21.1 Spectroscopic Identification of Organic compounds

Question Paper

Course	DP IB Chemistry
Section	21. Measurement & Analysis (HL only)
Topic	21.1 Spectroscopic Identification of Organic compounds
Difficulty	Medium

Time allowed: 70

Score: /56

Percentage: /100

Question 1a

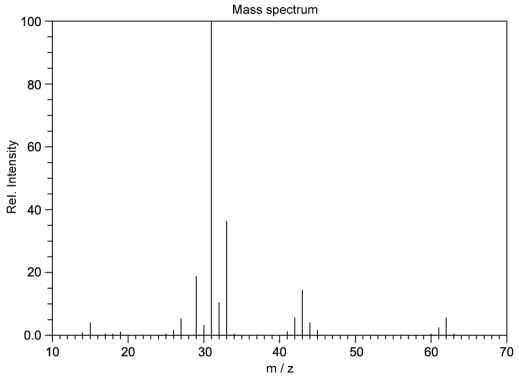
a)

Ethane-1,2-diol, $C_2H_6O_2$, can be distinguished from ethanedioic acid, $C_2H_2O_4$, by a number of analytic techniques including MS, IR and NMR

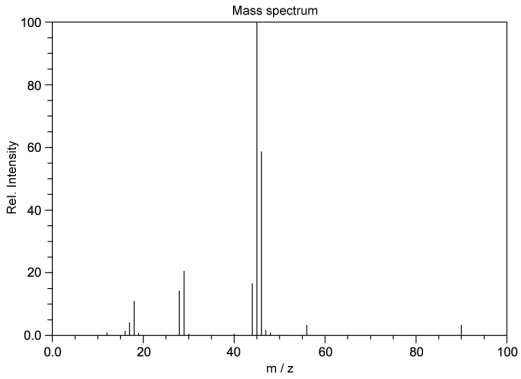
The MS of these molecules is shown below.

Which spectrum belongs to each molecule? Justify your answer.

Spectrum **A**



Spectrum **B**



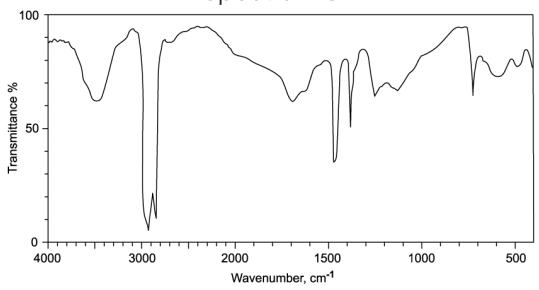
[2 marks]

Question 1b

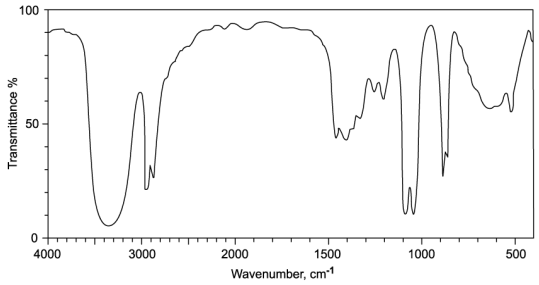
b)

The IR spectra of ethane-1,2-diol, $C_2H_6O_2$, and ethanedioic acid dihydrate, $C_2H_2O_4.2H_2O$, are shown in spectrum **C** and **D**. Use Section 26 of the Data Booklet to answer this question.

Spectrum **C**



Spectrum **D**



Which spectrum belongs to each molecule? Justify your answer.

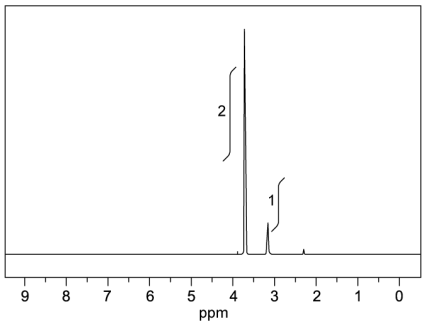
[2 marks]

Question 1c

c)

The ^1H NMR spectrum of ethane-1,2-diol is shown in spectrum **E**. Explain the significance of the spectrum.

Spectrum **E**



[3 marks]

Question 1d

d)
Predict the number of ^{1}H NMR signals and splitting pattern for ethanedioic acid.

[2 marks]

Question 2a

a)
During the production of an ^{1}H NMR spectrum, tetramethylsilane (TMS) is mixed with the sample.

i)
Draw the structural formula of TMS.

ii)
State two reasons why this chemical is suitable to be used as the standard reference compound.

