Structural Analysis (combined techniques) AS & A Level

Question Paper 1

Level	A Level
Subject	Chemistry
Exam Board	OCR
Module	
Topic	Structural Analysis(Combined techniques)
Paper	AS & A Level
Booklet	Question Paper 1

Time allowed: **69 minutes**

Score: **/51**

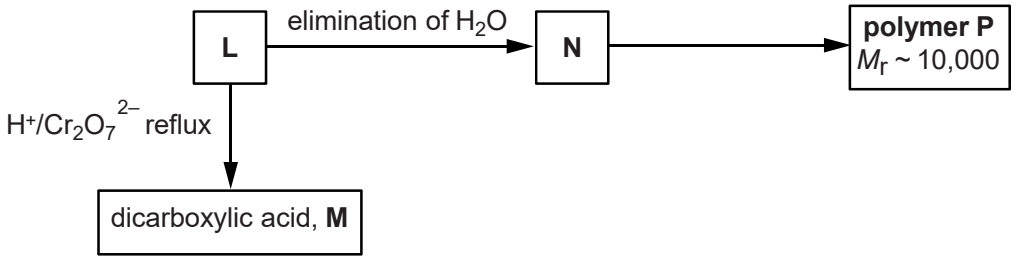
Percentage: **/100**

Grade Boundaries:

A*	A	B	C	D	E
>85%	73%	60%	47%	34%	21%

L, **M**, **N** and **P** are straight-chain organic compounds containing C, H and O only.

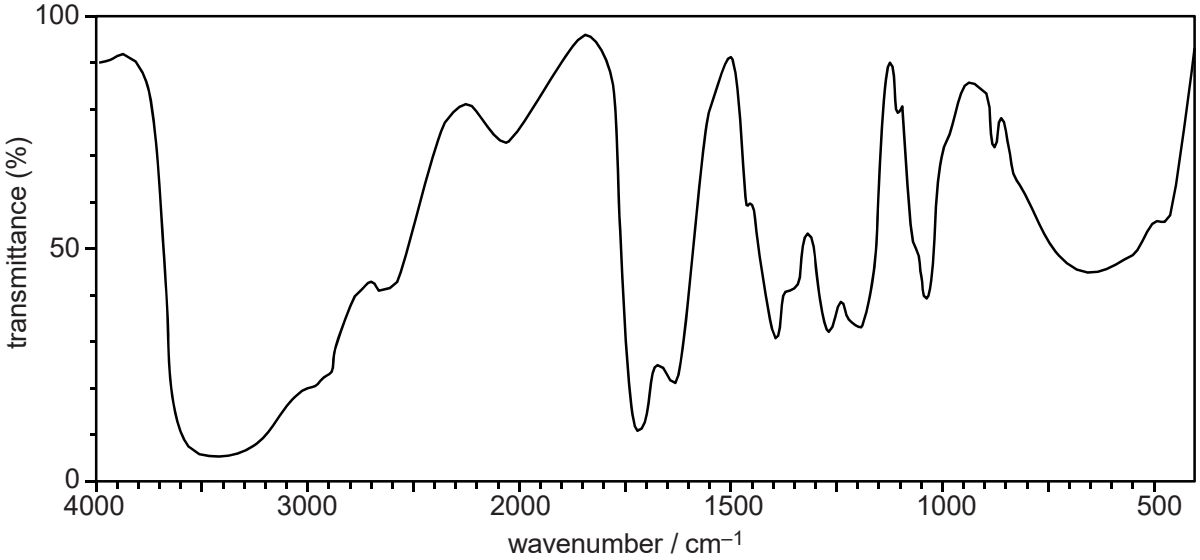
The flowchart shows reactions involving these compounds.



Analysis of compound **L** shows the following.

- Percentage composition by mass: C, 40.00%; H, 6.67%; O, 53.33%.
- Relative molecular mass of 90.0.
- The infrared spectrum below.

IR spectrum of **L**



(a) Calculate the empirical and molecular formulae of compound **L**.

Show your working. [3]

(b) Analyse the information and spectrum to determine the structures of **L** and **M**.

Include an equation for the reaction of **L** to form **M**. [5]

(c) Determine the structures of compounds **N** and **P**.

