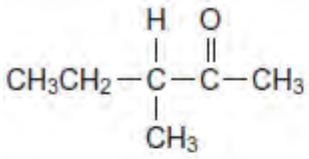
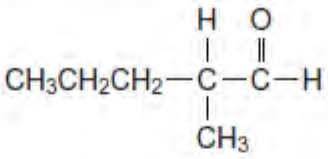
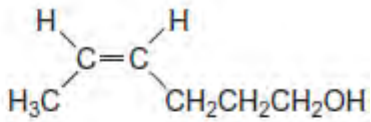
Q1. The following five isomers, **P**, **Q**, **R**, **S** and **T**, were investigated using test-tube reactions and also using n.m.r. spectroscopy.



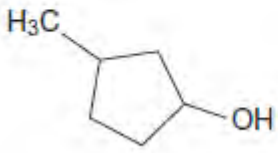
P



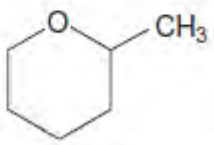
Q



R



S



T

(a) A simple test-tube reaction can be used to distinguish between isomers **P** and **S**.

Identify a reagent (or combination of reagents) you could use.
State what you would observe when both isomers are tested separately with this reagent or combination of reagents.

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(3)

(b) A simple test-tube reaction can be used to distinguish between isomer **Q** and all the other isomers.

Identify a reagent (or combination of reagents) you could use.
State what you would observe when **Q** is tested with this reagent or combination of reagents.

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(2)

(c) State which **one** of the isomers, **P**, **Q**, **R**, **S** and **T**, has the least number of peaks in its ^{1}H n.m.r. spectrum.
Give the number of peaks for this isomer.

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(2)

(d) Write the **molecular** formula of the standard used in ^{13}C n.m.r. spectroscopy.
Give **two** reasons why this compound is used.

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(3)

(e) **Figure 1** and **Figure 2** show the ^{13}C n.m.r. spectra of two of the five isomers.

