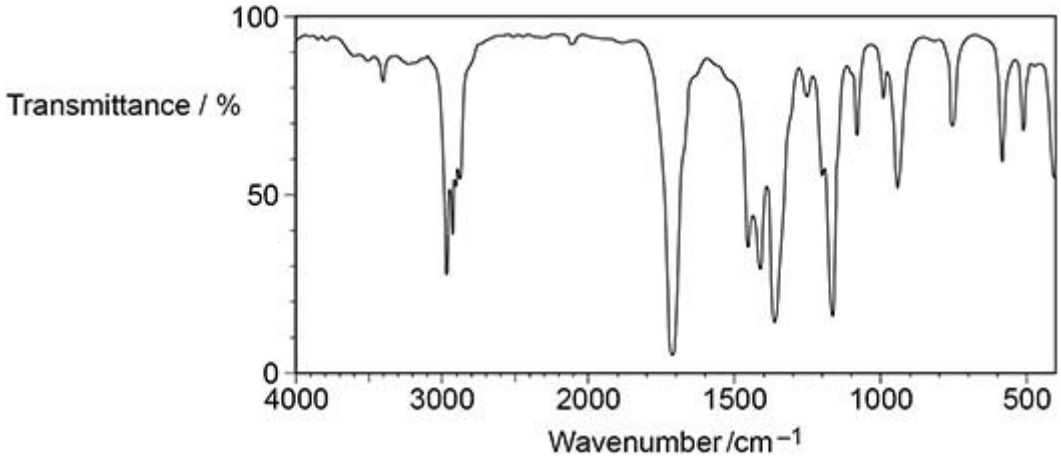
Q1.

This question is about spectroscopy.

(a) Compound **K** has molecular formula C_4H_8O
Figure 1 shows the infrared spectrum of **K**.

Figure 1



Which functional group does **K** contain?

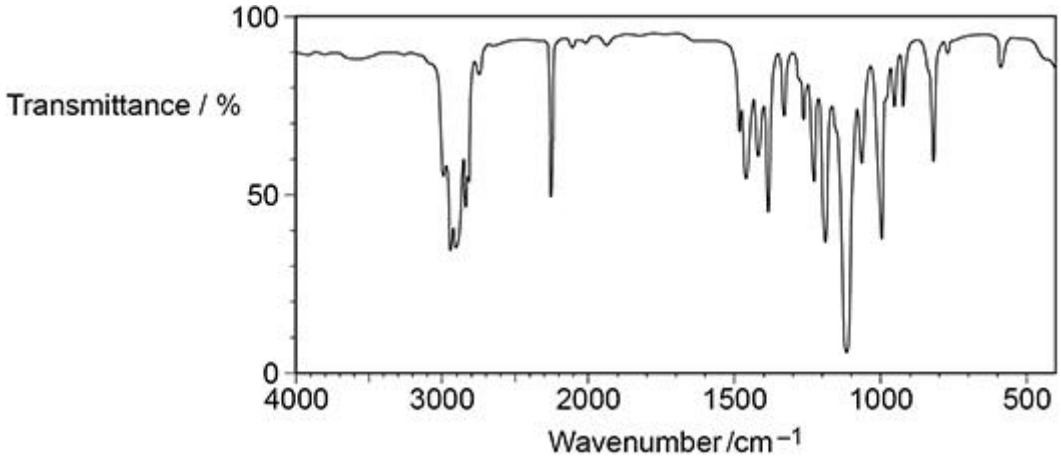
Tick (✓) **one** box.

Functional Group				
alcohol	alkene	amine	carbonyl	nitrile

(1)

(b) Compound **L** has molecular formula C_4H_7NO
Figure 2 shows the infrared spectrum of **L**.

Figure 2



L reacts with H_2 in the presence of a nickel catalyst to give compound **M**.

Suggest **three** ways in which the infrared spectrum of **M** is different from the infrared spectrum of **L**.