Estimate the number of repeat units in polymer **P** and write the equation for the formation of **P** from **N**. [4]

[Total 12 Marks]

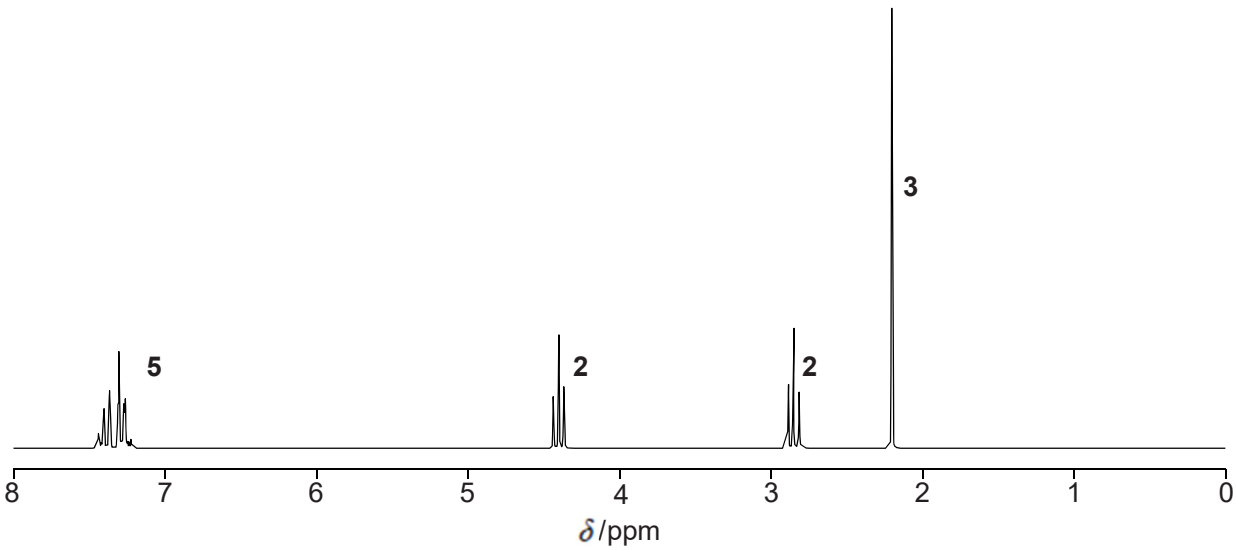
A chemist uses gas chromatography, GC, to separate the esters in a mixture. The esters are then analysed using different spectroscopic techniques.

(a) (i) How could the chemist use the results from GC to predict the number of esters in the mixture and their relative proportions? [1]

(ii) Why would there be some uncertainty about using GC alone to predict the number of esters in a mixture? [1]

(b) The chemist obtains a mass spectrum and a proton NMR spectrum of one of the esters separated by GC.

- The mass spectrum has a molecular ion peak at m/z = 164.
- The proton NMR spectrum is shown below.
  The numbers on the NMR spectrum represent the relative peak areas.



Analyse this information to identify the ester.

Include full details of your analysis of the proton NMR spectrum.

In your answer, you should use appropriate technical terms, spelled correctly. [9]

[Total 11 Marks]

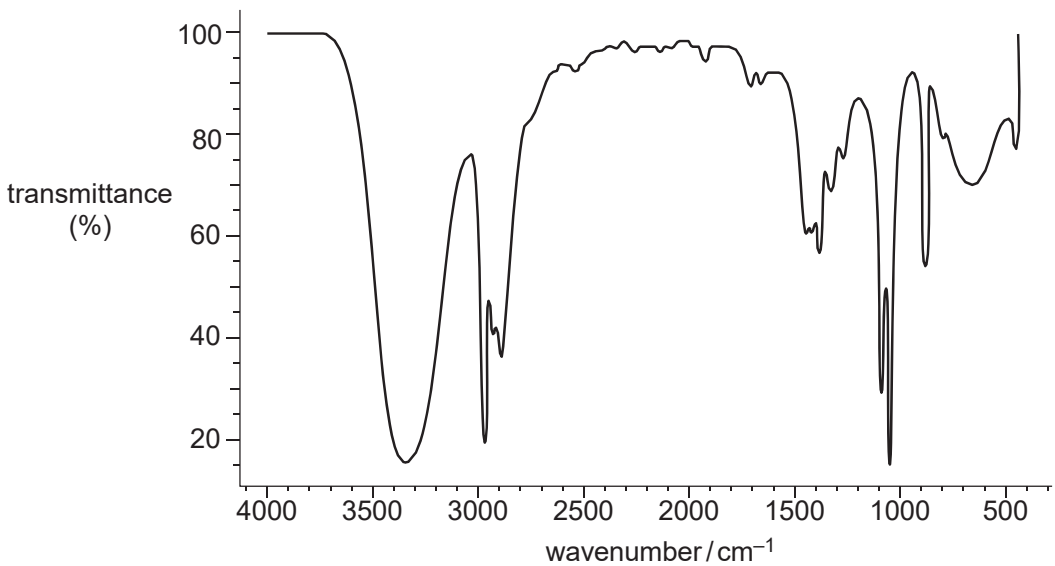
Compound **X** and compound **Y** react together to make an ester **Z**. Samples of **X** and **Y** were analysed by a research chemist. A summary of the chemist's results are shown below.

