(b) The mass spectrum shows a parent ion at 84. The molecular formula is C_nH_{2n}.

$$n(12.01) + 2n(1.01) = 84$$
$$14.03n = 84$$
$$n = 84/14.03 = 5.99$$

The molecular formula is C_6H_{12}.

The saturated non-cyclic compound with six carbons is C_6H_{14}, so the IHD = 1.

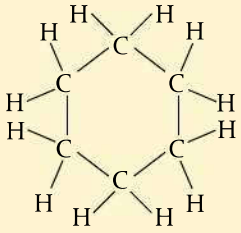
The molecule contains a C=C or a ring.

(c) The absence of peaks at 15 or 69 (84 – 15) suggests that the molecule probably does not contain a methyl group.

(d) The absorption close to 2900 cm^{-1} is due to the C–H bond.

The absence of an absorbance at 1600 cm^{-1} suggests that the molecule does not contain a C=C bond. It must, therefore, have a ring structure.

(e) The NMR spectra shows only one peak, so all the hydrogen atoms are in the same chemical environment. This confirms that the molecule has a ring structure. It is cyclohexane.



Practice questions

1 A burette reading is recorded as 27.70 ± 0.05 cm^3. Which of the following could be the actual value?

I 27.68 cm^3
II 27.78 cm^3
III 27.74 cm^3

A I and II only **B** I and III only **C** II and III only **D** I, II, and III

2 A piece of metallic aluminium with a mass of 10.044 g was found to have a volume of 3.70 cm^3. A student carried out the following calculation to determine the density.

$$\text{Density (g cm}^{-3}) = \frac{10.044}{3.70}$$

What is the best value the student could report for the density of aluminium?

A 2.715 g cm^{-3} **B** 2.7 g cm^{-3} **C** 2.71 g cm^{-3} **D** 2.7146 g cm^{-3}

3 Which experimental procedure is most likely to lead to a large systematic error?

A Determining the concentration of an alkali by titration with a burette.
B Measuring the volume of a solution using a volumetric pipette.
C Determining the enthalpy change of neutralization in a beaker.
D Measuring the volume of a gas produced with a gas syringe.

4 Which would be the best method to decrease the random uncertainty of a measurement in an acid–base titration?

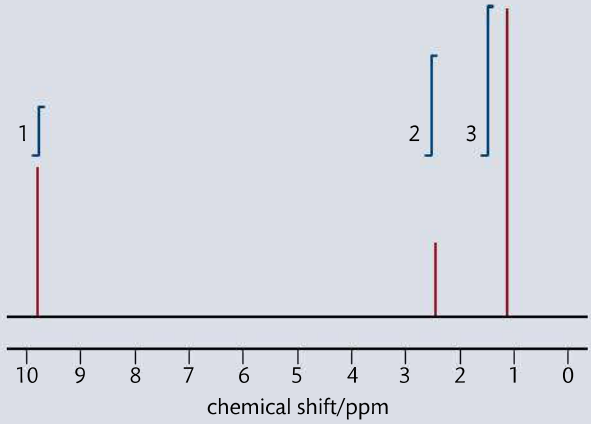
A repeat the titration
B ensure your eye is at the same height as the meniscus when reading from the burette

C use a different burette

D use a different indicator for the titration

5 The ^{1}H NMR spectrum of X with molecular formula C_3H_6O is shown below.

^{1}H NMR spectrum for question 5.



(a) Deduce which of the following compounds is X and explain your answer.

A $CH_3—CO—CH_3$

B $CH_3—CH_2—CHO$

C $CH_2=CH—CH_2OH$ (2)

(b) Deduce which one of the peaks in the ^{1}H NMR spectrum of X would also occur in the spectrum of one of the other isomers, giving your reasoning. (2)

(c) The infrared and mass spectra for X were also recorded.

(i) Apart from absorptions due to C—C and C—H bonds, suggest one absorption, in wavenumbers, that would be present in the infrared spectrum. (1)

(ii) Apart from absorptions due to C—C and C—H bonds, suggest one absorption, in wavenumbers, absent in this infrared spectrum but present in one of the other compounds shown in part (a). (1)

(d) Suggest the formulas and *m/z* values of two species that would be detected in the mass spectrum. (2)

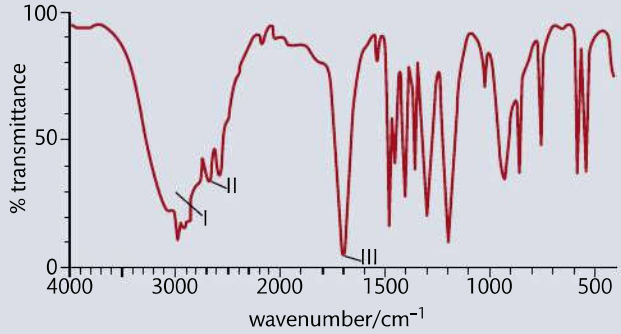
(Total 8 marks)

