Answers to exam-style questions

Topic 11

1 B

2 A

3 A

4 C

5 C

6 B

7 C

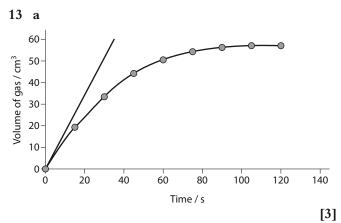
8 D

9 A

10 B

- 11 a Experiment B has produced the more precise values because there is a smaller spread of values. The range of values in experiment A is 53.2 49.2 = 4. The range of values in experiment B is 51.2 50.6 = 0.6. The smaller range in experiment B indicates more precise data. [2]
 - b The mean value in experiment A is 51.2. The mean value in experiment B is 50.9. The mean value in experiment B is closer to the literature value and therefore this is the more accurate experiment.
 [3]
- 12 a percentage error = $\frac{|\text{experimental value} \text{accepted value}|}{|\text{accepted value}|} \times 100$ $\text{percentage error} = \frac{|56.1 55.2|}{55.2} \times 100 = 1.6\%$ [1]
 - **b** percentage uncertainty due to random uncertainties = $\frac{0.5}{56.1} \times 100 = 0.9\%$

The percentage error (1.6%) is larger than that due to random uncertainties (0.9%) and therefore the student is not correct. This experiment contains systematic errors. [2]



b A tangent is drawn at the initial point of the graph as shown.

The gradient of this tangent is $\frac{56}{32} = 1.8 \,\text{cm}^3 \,\text{s}^{-1}$.

The initial rate of reaction is therefore $1.8 \,\mathrm{cm}^3 \,\mathrm{s}^{-1}$. This value is given to two significant figures, because the original data were given to two significant figures. The units are obtained by dividing the units on the γ -axis by those on the x-axis. [3]

- 14 a There is an absorption band in the range 1700–1750 cm⁻¹, which suggests the presence of a C=O group; so molecule I can be eliminated (also no O–H absorption in the spectrum).

 There is no very broad band absorption in the range 2400–3400 cm⁻¹, which is characteristic of carboxylic acids, so molecule III can be eliminated. There is no absorption band in the range 1000–1300 cm⁻¹, indicating that no C–O bond is present, so molecule IV (and III and I) can be eliminated. So this must be the spectrum of molecule II.
 - b Both propanal and propanone contain the same bonds and will have very similar absorption bands in the region around 1500 cm⁻¹. However, propanal has three peaks in its NMR spectrum (three different chemical environments for H) while propanone has only one, so they can be distinguished easily using NMR. Propanone has only one peak in the NMR spectrum because it is symmetrical and all the H atoms are chemically equivalent.

Note that the full structural formula must show the O–H bond. [1]

- **b** The three peaks arise because there are three different chemical environments for the protons (hydrogen atoms) in propan-2-ol. [2]
- c The integration trace gives the relative numbers of protons (hydrogen atoms) in each environment.
 This is obtained by finding the ratio of the heights of the vertical steps in the trace.

- ii The molecule is non-symmetrical and so there are five peaks in its NMR spectrum.
 The ratio of the areas under the peaks is the same as the ratio of the numbers of hydrogen atoms in each environment 3:1:1:2:3. [2]
- 16 a The relative molecular mass is obtained from the highest-mass peak in the mass spectrum 60 in this case.
 - **b** Z contains C, H and O and the only two possible combinations of these that add up to a relative molecular mass of 60 are C₃H₈O and C₂H₄O₂. [2]
 - **c** m/z 31 could be due to CH₃O⁺ or CH₂OH⁺; m/z 29 could be due to C₂H₅⁺ or CHO⁺ [2]
 - **d** The absorption band at about 3350 cm⁻¹ suggests the presence of an O–H bond. No absorptions in the range 1600–1800 cm⁻¹ suggests that there is no C=C or C=O present. [2]
 - **e** Z cannot have the formula C₂H₄O₂ because this requires the presence of a double bond. Therefore Z has the molecular formula C₃H₈O and possible structural formulas that contain an O–H group are:

f There are four different chemical environments for hydrogen atoms in propan-1-ol but only three in propan-2-ol because it is symmetrical. There are four peaks in the NMR spectrum, indicating four different chemical environments for hydrogen atoms – so **Z** must be propan-1-ol.

