

11.1 Spectroscopic Identification

Question Paper

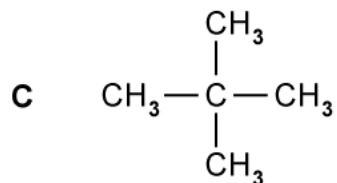
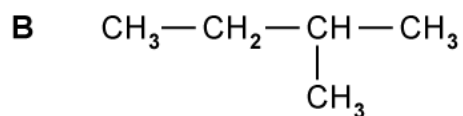
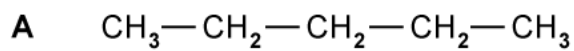
Course	DPIB Chemistry
Section	11. Measurements & Data Processes
Topic	11.1 Spectroscopic Identification
Difficulty	Easy

Time allowed: 40
Score: /33
Percentage: /100

Question 1a

a)

Three isomers of pentane are shown below.



Give the IUPAC names of isomers **B** and **C**.

[2]

[2 marks]

Question 1b

b)

Predict the number of different hydrogen environments in each of the isomers from part (a).

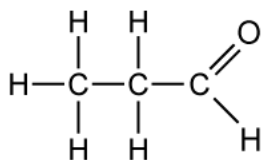
[3]

[3 marks]

Question 1c

c)

The displayed formula of propanal is shown.



State the number of ^1H NMR signals that would appear in the ^1H NMR of propanal and state the ratio of the area under the peaks in which they would appear.

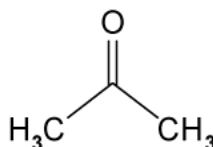
[2]

[2 marks]

Question 1d

d)

Propanal and propanone, shown below, both have the same molecular formula $\text{C}_3\text{H}_6\text{O}$.



Explain how propanone gives a different ^1H NMR spectrum compared to propanal.

[2]

[2 marks]

Question 1e

e)

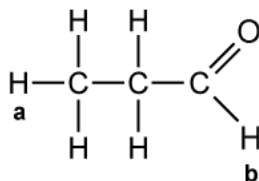
Using section 27 of the data booklet, state the chemical shift for the ^1H NMR of propanone.

[1]

[1 mark]

Question 2a

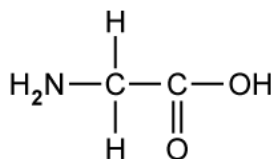
a)
Using section 27 of the data booklet, state the chemical shift for hydrogens **a** and **b** in the ^1H NMR of propanal.



[2 marks]

Question 2b

b)
The structure of the amino acid glycine is shown below.



State the number of peaks found in the ^1H NMR spectrum of glycine.

[1]

[1 mark]

Question 2c

c) State the ratio of the areas under the hydrogen peaks for glycine.

[1]

[1 mark]

Question 2d

d)

The chemical shift for the protons in the NH_2 protons in glycine is 1.0 - 4.5 ppm.

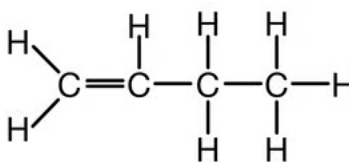
Using section 27 of the data booklet, predict the other ^1H NMR chemical shifts for glycine.

[1]

[1 mark]

Question 3a

a) Deduce the hydrogen deficiency of but-1-ene.



[1 mark]

Question 3b

b)

Phenol acid has the molecular formula $\text{C}_6\text{H}_6\text{O}$.

