Pages 234–236 Exam practice questions

1 a) Peak 1 is $C_2H_3^+$; peak 2 is $C_2H_5^+$; peak 3 is CH_2OH^+; peak 4 is $C_2H_5O^+$; peak 5 is $C_2H_5OH^+$. ([3] less [1] for each error)

b) $CH_3CH_2OH + e^-$ [1] $\rightarrow CH_3CH_2OH^+ + 2e^-$ [1]

c) i) $CH_3CH_2OH^+$ [1] $\rightarrow CH_3 + CH_2OH^+$ [1]

ii) The CH_3 fragment is an uncharged radical. [1] A mass spectrometer only detects ions. [1]

2 This question assesses a student's ability to show a coherent and logically structured answer with linkages and fully sustained line of reasoning. Assess the quality of the answer taking into account both the key points made (*up to 4 marks*) and the logic and coherence of the discussion (*up to 2 marks*).

Points to make in the answer:

- There is no broad −OH peak as expected for a carboxylic acid, which suggests that the product of oxidation is an aldehyde or a ketone and not a carboxylic acid.
- The different C=O absorptions for aldehydes and ketones are too close so which is formed cannot be decided from this spectrum.
- The oxidation was carried out with a limited amount of potassium dichromate(VI) in acid conditions.
- If the aldehyde, the product was distilled off as it formed to avoid further oxidation to the acid.
- Possible primary alcohols are $CH_3CH_2CH_2CH_2OH$ (butan-1-ol) or $(CH_3)_2CHCH_2OH$ (2-methylpropan-1-ol).
- If a ketone, the possible secondary alcohol is $CH_3CH_2CH(OH)CH_3$ (butan-2-ol).

3 a) i) There are two forms of chloroethane, $CH_3CH_2{}^{35}Cl$ (relative mass 64) and $CH_3CH_2{}^{37}Cl$ (relative mass 66). [1]

ii) The chlorine-35 isotope is three times as abundant as the chlorine-37 isotope. [1]

b) i) M_r = 97 uses the relative atomic mass of 35.5 for chlorine, which is the weighted average of the isotopes. [1] There is no individual Cl atom with this mass. [1]

ii) In a molecular ion of $C_2H_2Cl_2$ with two chlorine atoms the possibilities are: most likely two atoms of chorine-35 (96) [1]; next, one of chlorine-35 and one of chlorine-37 (98) [1]; and least likely two atoms of chlorine-37 (100). [1]

The adjacent peaks differ by two mass units and the expected ratio is 9 : 6 : 1.

iii) These two peaks are from fragments formed by the loss of one chlorine atom leaving a single chlorine atom in the fragment. [1] So the ratio of abundances corresponds to the ratio of abundances of the isotopes. [1]

4 **a)** M_r C_5H_{12} = 72.1483

M_r C_4H_8O = 72.1054

M_r $C_3H_4O_2$ = 72.0625 ([1] for all three)

So the molecular formula of the compound is $C_3H_4O_2$ [1]

b) Effervescence confirms the presence of acid group COOH [1] so the structure is $H_2C{=}CH{-}COOH$. [1]

5 The absorptions in their IR spectra at about 1720 cm^{-1} are due to C=O [1] so **A** and **B** are carbonyl compounds.

Apart from the molecular ion at m/z = 58, the mass spectrum of **A** had major peaks at m/z = 43 and 15, i.e. loss of 15 or CH_3 leaving $C_2H_3O^+$ or $CH_3C{=}O^+$ [1] and m/z = 15 is CH_3^+. So **A** is propanone, CH_3COCH_3. [1]

Apart from the molecular ion at m/z = 58, the mass spectrum of **B** had a major peak at m/z = 29, i.e. loss of 29 or CH_3CH_2 leaving CHO^+ [1] or loss of CHO leaving $CH_3CH_2^+$. So **B** is propanal CH_3CH_2CHO. [1]

The IR spectrum of **C** has absorptions at 1645 cm^{-1} (corresponding to a C=C bond) [1] and at 3300 cm^{-1} (corresponding to an O–H alcohol bond). [1]

Possible structures could in theory be $H_2C{=}CH{-}CH_2OH$ or $HC(OH){=}CH{-}CH_3$ or $H_2C{=}C(OH){-}CH_3$

Apart from the molecular ion at m/z = 58, the mass spectrum of **C** had major peaks at m/z = 57 and 31.

To form a fragment of m/z = 31 requires loss of 27 or $H_2C{=}CH{-}$ [1], so **C** is prop-2-en-1-ol, $H_2C{=}CH{-}CH_2OH$. [1]

6 **a)** **A**: hexan-3-one [1]

B: hex-1-ene [1]

C: hexan-1-ol [1]

D: 1-chlorohexane [1]

b) **i)** Warm, aqueous [1] NaOH [1]; nucleophilic substitution [1]

ii) Potassium dichromate(VI) in acid [1]

Peak at 3750–3200 cm^{-1} [1] due to O–H (alcohol) should have disappeared if reaction is complete. [1]

7 C: 54.5% H: 9.1% O: 36.4% [1]

$\frac{54.5}{12.0}$ $\frac{9.1}{1.0}$ $\frac{36.4}{16.0}$ [1]

= 4.54 = 9.1 = 2.28

Empirical formula = C_2H_4O [1]

M_r = 88, so molecular formula is $C_4H_8O_2$. [1]

IR peak at 3408 cm^{-1} is due to O–H (alcohol) [1] and peak at 1709 cm^{-1} is due to C=O. [1]

MS peak at m/z = 43 due to CH_3CO^+ [1] (cannot be $C_3H_7^+$ because X is not a carboxylic acid).

Possible structures = $CH_3COCH_2CH_2OH$ or $CH_3COCH(OH)CH_3$ [1]

Oxidation formed compound **Y** which gave an IR peak at 3087 cm^{-1}. This is due to O–H (acid). [1]

So **X** must be a primary alcohol, i.e. $CH_3COCH_2CH_2OH$. [1]

Y is CH_3COCH_2COOH. [1]