MERU UNIVERSITY OF SCIENCE AND TECHNOLOGY

P.O. Box 972-60200 – Meru-Kenya.
Tel: +254 (0)799529958, +254 (0)799529959, +254 (0)712524293
Website: www.must.ac.ke Email: info@must.ac.ke

University Examinations 2022/2023

FOURTH YEAR, SECOND SEMESTER EXAMINATION FOR THE DEGREE OF BACHELOR OF SCIENCE IN EDUCATION SCIENCE, BACHELOR OF SCIENCE IN CHEMISTRY

SCH 3452: ORGANIC SPECTROSCOPY

DATE: APRIL 2023 **TIME:2 HOURS**

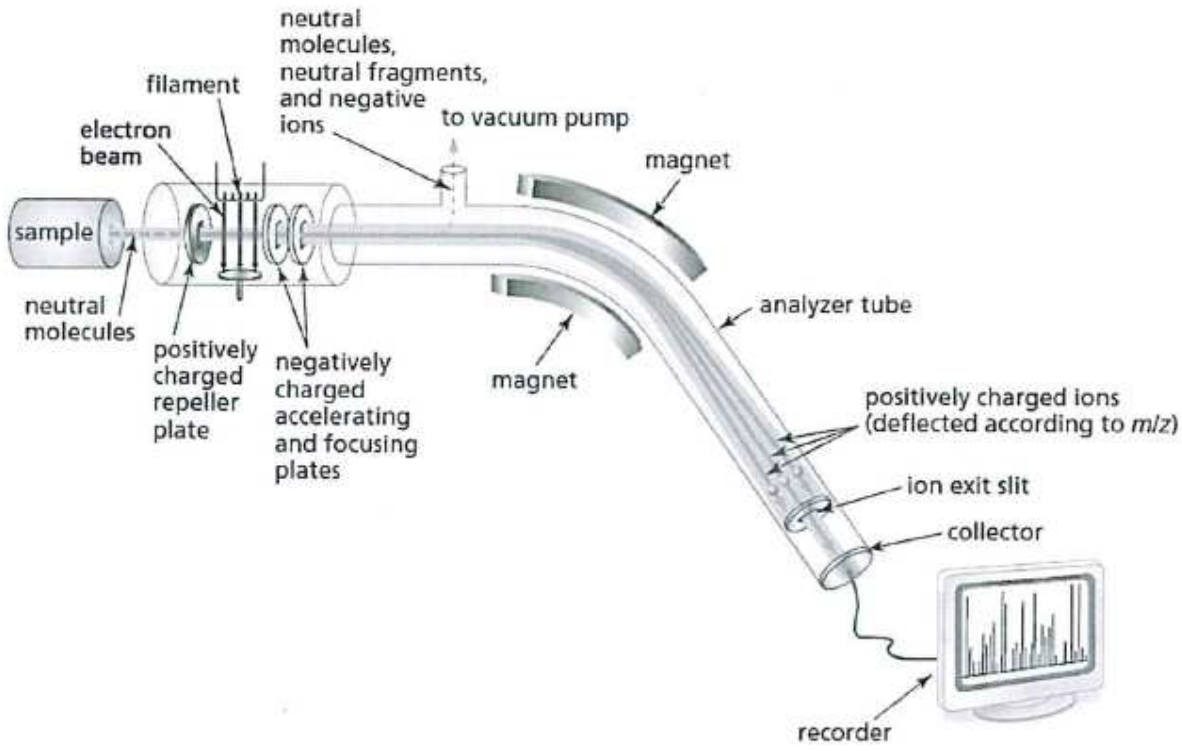
INSTRUCTIONS: *Answer question one and any other two questions. Useful data is provided are question 4*

QUESTION ONE (30 MARKS)

a) The following diagrams is a sketch of an instrument used in identification of organic compounds

(i) Name the instrument and what it is used for (2 marks)