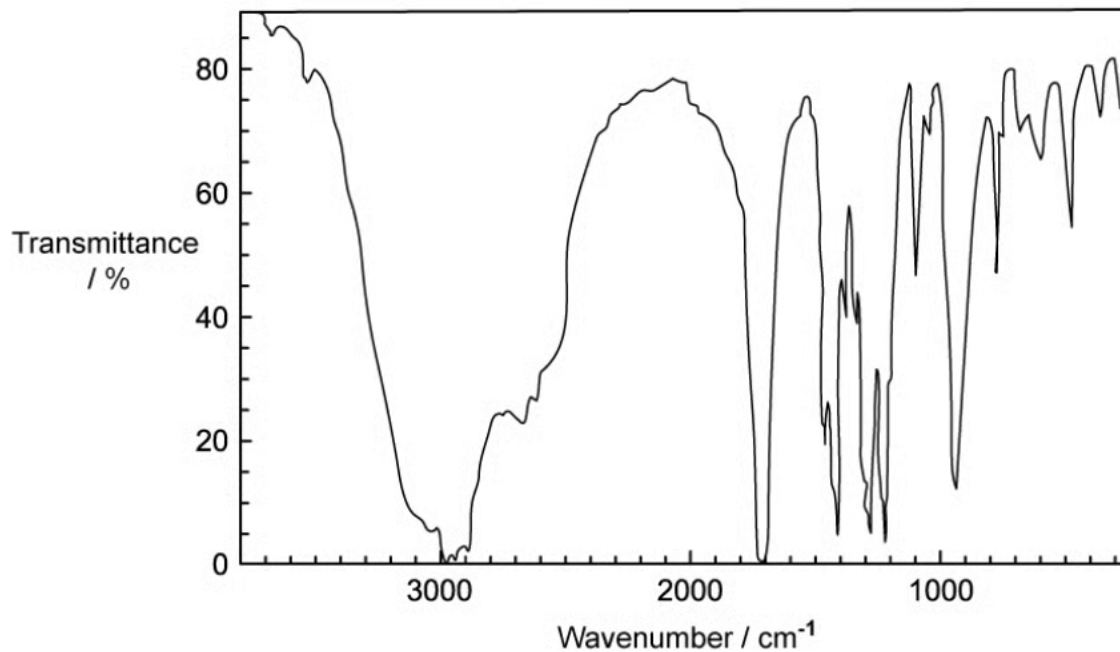
Deduce the index of hydrogen deficiency of phenol.

[1]

[1 mark]

Question 3c

c)
Under certain conditions, butan-1-ol can be oxidized to the compound with the infrared spectrum shown below.



Using section 26 of the data booklet, state the name of the compound that has produced the spectrum shown.

[1]

[1 mark]

Question 3d

d)
State what the molecular (parent) ion, M^+ peak, in the mass spectrum of a hydrocarbon containing ^{12}C and ^1H represents.

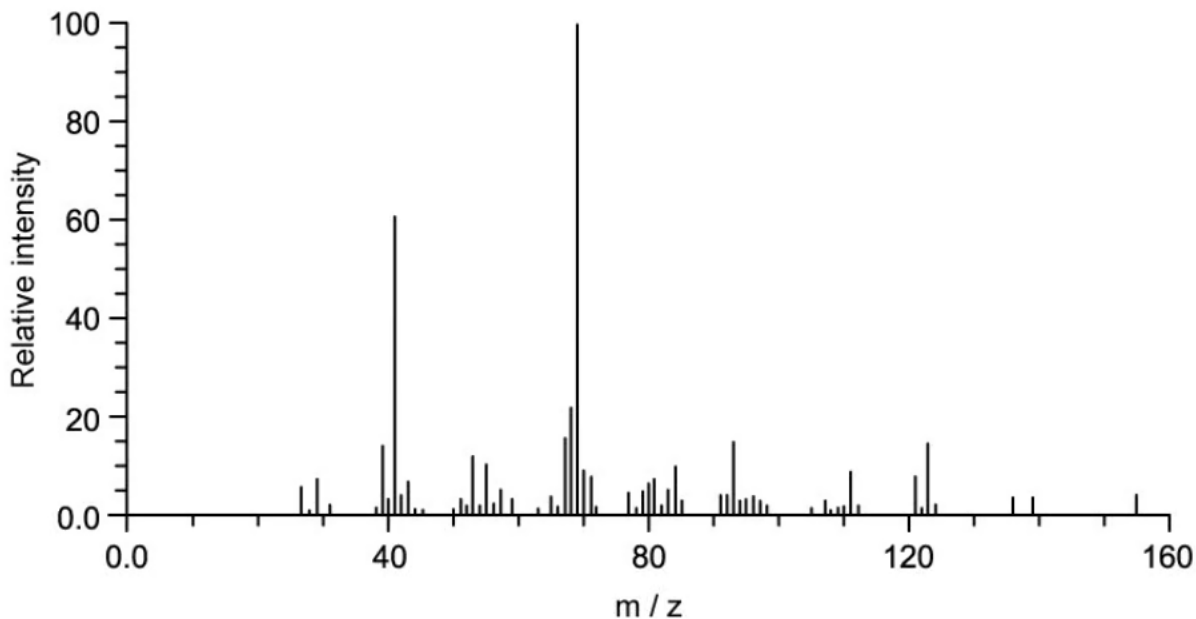
[1]