Figure 1

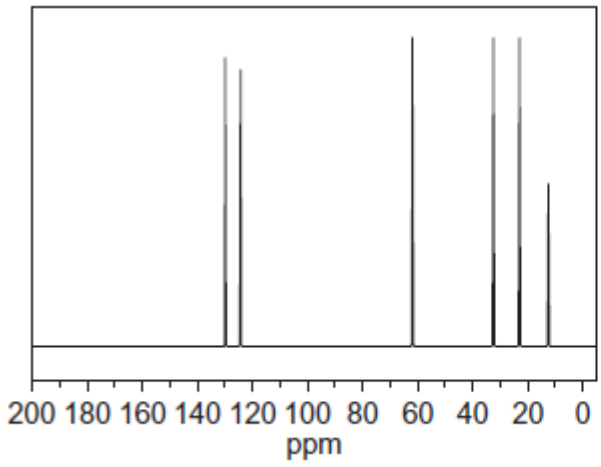
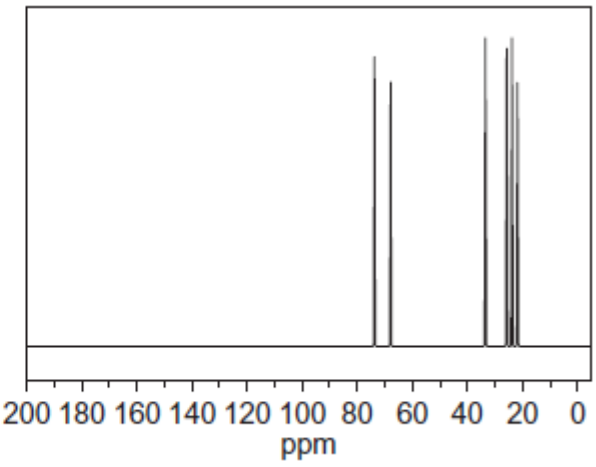
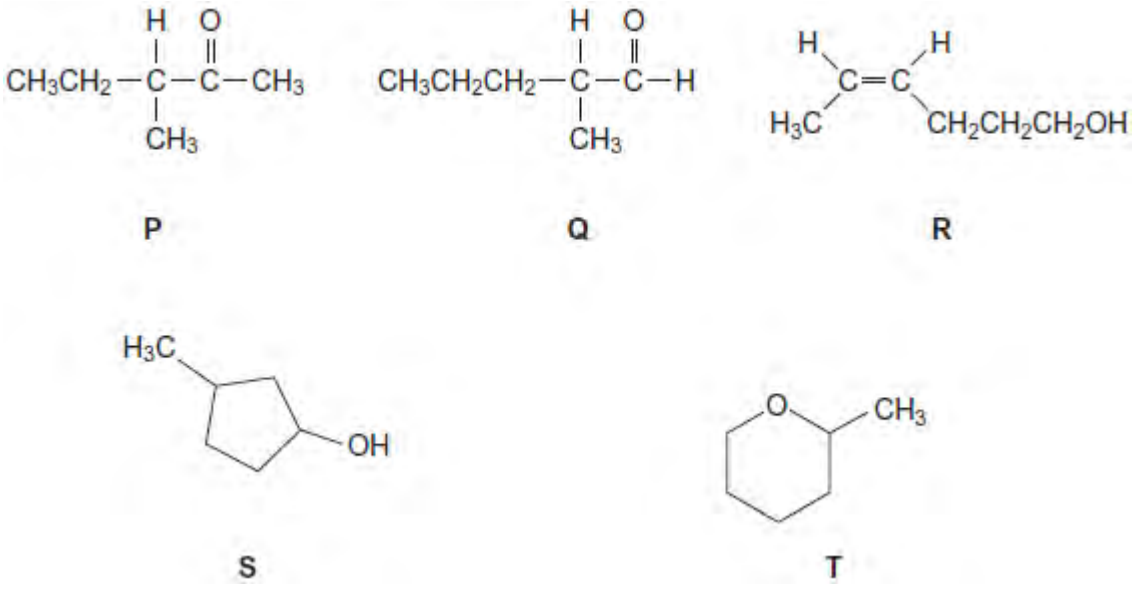


Figure 2



The structures of the five isomers are repeated to help you answer this question.



State which isomer produces the spectrum in **Figure 1** and which isomer produces the spectrum in **Figure 2**.

Explain your answer.

You do not need to identify every peak in each spectrum.
Use **Table C** on the Data Sheet to answer the question.

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(5)

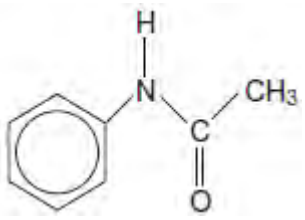
(f) **U** and **V** are other isomers of **P**, **Q**, **R**, **S** and **T**.
The ^{1}H n.m.r. spectrum of **U** consists of two singlets.
V is a cyclic alcohol that exists as optical isomers.

Draw the structure of **U** and the structure of **V**.

U **V**

(2)
(Total 17 marks)

Q2. The structure of N-phenylethanamide is



Use this structure to determine the number of peaks in the ^{13}C n.m.r. spectrum of N−phenylethanamide.

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(Total 1 mark)

Q3. This question concerns isomers of $C_6H_{12}O_2$ and how they can be distinguished using n.m.r. spectroscopy.

(a) The non-toxic, inert substance TMS is used as a standard in recording both ^{1}H and ^{13}C n.m.r. spectra.

(i) Give **two** other reasons why TMS is used as a standard in recording n.m.r. spectra.

Reason 1 .....

.....

Reason 2 .....

.....