(ii) Explain how it works (4 marks)



b) Explain the difference between alpha cleavage and McLafferty rearrangement in ketones (6 marks)

c) Explain the following terms (8 marks)

i) Stretching vibration

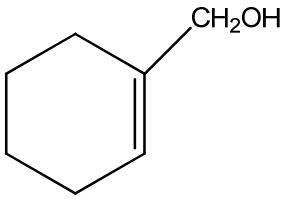
ii) Absorption bands

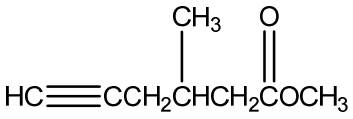
iii) Functional group region in IR

iv) Multiplet in nmr

d) The ^{1}H NMR peak of $CHCL_3$ was recorded on a spectrometer operating at 200 MHz providing the value of 1454 Hz. Convert 1454 Hz into δ units (4 marks)

e) Where might the following compounds have IR absorptions? (6 marks)

i) 

ii) 

QUESTION TWO (20 MARKS)

a) Explain the following terms (6 marks)

i) Chemical shif

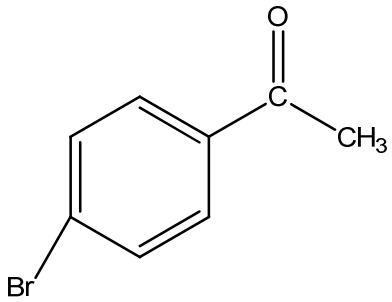
ii) Signal integration in nmr

iii) Spin-spin coupling

b) (i) Mention the number of peaks in the 1H NMR spectrum of 1,4-dimethyl-benzene (para-xylene or p-xylene (2 marks)

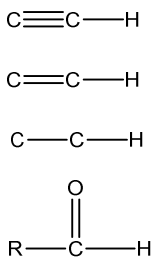
(ii) Mention the ratio of peak areas possible on integration of the spectrum (2 marks)

c) Predict the 13C chemical shifts for para-bromoacetophenone carbons and sketch the 13C spectrum for the molecule (10 marks)

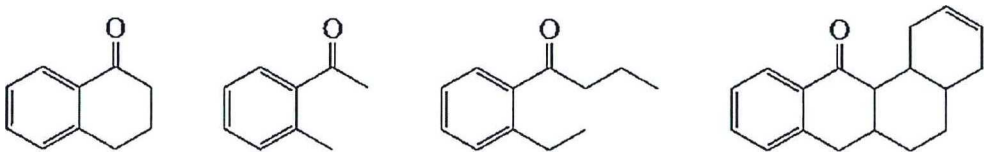


QUESTION THREE (20 MARKS)

a) Give the wavenumber where the following C – H stretching would occur in IR spectrum (4 marks)



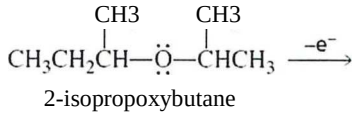
b) Draw the following compounds and highlight the conjugation patter on them (2 marks)



c) Fragmentation of 2-isopropoxybutane results into a molecular ion mainly in two ways:

- A C – C bond is cleaved heterolytically, with the electrons going to the more electronegative oxygen atom (14 marks)
- A C – C bond is cleaved homolytically at an a-carbon because this leads to a relatively stable cation since all its atoms have complete octets. (An a-carbon is the carbon bondend to the oxygen)

  Show the mechanism and sketch the mass spectrum expected (2 marks)