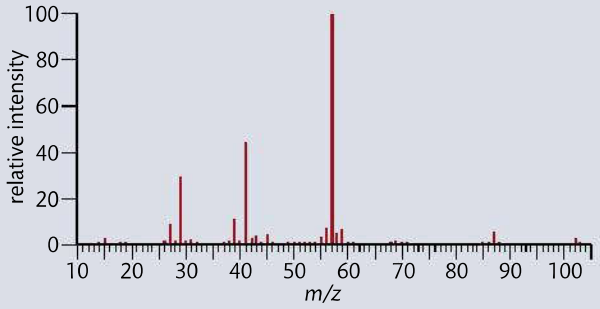
6 Infrared spectroscopy is commonly used as an analytical technique by inorganic, physical, and organic chemists.

(a) Explain why hydrogen bromide is IR active whereas bromine is IR inactive. (1)

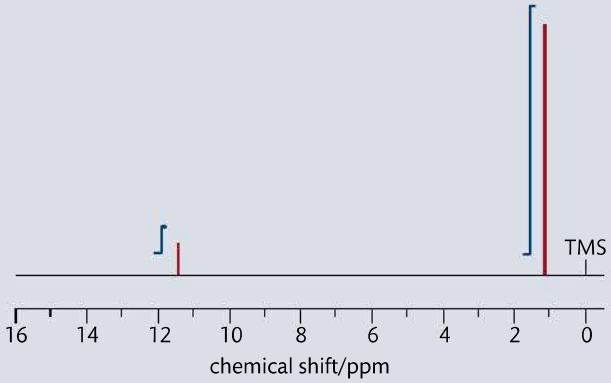
(b) The IR spectrum, mass spectrum, and ^{1}H NMR spectrum of an unknown compound, X, of molecular formula $C_5H_{10}O_2$, are as follows.

IR spectrum for question 6b.





Mass spectrum for question 6b.



^{1}H NMR spectrum for question 6b.

(i) In the IR spectrum, identify the bond responsible for each of the absorptions labelled I, II, and III. (3)

(ii) In the mass spectrum, deduce which fragments the *m/z* values at 102, 57, and 45 correspond to. (3)

(iii) Identify the peak at 11.5 ppm in the ^{1}H NMR spectrum. (1)

(iv) State what information can be obtained from the integration traces in the ^{1}H NMR spectrum about the hydrogen atoms responsible for the peak at 1.2 ppm. (1)

(v) Deduce the structure of X. (1)

(vi) $CH_3COOCH_2CH_2CH_3$ is an isomer of X. Deduce two differences between the ^{1}H NMR spectrum of this isomer and that of X. (2)

(Total 12 marks)

7 Infrared (IR) spectroscopy is widely used as a technique in analytical chemistry. Explain what happens at a molecular level during the absorption of IR radiation by carbon dioxide, CO_2. (3)

8 Compounds A and B are alcohols with the molecular formula C_3H_8O. The following information was obtained from a mass spectrum of each alcohol.

A: peaks at *m/z* = 29, 31, 60

B: peaks at *m/z* = 45, 60

(a) Deduce the formula of the species responsible for the peak at *m/z* = 60. (1)

(b) Deduce the formula of the species with *m/z* = 31. (1)

(c) Deduce the structure of each alcohol.

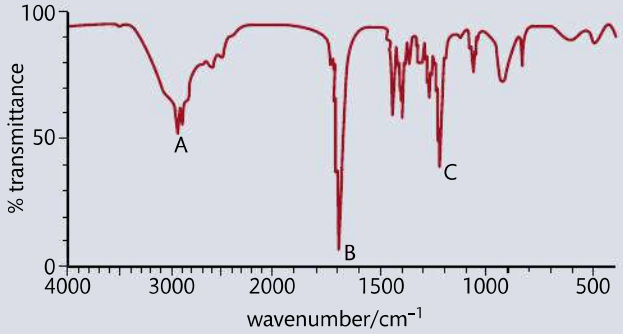
Structure of A

Structure of B (2)

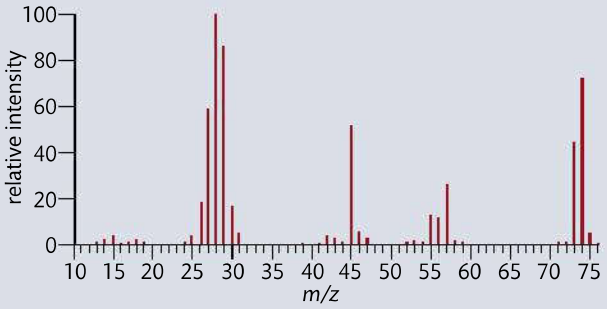
(Total 4 marks)

9 The IR spectrum, mass spectrum, and ^{1}H NMR spectrum of an unknown compound, X, of molecular formula $C_3H_6O_2$ are as follows.