Analysis of compound X

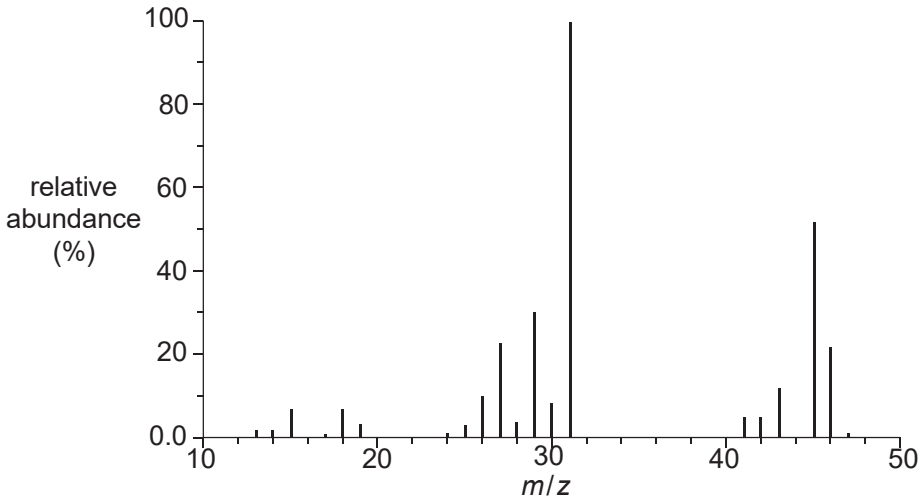
type of analysis	evidence
infrared spectroscopy	absorption at 1720 cm^{-1} and a very broad absorption between 2500 and 3300 cm^{-1}
percentage composition by mass	C, 48.65%; H, 8.11%; O, 43.24%
mass spectrometry	molecular ion peak at m/z = 74.0

Analysis of compound Y

infrared spectrum of **Y**



mass spectrum of **Y**



Use this information to suggest the identity of compound **X**, compound **Y** and ester **Z**.

In your answer you should make clear how your explanation is linked to the evidence. [10]

[Total:10 Marks]

Forest fires release a large number of organic compounds into the atmosphere, many in very small quantities.

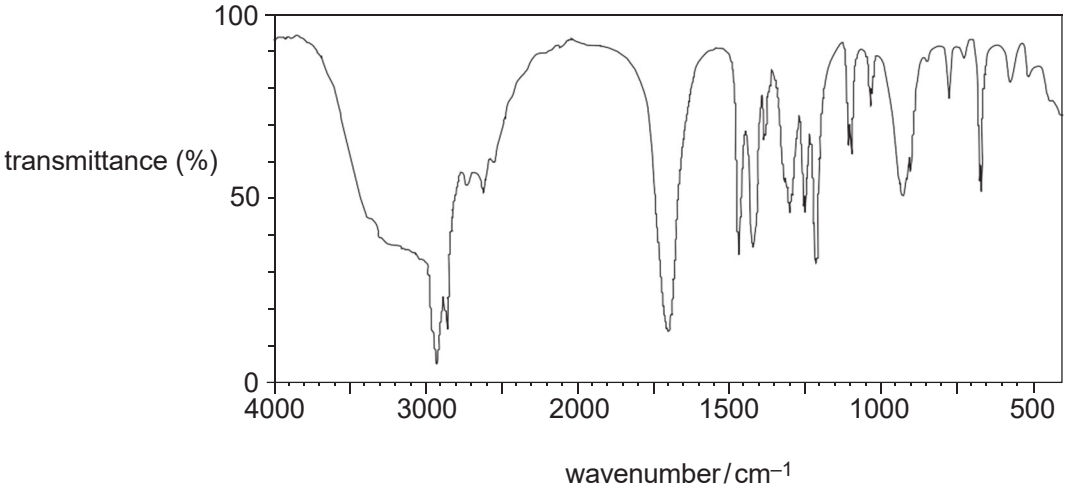
(a) Compounds in the smoke from forest fires can be analysed using GC-MS.
Explain how GC-MS enables the compounds to be identified. [2]

(b) Compound **F** was found to be present in the smoke.
Compound **F** contains C, H and O only and contains 54.2% oxygen by mass.
The molar mass of compound **F** is 118.0 g mol^{-1}.

