UNIVERSITY OF SWAZILAND
SECOND SEMESTER FINAL EXAMINATION 2012

TITLE OF PAPER	:	Applied Spectroscopy
COURSE NUMBER	:	C603
TIME	:	Three Hours
INSTRUCTIONS	:	Answer any FOUR Questions. Each Question carries 25 Marks.

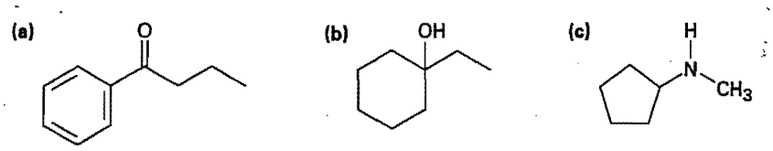
This Paper contains five (5) pages.

You must not open this paper until the Chief Invigilator so has granted permission to do.

SECTION A : MASS SPECTROMETRY AND INFRARED SPECTROSCOPY

Question 1

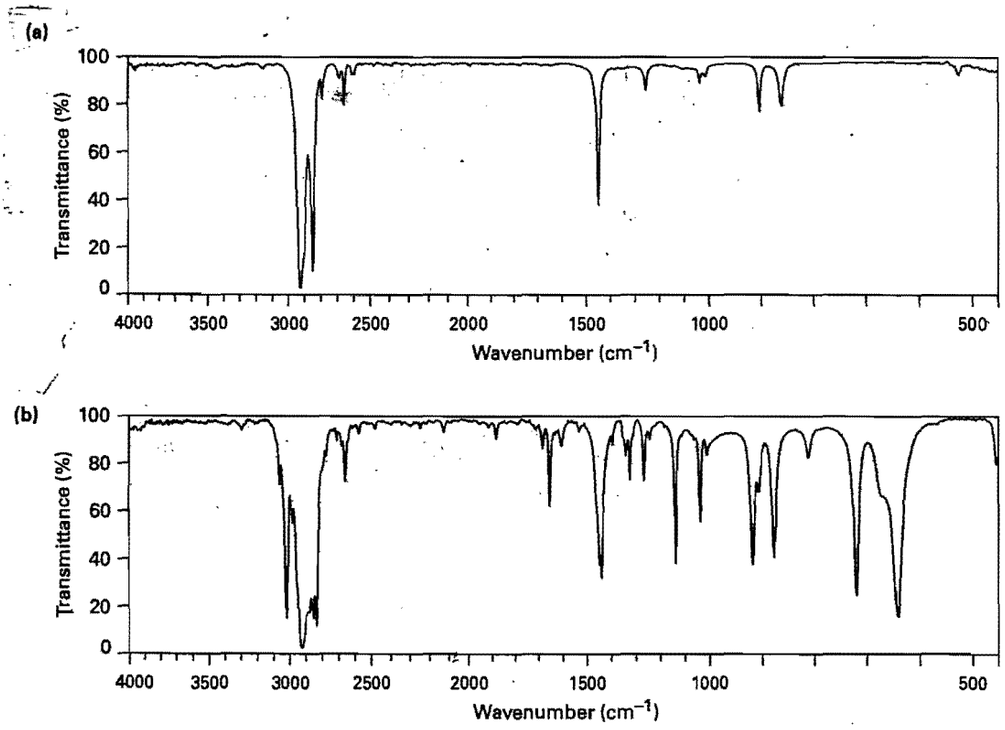
(a) What fragments might you expect in the mass spectra of the following compounds? Explain how the fragments and their m/z values arise. [18 marks]



(b) Assume that you are in the laboratory carrying out the catalytic hydrogenation of cyclohexene to cyclohexane. Explain how you would use a mass spectrometer to determine when the reaction is finished? [7 marks]

Question 2

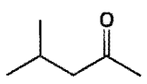
(a) Two infrared spectra are shown. One is the spectrum of cyclohexane, and the other is the spectrum of cyclohexene. Identify them and explain your answer. [12 marks]



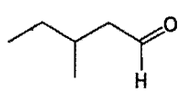
(b) Assume that you are carrying out the base-induced dehydrobromination of 3-bromo-3-methylpentane to yield an alkene. How could you use IR spectroscopy to tell which of the two possible elimination products is formed. [13 marks]

Question 3

(a) 4-Methyl-2-pentanone and 3-Methylpentanal are isomers. Explain how you could tell them apart both by mass spectrometry and by infrared spectroscopy. [18 marks]