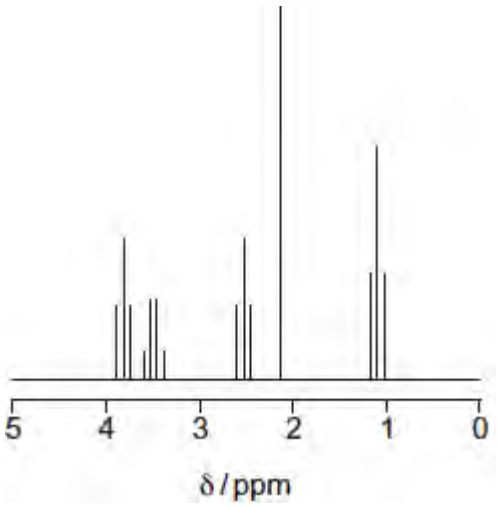
(2)

(ii) Give the structural formula of TMS.

(1)

(b) The proton n.m.r. spectrum of compound **P** ($C_6H_{12}O_2$) is represented in **Figure 1**.

Figure 1



The integration trace gave information about the five peaks as shown in **Figure 2**.

Figure 2

δ / ppm	3.8	3.5	2.6	2.2	1.2
Integration ratio	2	2	2	3	3

(i) Use **Table 2** on the Data Sheet, **Figure 1** and **Figure 2** to deduce the structural fragment that leads to the peak at δ 2.2.

(1)

(ii) Use **Table 2** on the Data Sheet, **Figure 1** and **Figure 2** to deduce the structural fragment that leads to the peaks at δ 3.5 and 1.2.

(1)

(iii) Use **Table 2** on the Data Sheet, **Figure 1** and **Figure 2** to deduce the structural fragment that leads to the peaks at δ 3.8 and 2.6.

(1)

(iv) Deduce the structure of **P**.

(1)

(c) These questions are about different isomers of **P** ($C_6H_{12}O_2$).

(i) Draw the structures of the two esters that both have only two peaks in their proton n.m.r. spectra. These peaks both have an integration ratio of 3:1.

Ester 1

Ester 2

(2)

(ii) Draw the structure of an optically active carboxylic acid with five peaks in its ^{13}C n.m.r. spectrum.

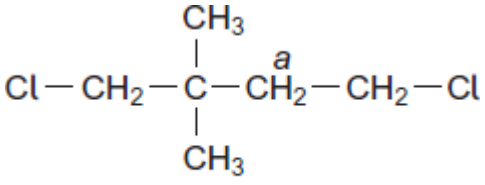
(1)

(iii) Draw the structure of a cyclic compound that has only two peaks in its ^{13}C n.m.r. spectrum and has no absorption for C = O in its infrared spectrum.

(1)
(Total 11 marks)

Q4. N.m.r. spectroscopy can be used to study the structures of organic compounds.

(a) Compound **J** was studied using ^{1}H n.m.r. spectroscopy.



J

(i) Identify a solvent in which **J** can be dissolved before obtaining its ^{1}H n.m.r. spectrum.

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(1)

(ii) Give the number of peaks in the ^{1}H n.m.r. spectrum of **J**.

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(1)

(iii) Give the splitting pattern of the protons labelled *a*.

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(1)

(iv) Give the IUPAC name of **J**.

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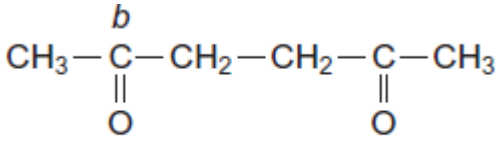
(1)

(b) Compound **K** was studied using ^{13}C n.m.r. spectroscopy.



K

(i) Give the number of peaks in the ^{13}C n.m.r. spectrum of **K**.

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(1)

(ii) Use **Table 3** on the Data Sheet to suggest a δ value of the peak for the carbon labelled *b*.

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(1)

(iii) Give the IUPAC name of **K**.

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(1)

(Total 7 marks)

Q5. The infrared spectrum (**Figure 1**) and the ^{1}H NMR spectrum (**Figure 2**) of compound **R** with molecular formula $C_6H_{14}O$ are shown.

