	
C-N	40-60
<i>Halogens</i>	
C-F	70-80
C-Cl	25-50
C-Br	10-40
C-I	-20-10
<i>Carbonyls, C=O</i>	
R <sub>2</sub> C=O	190-220
RXC=O (X = O or N)	150-180