[1 mark]

Question 4a

a) Geraniol is an organic molecule that contains alkene and alcohol functional groups.

The mass spectrum of geraniol is shown below.



i) State how this mass spectrum can be used to confirm the molar mass of geraniol. [1]

ii) Give the formula of an ion that could be responsible for the peak at $m/z = 69$. [1]

[2 marks]

Question 4b

b)

A sample of propan-2-ol was heated under reflux with potassium dichromate(VI) acidified with sulfuric acid, and then the mixture was distilled.

Apart from the peaks due to the C—C and C—H bonds, what peak(s) would be present in the infrared spectrum of the distillate.

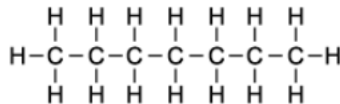
[1]

[1 mark]

Question 4c

c)

The compound shown below can be analysed to obtain infrared and mass spectra.



Using section 28 of the data booklet, suggest the molecular formulae of the ions responsible for peaks in the mass spectrum with the following m/e values.

i) 15 [1]

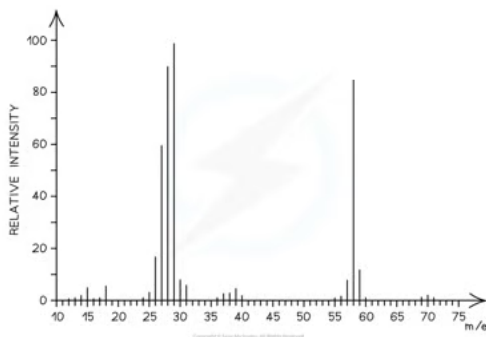
ii) 100 [1]

[2 marks]

Question 4d

d)

The mass spectrum shown below was obtained for propanal, $\text{CH}_3\text{CH}_2\text{CHO}$.



i) Use the mass spectrum to show that the empirical and the molecular formulae of the compound mentioned are the same. [1]

ii) Using section 28 of the data booklet, suggest the species responsible for the peak at $m/z = 29$. [1]

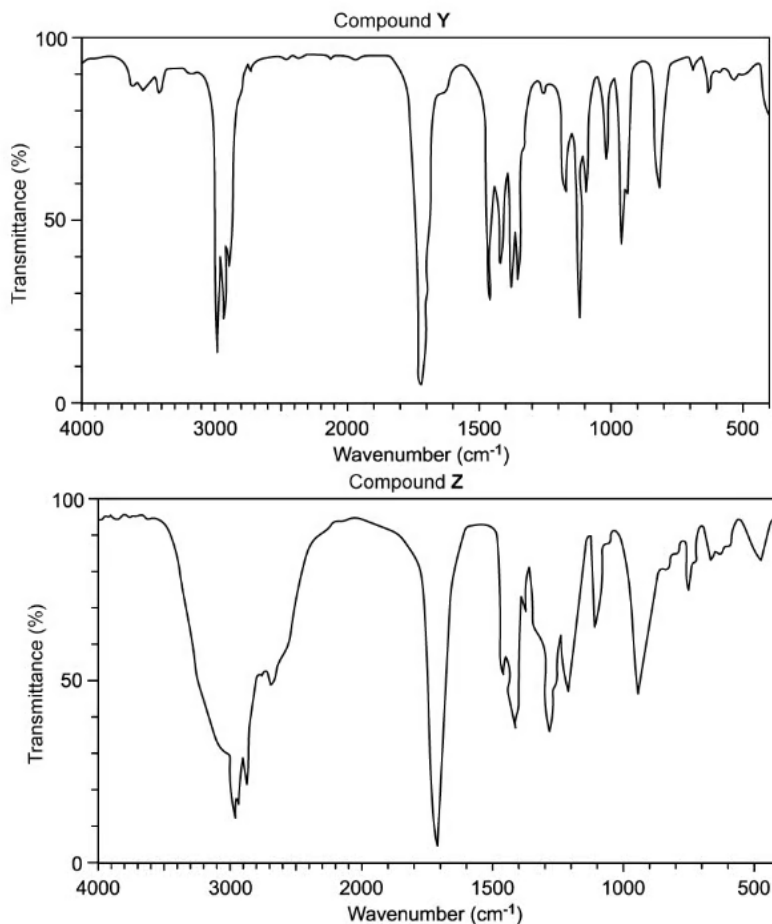
[2 marks]