Figure 1

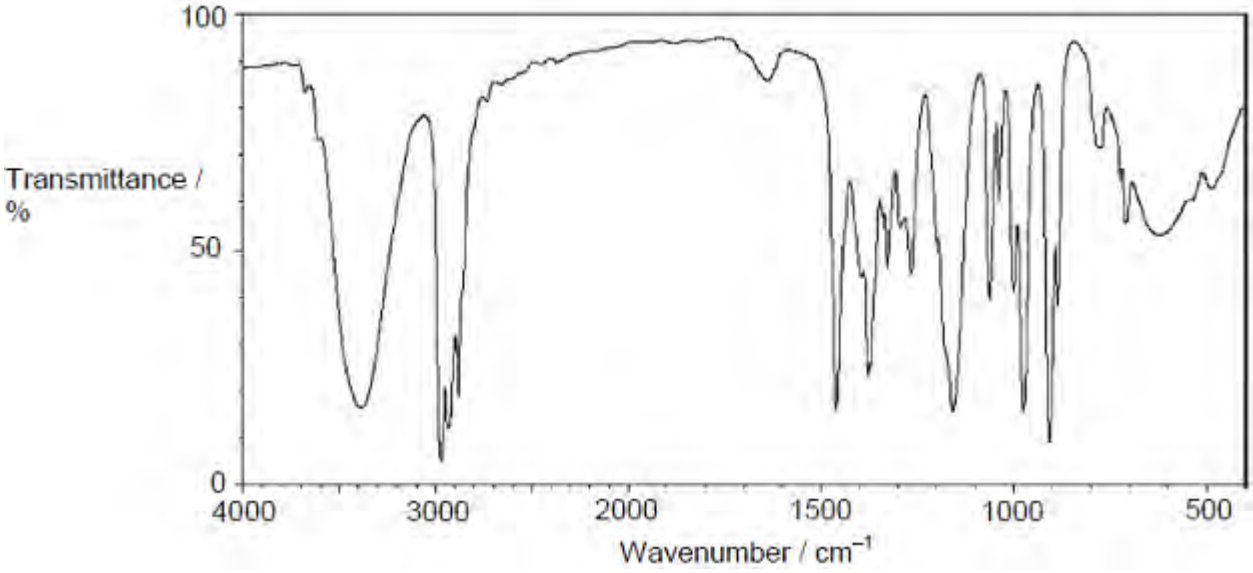
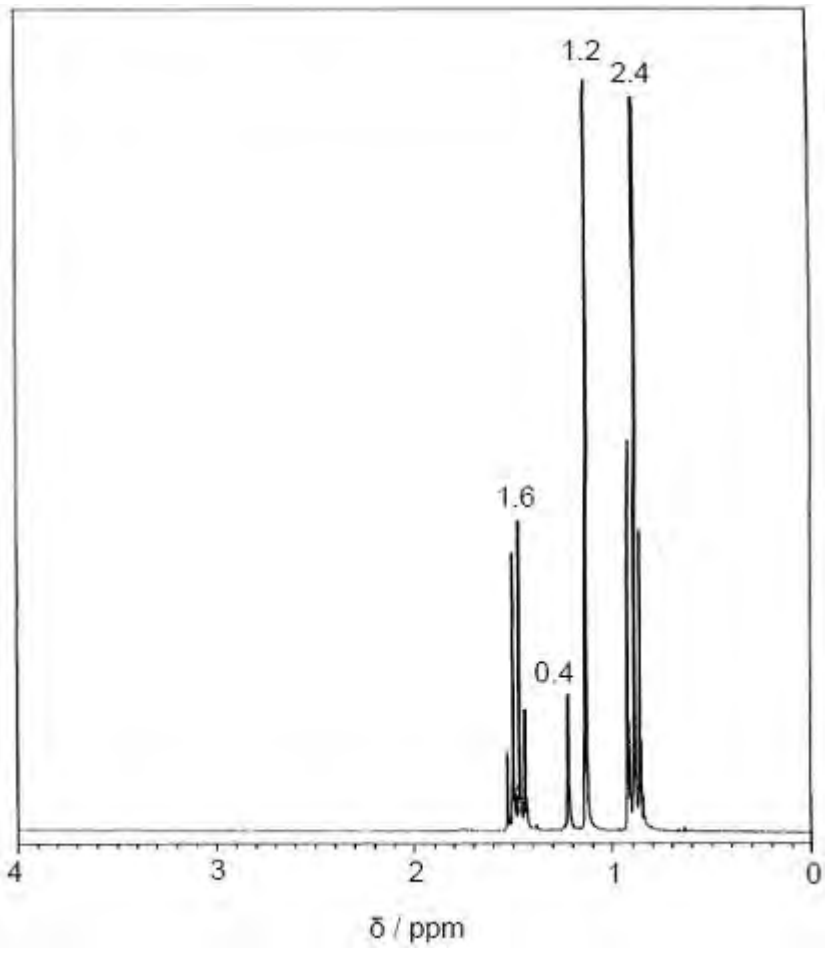