[3 marks]

Question 2b

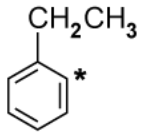
b)
Predict the number of peaks in the ^{1}H NMR spectrum of 1,3-dichlorobenzene.

[1 mark]

Question 2c

c)
The structural formula of ethylbenzene is shown below in **Figure 1**.

Figure 1



i)
Predict the number of peaks in the ^{1}H NMR spectrum of ethylbenzene

ii)
One of the hydrogen atoms in the structure of ethylbenzene shown above is labelled with an asterisk (*).
Use Section 27 from the Data Booklet to suggest a range of **δ** values for the peak due to this proton in the ^{1}H NMR spectrum of ethylbenzene.

[2 marks]

Question 2d

d)
Predict the splitting patterns of the signals due to the ethyl group found in the ^{1}H NMR spectrum of ethylbenzene.

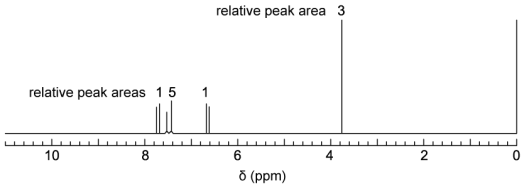
[1 mark]

Question 3a

a)

Methyl cinnamate, $C_{10}H_{10}O_2$, is a white crystalline solid used in the perfume industry. A sample of methyl cinnamate was analysed by ^1H NMR spectroscopy.

A simplified spectrum is shown below.

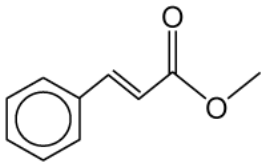


i)

Name the compound responsible for the peak at a chemical shift of 0 ppm. State its purpose.

ii)

Identify the proton environment that causes the peak at a chemical shift of 3.8 ppm by circling it on the structure of methyl cinnamate shown. Justify your answer.



[5 marks]

Question 3b

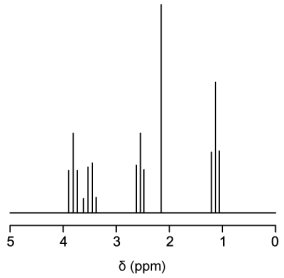
b)
This question is about the use of ^{1}H NMR spectroscopy to distinguish between isomers of $C_6H_{12}O_2$.

Draw the two esters with formula $C_6H_{12}O_2$ that each have only two peaks, both singlets, in their ^{1}H NMR spectra. The relative peak areas are 3:1 for both esters.

[2 marks]

Question 3c

c)
The high resolution ^{1}H NMR spectrum of another isomer of $C_6H_{12}O_2$ is shown below.



The integration values for the peaks in the ^{1}H NMR spectrum of this isomer, are given below.

Chemical shift, δ/ppm	3.8	3.5	2.6	2.2	1.2
Integration value	0.6	0.6	0.6	0.9	0.9
Splitting pattern	triplet	quartet	triplet	singlet	triplet

i)
Deduce the simplest ratio of the relative numbers of protons in each environment in the isomer.

ii)
Use Section 27 from the Data Booklet and the information given to deduce the part of the isomer that causes the signal at δ= 3.5 and the part of the structure at the isomer that causes the signal at δ=1.2.

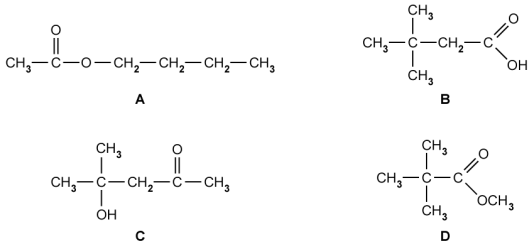
Explain why the splitting patterns of these peaks are produced.

[5 marks]

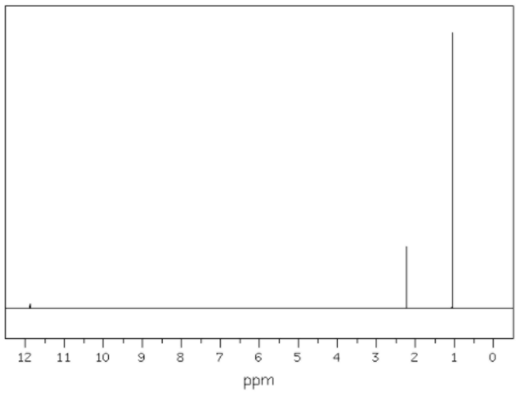
Question 3d

d)

Four isomers of $C_6H_{12}O_2$ are shown below.



Which isomer matches the ^1H NMR spectrum below? Justify your choice.