2-isopropoxybutane

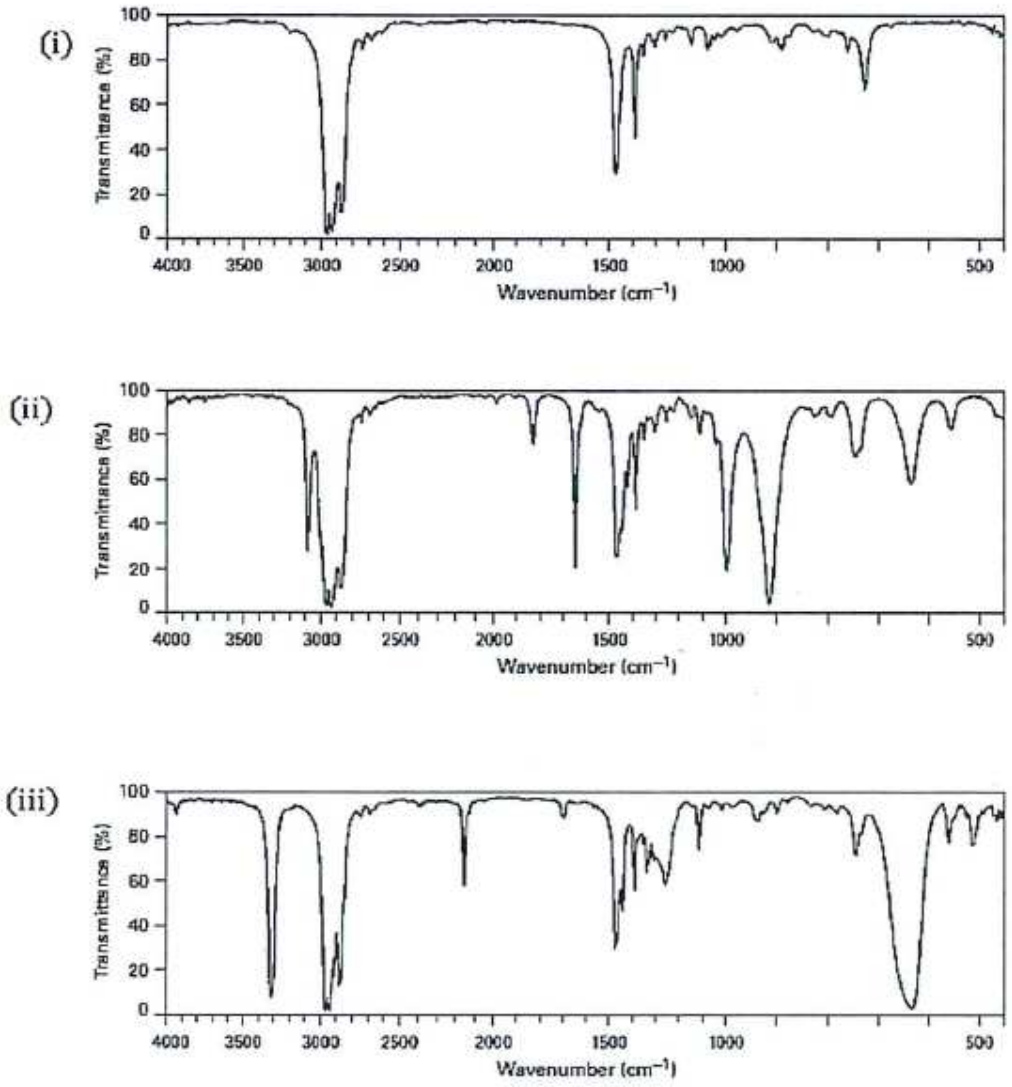
QUESTION FOUR (20 MARKS)

a) The amount of UV light absorbed is expressed as the sample's molar absorptivity ($\mathcal{E}$), define the equation (4 marks)

b) Explain what happens when a molecule absorbs UV radiation (4 marks)

c) Methyl 2, 2 – dimethylpropanoate $(CH_3)_3CCO_2CH_3$ has two peaks in its 1H NMR spectrum. What are their approximate chemical shifts? (4 marks)

d) Look at the IR spectra of 1-hexene and 1-hexyne and hexane in the figure below. Identify and explain which spectrum belongs to which compound (8 marks)