1 _____

_____

2 _____

_____

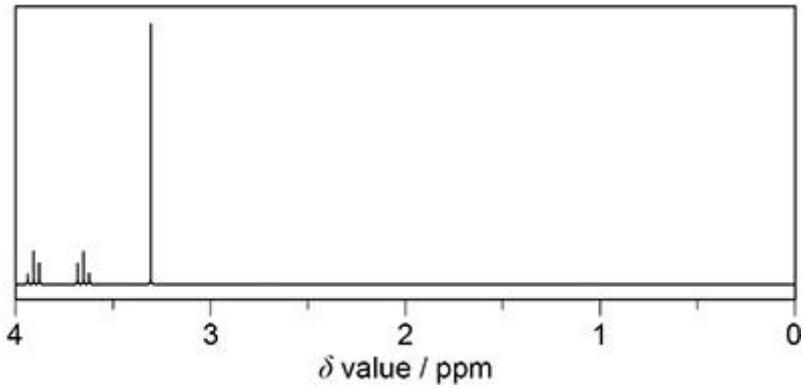
3 _____

_____

(3)

(c) **Figure 3** shows the ^1H NMR spectrum of **Q**, C_3H_7ClO

Figure 3



The table below shows the chemical shifts (δ values) and integration values for each peak.

δ value / ppm	3.95	3.65	3.35
Integration value	0.6	0.6	0.9

Deduce the structure of **Q**.

Explain your answer.

_____

_____

_____

_____

_____

(5)

(Total 9 marks)

Q2.

This question is about NMR spectroscopy.

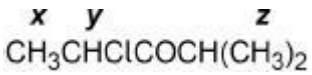
(a) A compound is usually mixed with $Si(CH_3)_4$ and either CCl_4 or $CDCl_3$ before recording the compound's ^1H NMR spectrum.

State why $Si(CH_3)_4$, CCl_4 and $CDCl_3$ are used in ^1H NMR spectroscopy.

Explain how their properties make them suitable for use in ^1H NMR spectroscopy.

(6)

(b) Deduce the splitting pattern for each of the peaks given by the H atoms labelled ***x***, ***y*** and ***z*** in the ^{1}H NMR spectrum of the compound shown.



x _____

y _____

z _____

(3)

(c) Suggest why it is difficult to use **Table B** in the Data Booklet to predict the chemical shift (δ value) for the peak given by the H atom labelled ***y***.

_____

_____

_____

_____

(1)

(d) Two isomers of $CH_3CHClCOCH(CH_3)_2$ each have two singlet peaks only in their ^{1}H NMR spectra.
In both spectra the integration ratio for the two peaks is 2:9

Deduce the structures of these two isomers.

Isomer 1

Isomer 2

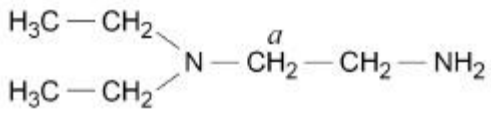
(2)

(Total 12 marks)

Q3.

There are several isomers with the molecular formula $C_6H_{16}N_2$

(a) One isomer is shown.



Give the number of peaks in the ^{13}C NMR spectrum of this isomer.

State and explain the splitting pattern of the peak for the hydrogens labelled *a* in its ^{1}H NMR spectrum.

Number of ^{13}C peaks

_____

Splitting pattern

_____

Explanation

_____

_____

_____

_____

(3)

(b) Draw the structure of the isomer of $C_6H_{16}N_2$ used to make nylon 6,6

(1)

(c) Draw the structure of the isomer of $C_6H_{16}N_2$ that contains two **primary** amine groups and has only two peaks in its ^{13}C NMR spectrum.

(1)

(d) Draw the structure of the isomer of $C_6H_{16}N_2$ that contains two **tertiary** amine groups and has only two peaks in its ^{13}C NMR spectrum.

(1)

(Total 6 marks)

Q4.

How many peaks are there in the ^{13}C NMR spectrum of 1,4-dimethylbenzene?

A 8 ⬭

B 4 ⬭

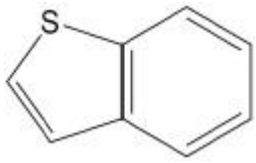
C 3 ⬭

D 2 ⬭

(Total 1 mark)

Q5.

How many peaks does this compound have in its ^{13}C spectrum?



A 5 ⬭

B 6 ⬭

C 7 ⬭

D 8 ⬭

(Total 1 mark)

Q6.

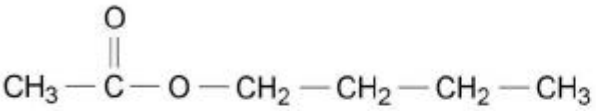
^{1}H NMR, ^{13}C NMR and infrared spectroscopy are used in organic chemistry to distinguish between compounds and to identify them.

(a) Give the skeletal formula of the compound that is used as the standard when recording a ^{13}C NMR spectrum.