Question 5a

a) This question is about some isomeric alcohols with the molecular formula $C_5H_{12}O$.

Some alcohols were heated with potassium dichromate(VI) and sulfuric acid. The organic compounds were separated from the reaction mixtures and purified.

The infrared spectra of two of these organic compounds are shown below.



Using section 26 of the data booklet, deduce the type of compound responsible for each spectrum.

Include in your answer references to wavenumbers and their corresponding bonds.

[2]

[2 marks]

Question 5b

b)

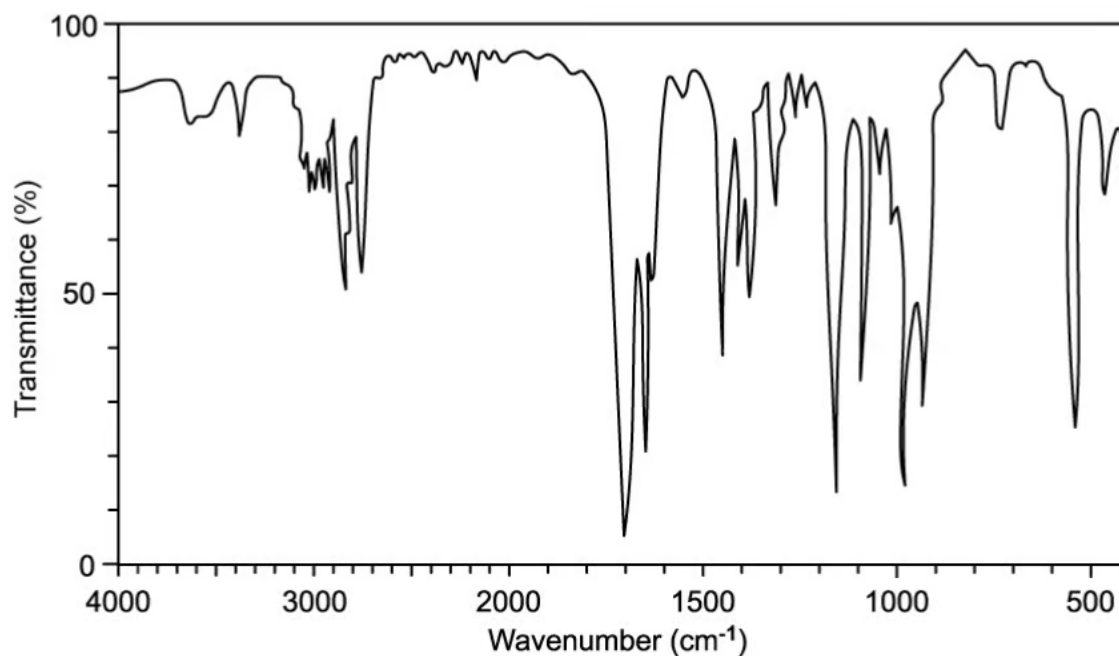
State what is meant by the term 'fingerprint region' on infrared spectra and explain how this can be used to identify primary, secondary and tertiary halogenoalkanes.

[2]

[2 marks]

Question 5c

c) The infrared spectrum a student obtained of an organic molecule which contains carbon, hydrogen and oxygen atoms is shown below.