[2 marks]

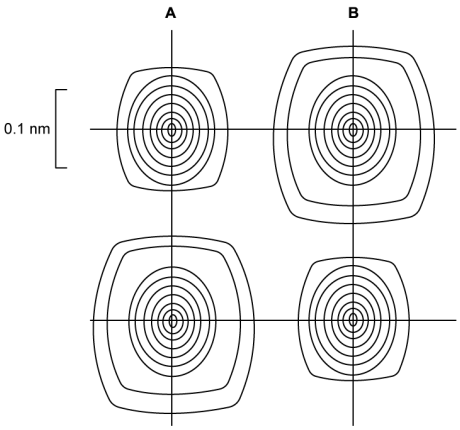
Question 4a

a)
X- ray crystallography is a spectroscopy technique use to determine structural Information. State **two** pieces of information found by this technique.

[1 mark]

Question 4b

b)
X ray crystallography enables chemists to produce electron density maps for substances, such as sodium chloride, shown below.



Estimate the interionic bond length and state which of the two patterns, **A** or **B**, belongs to the chloride ion.

[2 marks]

Question 4c

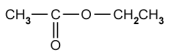
c)
Using Sections 26 & 27 of the Data Booklet and other sources, state three pieces of different spectroscopic evidence that would give structural information to identify benzene.

[3 marks]

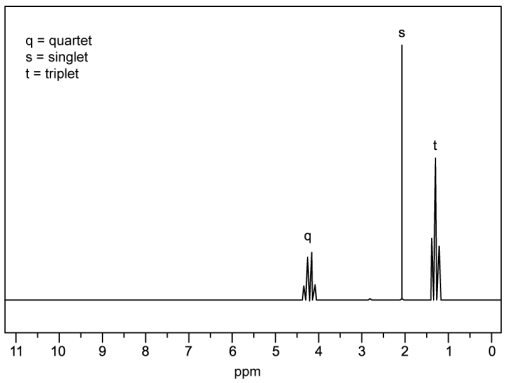
Question 4d

d)

The ester shown below was analysed by high resolution ^{1}H NMR spectroscopy.



The ^{1}H NMR spectrum shown was produced for this ester.



Explain the splitting pattern marked on the spectrum.

[3 marks]

Question 5a

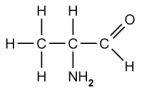
a)
An isomer with the molecular formula $C_5H_{10}O_2$ was analysed by infrared spectroscopy, to confirm it was a carboxylic acid.
i)
Give the wavenumbers of **two** characteristic absorptions for a carboxylic acid. Indicate the bond responsible for each absorption. Suggest why one of the absorptions is broad.

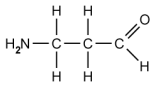
ii)
The ^{1}H NMR spectrum of this isomer contains only two peaks with the integration ratio 9:1. Using this information from the spectra, deduce the structure of the isomer.

[4 marks]

Question 5b

b)
This question is about two aldehydes, 2–aminopropanal and 3–aminopropanal.


2-aminopropanal


3-aminopropanal

Explain how ^{1}H NMR spectra can be used to distinguish between these two aldehydes. You need to reference the splitting patterns and integration pattern in your answer.

[5 marks]

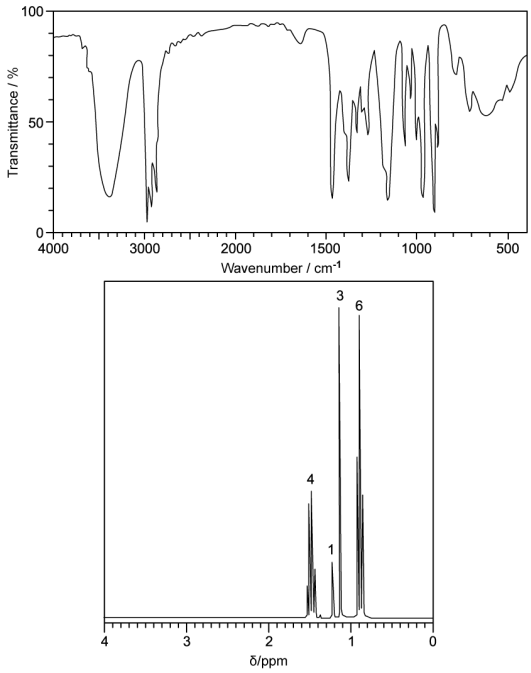
Question 5c

c)
Suggest how the two isomers in part b) could be distinguished using mass spectroscopy.

[1 mark]

Question 5d

d)
A compound **X** has a molecular formula of $C_6H_{14}O$. The infrared spectrum and ^1H NMR spectrum of compound **X** are shown below.



Use Section 26 from the Data Booklet, deduce the structure of compound **X**. Justify each of your deductions.

[7 marks]