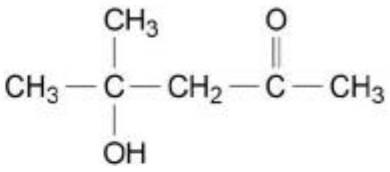
(1)

(b) Four isomers of $C_6H_{12}O_2$, **P**, **Q**, **R** and **S**, shown in **Figure 1**, were analysed by
^{13}C NMR spectrometry.

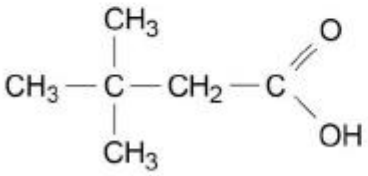
Figure 1



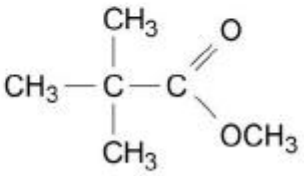
P



Q



R



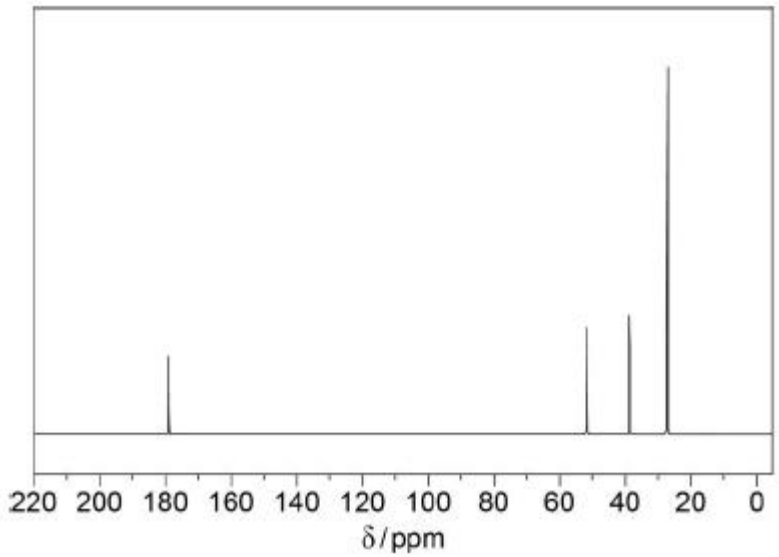
S

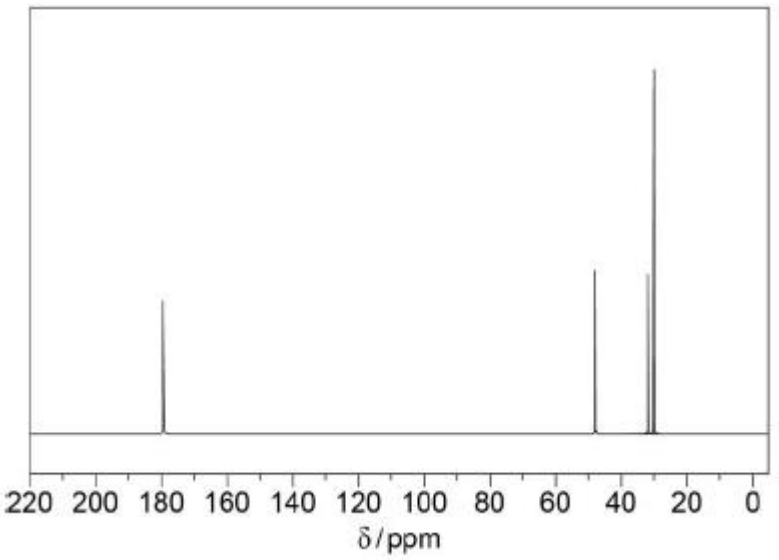
The ^{13}C NMR spectra of three of these isomers are shown in **Figure 2**.

