Analytical chemistry year 12



3 Marks

- An organic compound was analysed and found to contain the following percentage composition by mass.
 36.36% O, 9.10% H, 54.54% C.
 Its mass and NMR spectra are given on the right.
 - a) Calculate the empirical formula of the compound C_2H_4O
 - b) With reference to the mass spectrum, above, find the molecular formula of the compound *Molecular mass is 88 as shown by the heaviest fragment on the mass spectrum, while empirical formula is 44. Hence the molecular formula is* $C_4H_8O_2$
 - c) Using the NMR and IR spectra on the right, identify the molecule by drawing its molecular structure.

The IR spectrum clearly shows O-H and C=O bonds. The ¹H NMR spectrum shows four hydrogen environments.



2+2+2=6 marks

5) A compound has a molecular mass of 62 and vaporises at around 120°C. Stephen and Jonathon need to isolate this compound from a mixture and identify its molecular structure. Two techniques have been discussed, GC and HPLC.

a) Discuss the similarities and the differences between the two techniques. Both have stationary and mobile phases and substances are identified by retention time.

- HPLC liquid mobile phase under high pressure, solid stationary phase. Useful for high molecular weight compounds.
- GC gas mobile phase, solid or liquid stationary phases. Useful for low molecular weight (<300) compounds that can be vapourised without decomposing. It is the most sensitive of all chromatographic techniques.

b) Identify the appropriate technique and discuss why. Since the molecule has a low molecular weight and vaporises at about 120^oC without decomposing it can be separated by GC.

6) A compound is to be analysed to determine its functional groups.a) Which is the most appropriate analytical technique?*IR spectroscopy*

1 mark

2 marks

2 marks

b) It was determined that the compound was a hydrocarbon. Which two techniques are best used to determine its structure?

¹H NMR and Mass spectrometry (in Mass spectrometry the difference in mass between fragment ions can give information about the structure of the molecule) Or ¹H NMR and ¹³C NMR

2 marks

7) A mixture of high molecular mass, organic compounds, mainly enzymes, is to be analysed.

a) Which is the most appropriate analytical technique to separate the components?

HPLC

1 mark

b) Give reasons why you selected the method above.
HPLC is used for medium to high molecular weight compounds.
Samples can be easily dissolved in a suitable solvent.

8) The mass spectrum of an unknown element is shown on the right.

Calculate the relative atomic mass of the element.

Three isotopes exist of atomic mass 29, 31,33 At relative percentage of 20%, 50% and 30% Respectively.

(29 X 20 + 31 X 50 + 33 X 30)/100 = 31.20



2 marks

Absorbance	Concentration% m/v
0.01	0.000
0.21	0.003
0.39	0.006
0.61	0.009
0.80	0.012
0.90	0.015

9) Below is a table of absorbance of known concentrations of mercury.

a) Construct a calibration curve





- b) A 450.0 g sample of shark meat was crushed and dissolved in 30.00 mL of 1.00 M HCl. The mixture was then filtered and the filtrate was made up to 50.00 mL with distilled water. A 25.00 mL sample of the final filtrate was taken and placed in a 250.0 mL volumetric flask and made up to the mark with distilled water. A 2.00 mL sample was analysed in a UV-visible spectrometer and an absorbance of 0.35 was obtained.
 - i) What is the concentration, in % m/v of the 2.00 mL sample?

0.0052% or 0.0052g/100mL

ii) What is the mass of mercury in the 250.0 volumetric flask? (0.0052/100) X 250 = 0.0130g

iii) What is the mass of mercury in the original sample of shark meat? $0.0130 \times 2 = 0.0260 \text{ g}$

iv) What is the concentration of mercury in the shark meat in ppm 0.0260/0.450 = 0.578 g/kg = 578 mg/kg = 578ppm

1+2+2+2 =7 marks

c) A substance was isolated from the meat and analysed. It was found to be a hydrocarbon of molecular mass between 60 and 70. Its ¹H NMR is shown below. Identify the hydrocarbon.



Pentane

2 marks