Figure 2



The relative integration values for the NMR peaks are shown on **Figure 2**.

Deduce the structure of compound **R** by analysing **Figure 1** and **Figure 2**.
Explain each stage in your deductions.

Use **Table A** and **Table B** on the Data Sheet.

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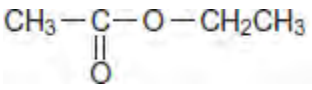
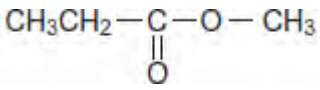
(Total 8 marks)

Q6.(a) **Ester 1** and **Ester 2** were studied by ^{1}H n.m.r. spectroscopy.

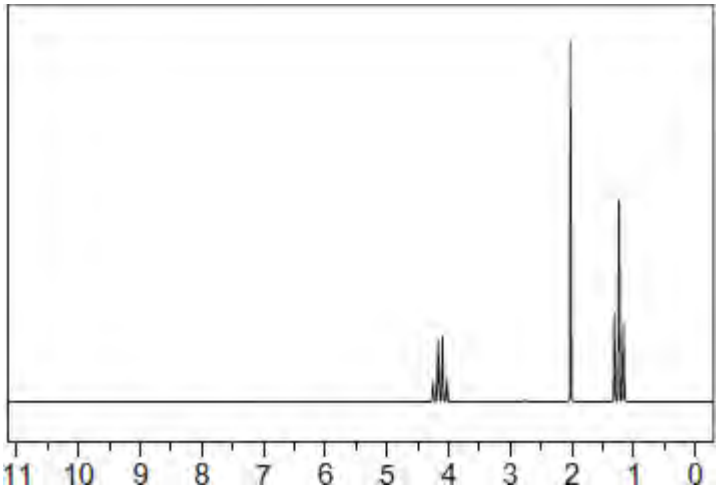


Ester 1



Ester 2

One of the two esters produced this spectrum.



Deduce which of the two esters produced the spectrum shown. In your answer, explain the position and splitting of the quartet peak at δ = 4.1 ppm in the spectrum.

Predict the δ value of the quartet peak in the spectrum of the other ester.

Use **Table B** on the Data Sheet.

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(4)

(b) Cetrimide is used as an antiseptic.

$[CH_3(CH_2)_{15}N(CH_3)_3]^+ Br^-$

cetrimide

Name this type of compound.

Give the reagent that must be added to $CH_3(CH_2)15NH_2$ to make cetrimide and state the reaction conditions.

Name the type of mechanism involved in this reaction.

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(4)

(c) Give a reagent that could be used in a test-tube reaction to distinguish between benzene and cyclohexene.
Describe what you would see when the reagent is added to each compound and the test tube is shaken.

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(3)
(Total 11 marks)

Q7. Which amine has only **three** peaks in its proton NMR spectrum?

A Methylamine ⬭

B Trimethylamine ⬭

C Diethylamine ⬭

D Propylamine ⬭

(Total 1 mark)