USEFUL DATA

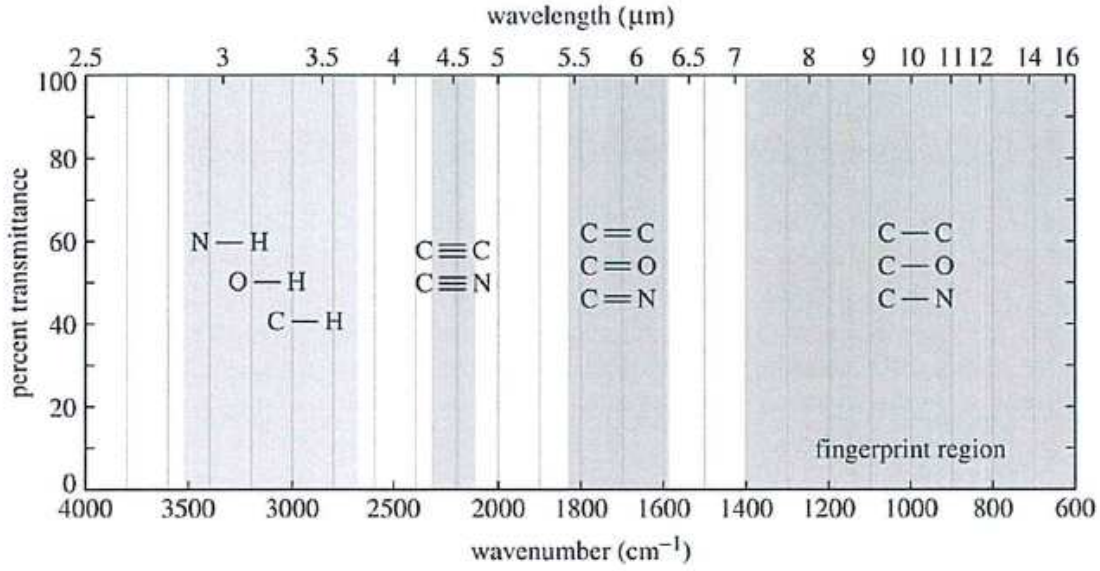
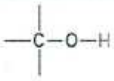
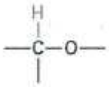
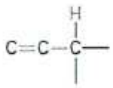
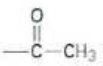
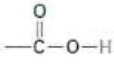
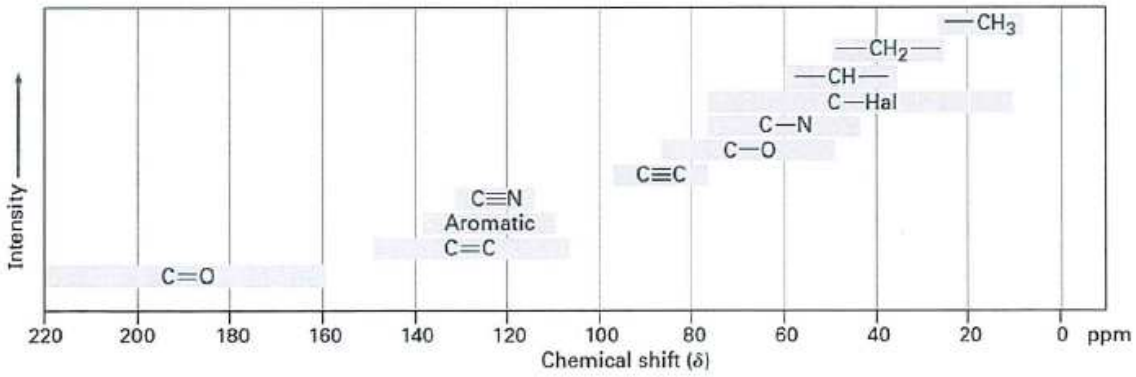


TABLE 13-3 Correlation of ^1H Chemical Shift with Environment

Type of hydrogen		Chemical shift (δ)	Type of hydrogen		Chemical shift (δ)
Reference	$Si(CH_3)_4$	0	Alcohol		2.5–5.0
Alkyl (primary)	$-CH_3$	0.7–1.3			
Alkyl (secondary)	$-CH_2-$	1.2–1.6			
Alkyl (tertiary)		1.4–1.8	Alcohol, ether		3.3–4.5
Allylic		1.6–2.2			
Methyl ketone		2.0–2.4	Vinylic		4.5–6.5
Aromatic methyl	$Ar-CH_3$	2.4–2.7	Aryl	Ar—H	6.5–8.0
Alkynyl	$-C\equiv C-H$	2.5–3.0	Aldehyde		9.7–10.0
Alkyl halide		2.5–4.0	Carboxylic acid		11.0–12.0


Intensity
—CH3
—CH2—
—CH—
C—Hal
C—N
C—O
C≡C
C≡N
Aromatic
C=C
C=O
220
200
180
160
140
120
100
80
60
40
20
0
ppm
Chemical shift (δ)