(i) Using the information, show that the molecular formula of compound **F** is $C_4H_6O_4$.

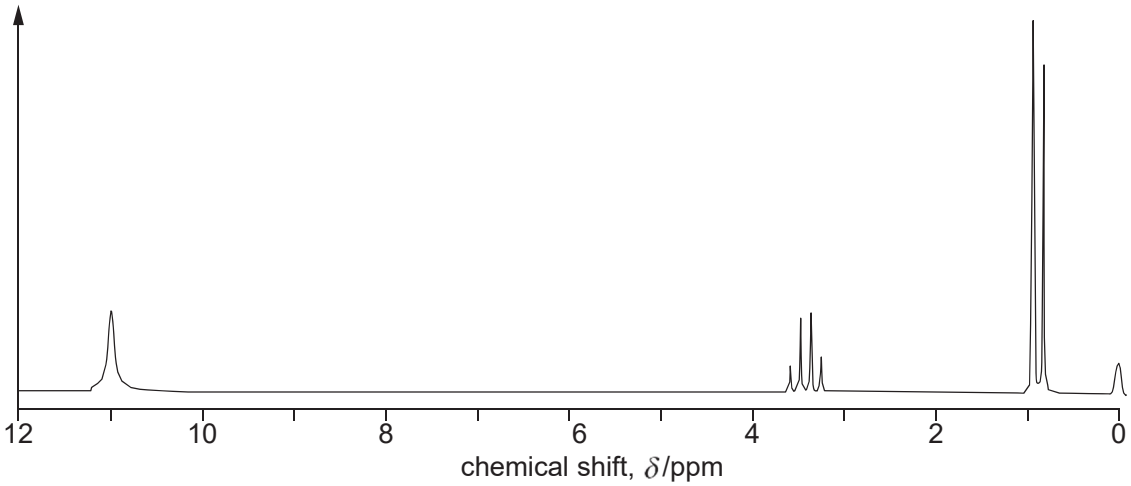
Show all of your working. [2]

(ii) The infrared spectrum of compound **F** is shown below.



Using this spectrum, name the functional group present in compound **F**. [1]

(c) Compound **F**, $C_4H_6O_4$, was dissolved in deuterated dimethylsulfoxide, $(CD_3)_2SO$, and some tetramethylsilane, TMS, was added. The proton NMR spectrum of compound **F** is shown below.



The peak centred at δ = 3.4 ppm would normally be expected at a chemical shift value about 1 ppm to the right, i.e. 2.4 ppm.

(i) Using the chemical shifts and splitting patterns, deduce the structural formula of compound **F**.

Explain your reasoning. [4]

(ii) Explain why deuterated dimethylsulfoxide, $(CD_3)_2SO$, is used as the solvent rather than $(CH_3)_2SO$..

[1]

(iii) State why TMS was added.

[1]

(iv) A second proton NMR spectrum of compound **F** was obtained after adding a few drops of D_2O.

What difference would you expect to see between the proton NMR spectra of compound **F** obtained with and without D_2O?

[1]

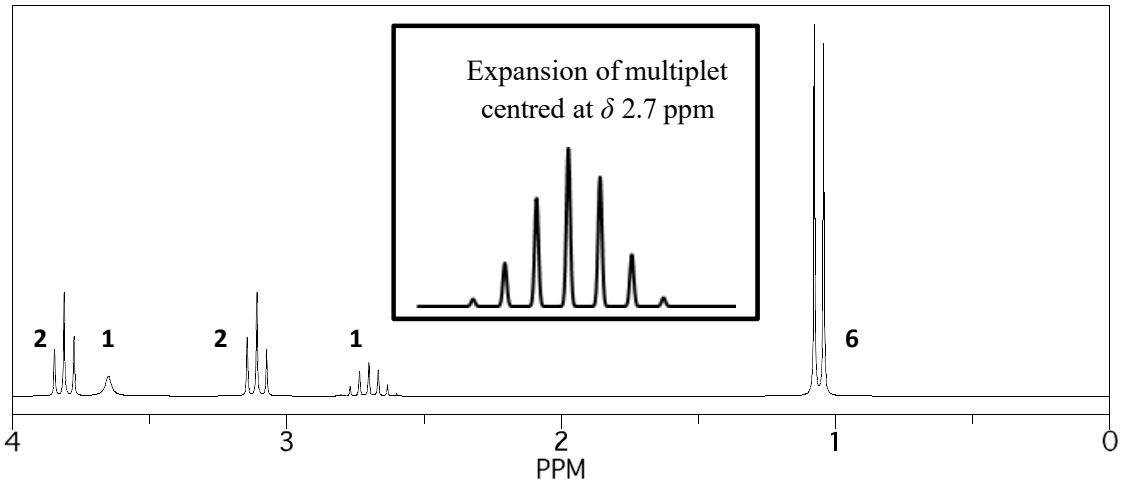
[Total 12 Marks]

A chemist isolates compound **L**, with empirical formula C_3H_6O, and sends a sample for analysis. The analytical laboratory sends back the following spectra.