We could also measure the vertical heights of the steps in the integration trace – this works out to be 1:2:2:3, which corresponds with the numbers of hydrogen atoms in each environment in propan-1-ol. [4]

- 17 a The signal caused by the proton (hydrogen atom) in bold type is not split by the protons on the same carbon atom because they are chemically equivalent. There is one hydrogen atom on the adjacent carbon atom, so the signal due to the bold proton is split into a 1:1 doublet (if we add 1 to the number of hydrogens on the adjacent carbon atom we get 2 i.e. a doublet). [2]
 - **b** This can be approached in two ways. The first is to draw the isomers of $C_4H_{10}O$:

H-C-H H-C-H H-C-H H-C-H

There are two sets of peaks in the NMR spectrum and only two of these isomers (**I** and **III**) have two different chemical environments for hydrogen. These can be distinguished by using the integration trace. The ratio of the heights of the steps is 1:1.5, or 2:3, so the compound must be isomer **I**. This has hydrogen atoms (protons) in two different chemical environments and the numbers of protons in each are in the ratio 4:6, or 2:3.

The second way is to consider the splitting pattern and the integration trace. The ratio of the heights of the steps is 1:1.5, or 2:3. There are 10 protons (hydrogen atoms) in this molecule and

if they are divided in the ratio 2:3 there are 4 protons in one chemical environment and 6 in the other. The splitting pattern is a quartet and a triplet – the quartet indicates three hydrogen atoms on the adjacent carbon atom, and the triplet indicates two hydrogen atoms on the other adjacent carbon atom. These two peaks together are characteristic of an ethyl group, CH₃CH₂. So with ten protons there must be two ethyl groups, and the compound is isomer **I**. [4]

c The isomers are:

Isomer I has two different chemical environments for hydrogen atoms, so there will be two sets of peaks in its NMR spectrum. The ratio of the areas under these peaks will be 1:1. There are no hydrogen atoms on adjacent carbon atoms, so the spectrum will consist of two singlets.

Isomer **II** has three different chemical environments for hydrogen atoms, so there will be three sets of peaks in its NMR spectrum. The ratio of the areas under these peaks will be 3:2:1. There are three hydrogen atoms on one carbon atom and two on the adjacent carbon atom, so the peak with area 3 will be a triplet and the peak with area 2 will be a quartet – the third peak will be a singlet. The quartet will have a chemical shift similar to that of three of the protons in isomer I because the protons (hydrogen atoms) are in the same type of environment but all other chemical shifts will occur in different ranges. **[5]**

d The isomers are:

The NMR spectrum shows three sets of peaks and so there are three different chemical environments for hydrogen atoms (protons). This

means that isomer **III** can be eliminated because it has four different environments.

The ratio of the heights of the vertical steps in the integration trace is 3:2:3. There is a total of 8 hydrogen atoms in one molecule so this ratio indicates the numbers in each environment. This means isomer **IV** can be eliminated because its ratio of hydrogen atoms in different environments is 6:1:1.

The splitting pattern is singlet, quartet, triplet. Putting this together with the information from the integration trace we can say the following about atom arrangements – there are three Hs with no Hs on an adjacent carbon atom; two Hs with three Hs on an adjacent carbon atom; and three Hs with two Hs on an adjacent carbon atom. The latter two signals indicate the presence of an ethyl group. Both isomers I and II have the splitting pattern shown in the spectrum and so they have to be distinguished using chemical shifts.

If we consider the singlet in the spectra of isomers **I** and **II**, we can predict the following chemical shifts using Table **11.14**:

The singlet in the spectrum occurs at δ 3.7 ppm, so we can conclude that the compound responsible for the spectrum is isomer **II** – methyl propanoate. [6]