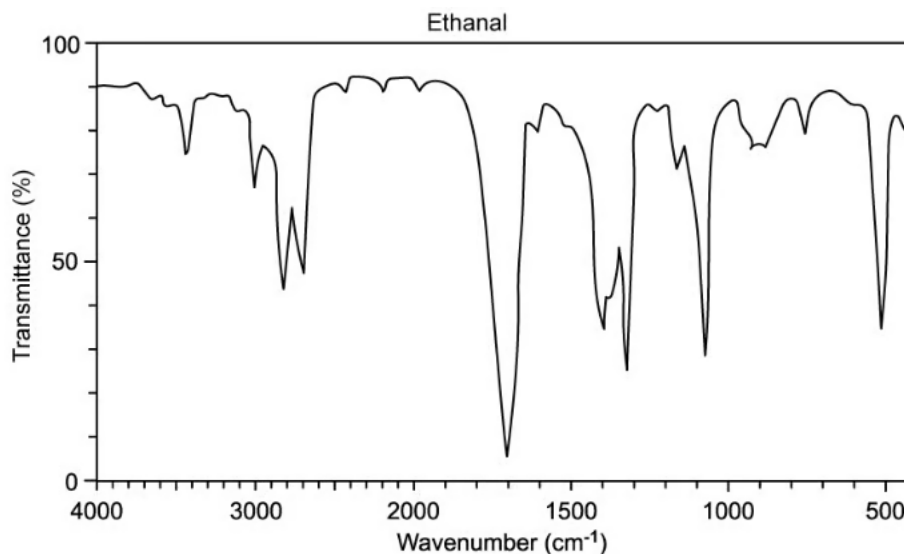
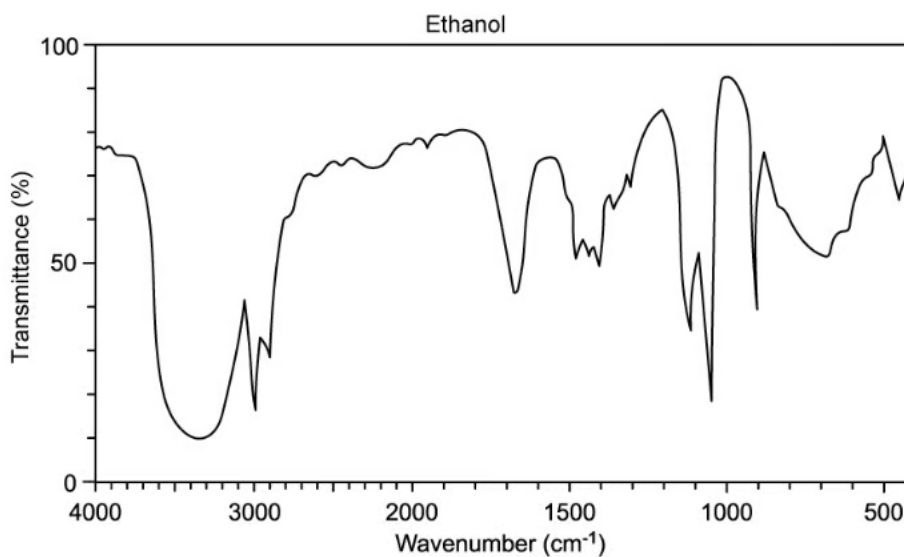
Use section 26 of the data booklet and information from the infrared spectrum to explain how the student deduced that the spectrum shows the presence of a carbonyl group.

[1]

[1 mark]

Question 5d

d) In an experiment to prepare a sample of ethanal, CH_3CHO , ethanol, $\text{C}_2\text{H}_5\text{OH}$, is reacted with acidified potassium dichromate (VI) and the reaction mixture is distilled. The infrared spectra for ethanol and ethanal are shown below.



i) State the bonds that give rise to the absorption in the ethanol spectrum at 3400 cm^{-1} and the absorption in the ethanal spectrum at 1720 cm^{-1} . [1]

ii) Explain why the absorption at 3400 cm^{-1} in the ethanol spectrum does not appear in the spectrum for ethanal. [1]

[2 marks]