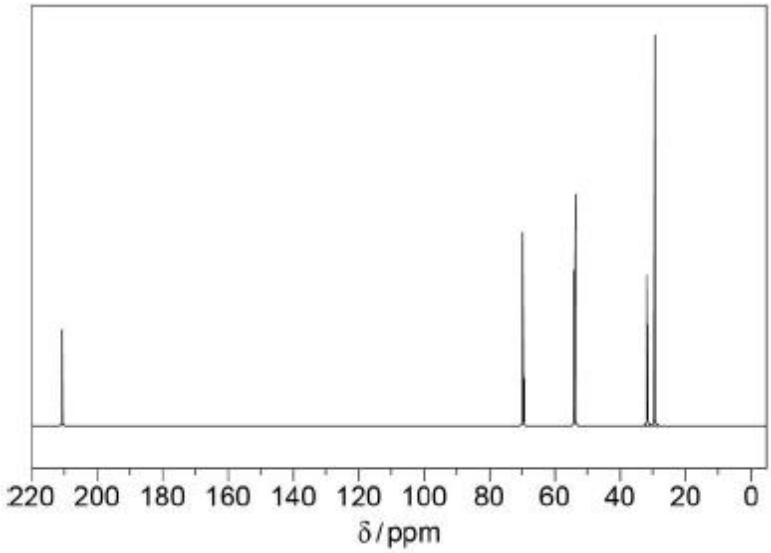
Use **Table C** in the Data Booklet to help you to identify which isomer produces each spectrum.

Write the letter of each isomer opposite its spectrum in **Figure 2**.