4-Methyl-2-pentanone



3-Methylpentanal

(b) Assume that you are carrying out the dehydration of 1-methylcyclohexanol to yield 1-methylcyclohexene. Explain clearly how you could use infrared spectroscopy to determine when the reaction is complete. [7 marks]

SECTION B : NUCLEAR MAGNETIC RESONANCE (^1H AND ^{13}C NMR SPECTROSCOPY)

Question 4

Briefly describe the following aspects of nuclear magnetic resonance (NMR) spectroscopy.

i.	Theory	[10 marks]
ii.	Nature of NMR absorptions	[5 marks]
iii.	NMR spectra	[5 marks]
iv.	Operation of an NMR Spectrometer.	[5 marks]

Question 5

Compound A, a hydrocarbon with $M^+ = 96$ in its mass spectrum, has the ^{13}C spectral data given below. On reaction with BH_3 followed by treatment with basic H_2O_2, A is converted into B, whose ^{13}C spectral data are also given below. Propose structures for A and B. Show reasons that support your proposal.

Compound A [13 marks]

Broadband – decoupled ^{13}C NMR : 26.8, 28.7, 35.7, 106.9, 149.7 δ

Dept - 90: No peaks

Dept – 135 : No positive peaks; negative peaks at 26.8, 28.7, 35.7, 106.9 δ

Compound B [12 marks]

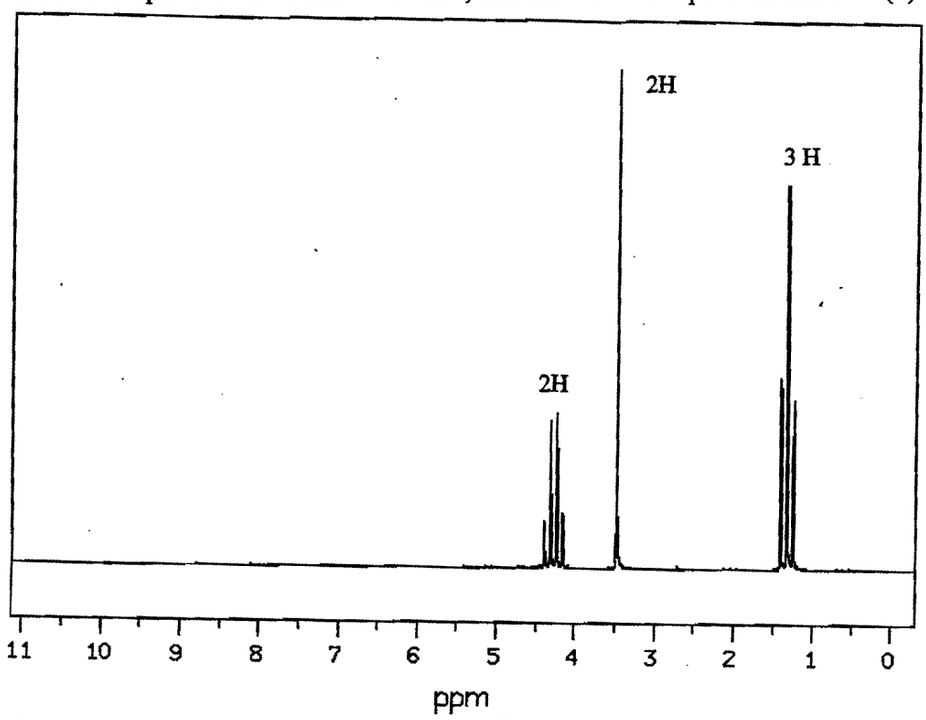
Broad band-decoupled ^{13}C NMR : 26.1, 26.9, 29.9, 40.5, 68.2 δ

Dept – 90 : 40.5 δ

Dept – 135 : positive peak at 40.5 δ ; negative peaks at 26.1, 26.9, 29.9, 68.2 δ

Question 6

To answer the following questions, consider the data and H^1 NMR spectrum below. The mass spectrum of this compound shows a molecular ion at m/z = 113 ; the IR spectrum has characteristic absorption at 2270 and 1735 cm^{-1}, and the ^{13}CNMR spectrum has five (5) signals.



(a) Based on the mass spectral data and the IR data, what functional groups are present in this compound? [4 marks]

(b) How many types of non-equivalent protons are there in this molecule? [4 marks]

(c) Comment or describe the signal at 3.5 delta in terms of integration, splitting pattern and chemical shift. [4 marks]

(d) Describe the signals at 4.3 delta and 1.3 delta in terms of their integration splitting and chemical shift. [4 marks]

(e) What is the significance of ^{13}C NMR data? [4 marks]

(f) Analyze all the information deduced from the data provided and then propose a structure for this compound? [5 marks]