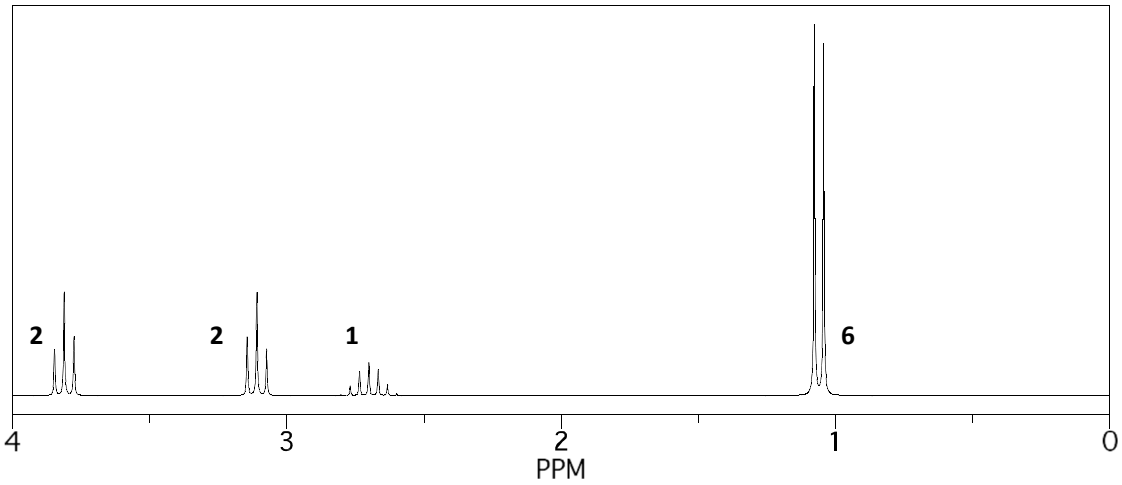
Mass spectrum
Molecular ion peak at *m*/*z* = 116.0.

^{1}H NMR spectra
The numbers next to each signal represent the number of ^{1}H responsible for that signal.
Two ^{1}H NMR spectra were obtained: one without D_2O and one with D_2O added.

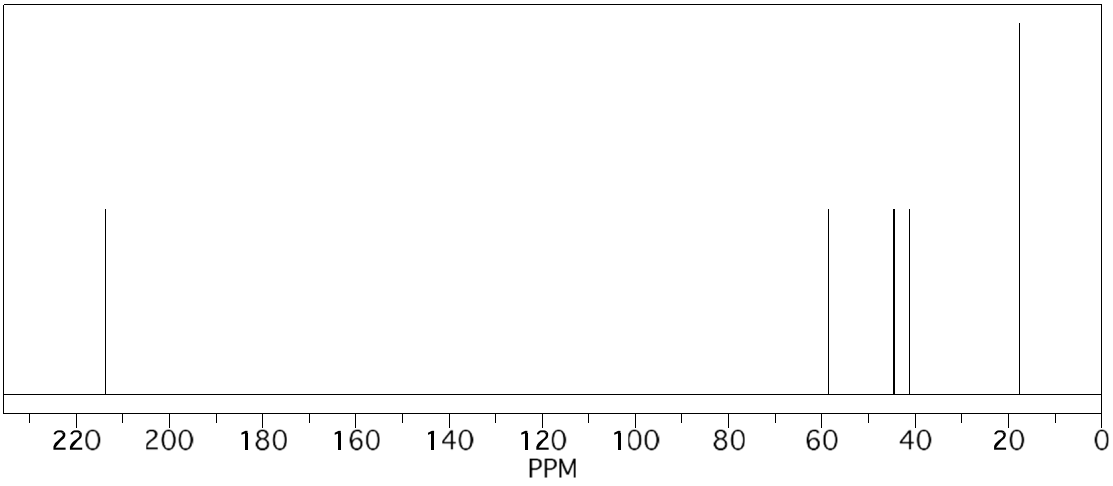
^{1}H NMR spectrum with no D_2O:



^{1}H NMR spectrum with D_2O added:



^{13}C NMR spectrum:



Use the information provided to suggest a structure for compound **L**.

Give your reasoning. **[6]**

[Total 6 Marks]