Figure 2



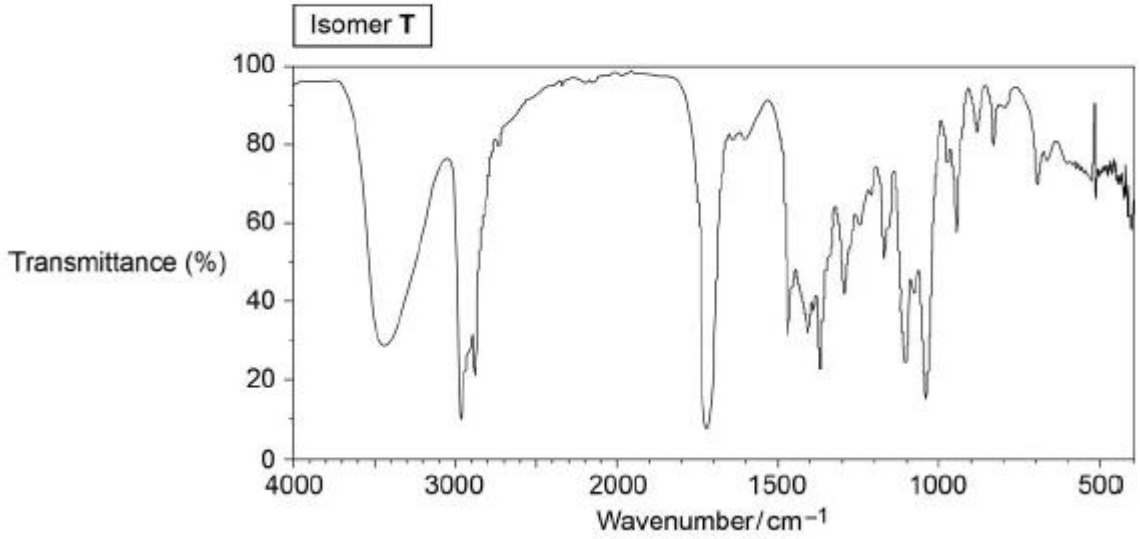


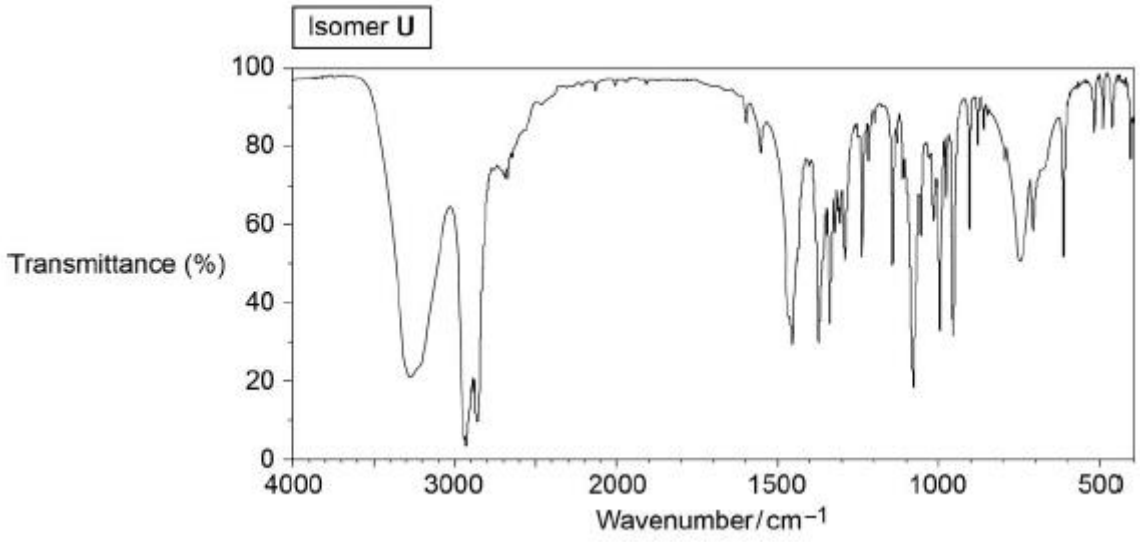


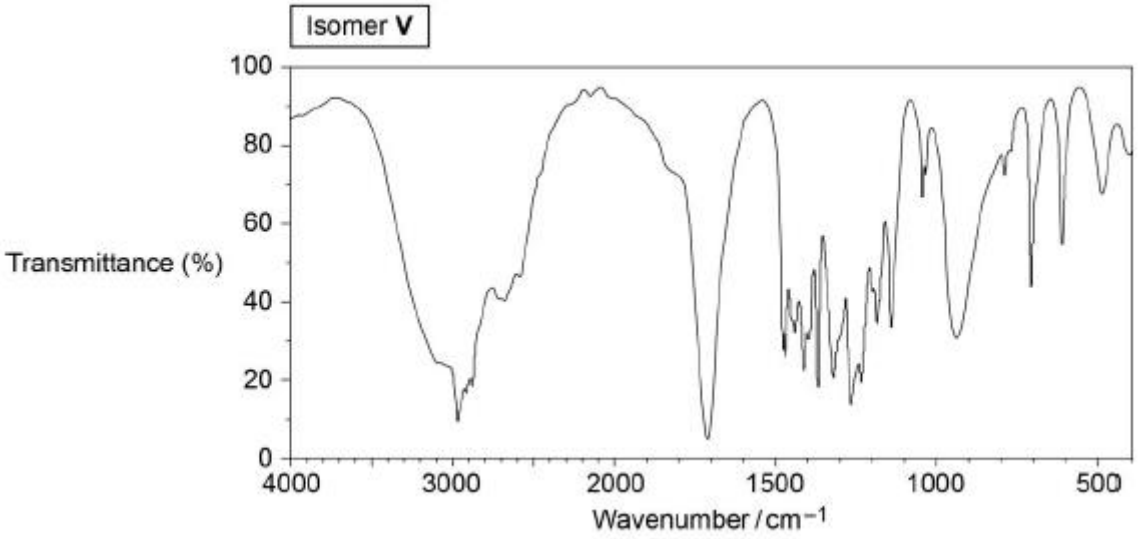
(3)

(c) The infrared spectra shown in **Figure 3** are those of three different isomers of $C_6H_{12}O_2$, isomers **T**, **U** and **V**.

Figure 3







Identify the functional group(s) present in each isomer **T**, **U** and **V** of $C_6H_{12}O_2$ using **Table A** in the Data Booklet.

Explain your answer.

(6)

(d) The integration values for the peaks in the ^{1}H NMR spectrum of **X**, a different isomer of $C_6H_{12}O_2$, are given in the table below.

Chemical shift, δ/ppm	3.7	3.5	2.6	2.2	1.1
Integration value	0.6	0.6	0.6	0.9	0.9
Splitting pattern	triplet	quartet	triplet	singlet	triplet

Deduce the simplest ratio of the relative numbers of protons in each environment in compound **X**.

(1)

(e) Use the data in the table above and **Table B** in the Data Booklet to help you answer this question.

Deduce the part of the structure of **X** that causes the signal at δ= 3.5 and the part of the structure at **X** that causes the signal at δ=2.2.

Explain the splitting patterns of these peaks.

Signal at δ= 3.5

Signal at δ= 2.2

(4)

(f) Deduce the structure of compound **X**, $C_6H_{12}O_2$

Use your answer from part **(e)** to help you.

You are **not** required to explain how you deduced the structure.

_____

_____

_____

_____

(2)

(Total 17 marks)

Q7.

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

A Methylamine ⬭

B Trimethylamine ⬭

C Diethylamine ⬭

D Propylamine ⬭