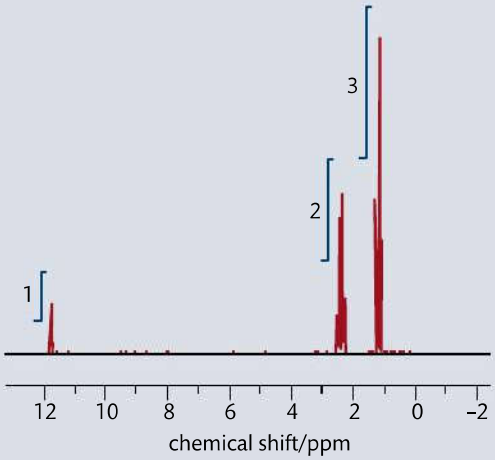
IR spectrum for question 9.



Mass spectrum for question 9.



^{1}H NMR spectrum for question 9.



(a) Identify the bonds responsible for the peaks A, B, and C in the IR spectrum of X. (2)

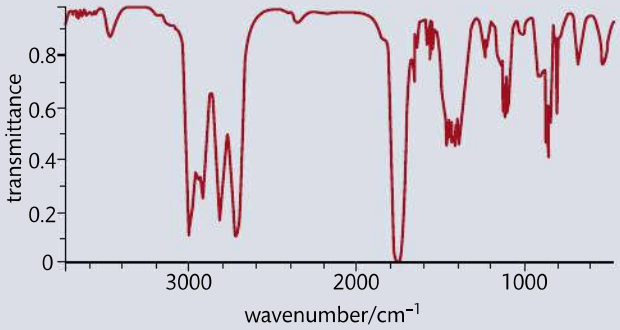
(b) In the mass spectrum of X, deduce which ions the *m*/*z* values at 74, 45, and 29 correspond to. (3)

(c) Identify the peak at 11.73 ppm in the ^{1}H NMR spectrum. (1)

(d) Deduce the structure of X. (1)

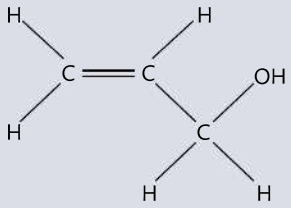
(*Total 7 marks*)

10 The infrared spectrum of a substance, X, with empirical formula C_3H_6O is given below.



IR spectrum for question 10.

(a) Explain why the structural formula of X cannot be:



(2)

(b) The ^1H NMR spectrum of X consists of three peaks. Deduce the structural formula of X and the relative areas under each peak. (2)

(*Total 4 marks*)

11 Butan-1-ol, butan-2-ol, 2-methylpropan-1-ol, and 2-methylpropan-2-ol are four structural isomers with the molecular formula $C_4H_{10}O$.

(a) Details of the ^1H NMR spectra of two of these alcohols are given below.

Spectrum 1

Two peaks: One at 1.3 ppm (relative to the TMS reference) with an integration trace of nine units, and the other at 2.0 ppm with an integration trace of one unit.

Spectrum 2

Four peaks: The first at 0.9 ppm with an integration trace of six units, the second at 1.7 ppm with an integration trace of one unit, the third at 2.1 ppm with an integration trace of one unit, and the fourth at 3.4 ppm with an integration trace of two units.

Consider the proton environments present in each of the alcohol molecules when answering the following questions.

(i) Identify which alcohol gives spectrum 1 and explain your answer by stating which hydrogen atoms in the molecule are responsible for each of the two peaks. (3)

(ii) Deduce which alcohol gives spectrum 2. Explain which particular hydrogen atoms in the molecule are responsible for the peaks at 0.9 ppm and 3.4 ppm. (3)

(b) The mass spectrum of one of the alcohols shows peaks at *m/z* values of 74, 59, and 45.

(i) Deduce which two of the alcohols could produce this spectrum and identify the species responsible for the three peaks. (4)

(ii) The spectrum also shows a significant peak at $m/z = 31$. Suggest which alcohol is responsible for this spectrum and deduce the species responsible for the peak at $m/z = 31$. (2)

(c) Explain why the infrared spectra of all four alcohols are very similar. (2)

(*Total 14 marks*)

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