# A-Level Chemistry

## Hydrogen NMR

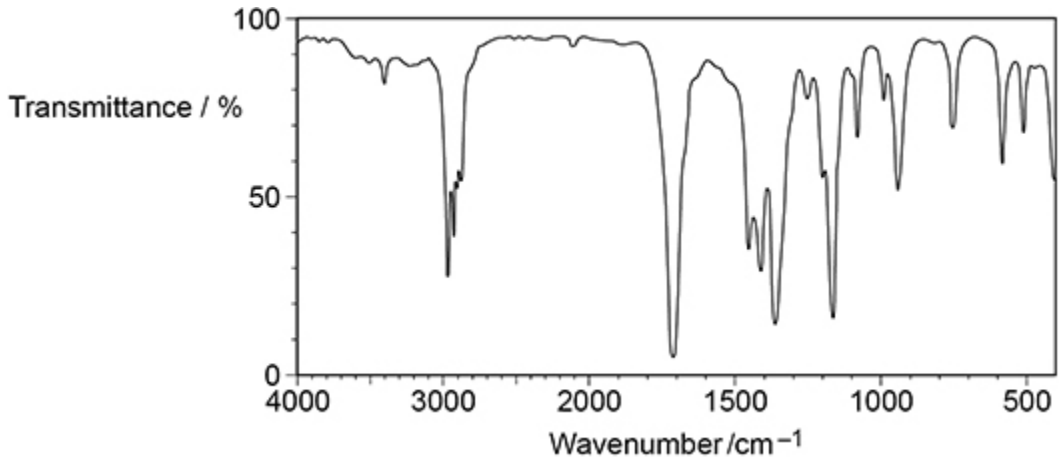
### Question Paper

**Time available: 62 minutes**
**Marks available: 59 marks**

**1.** 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?

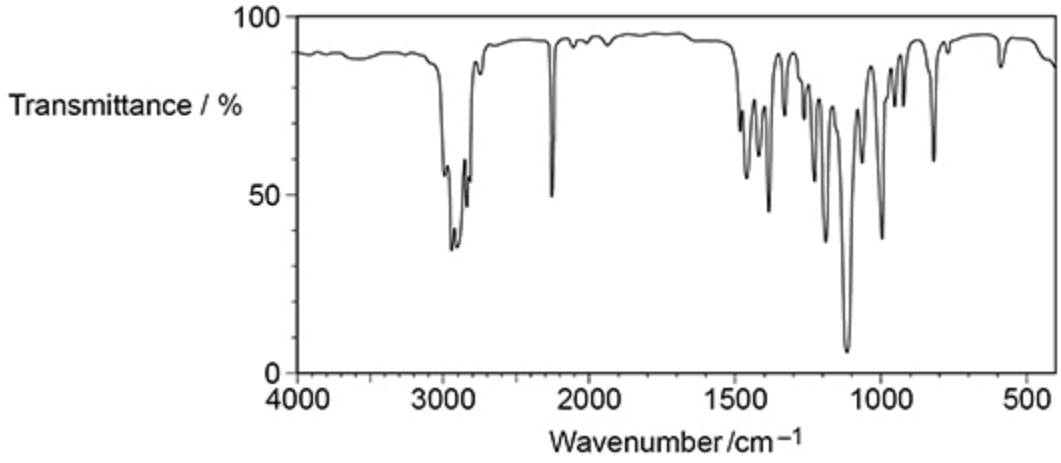
Tick (✓) **one** box.

| 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 _____

_____

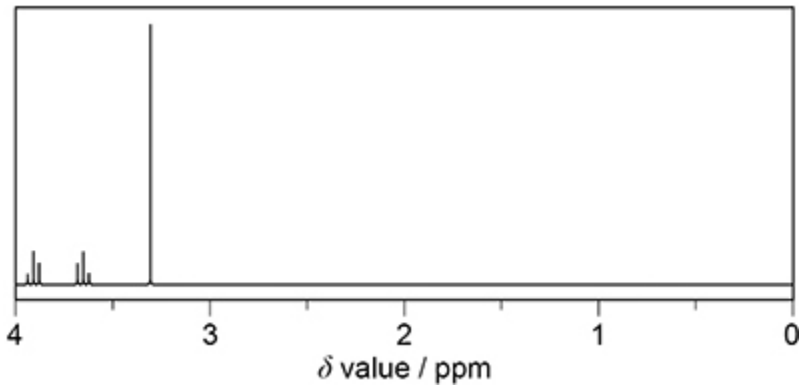
3 _____

_____

**(3)**

(c) **Figure 3** shows the $^{1}H$ 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)**

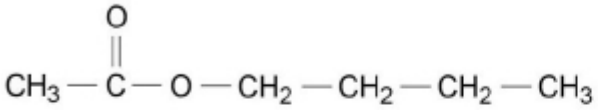
**2.** $^{1}H$ NMR, $^{13}C$ NMR and infrared spectroscopy are used in organic chemistry to distinguish between compounds and to identify them.

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

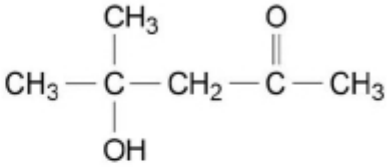
**(1)**

(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.

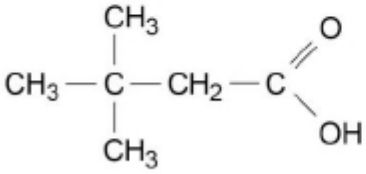
**Figure 1**



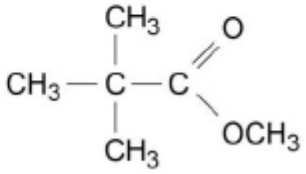
**P**



**Q**



**R**



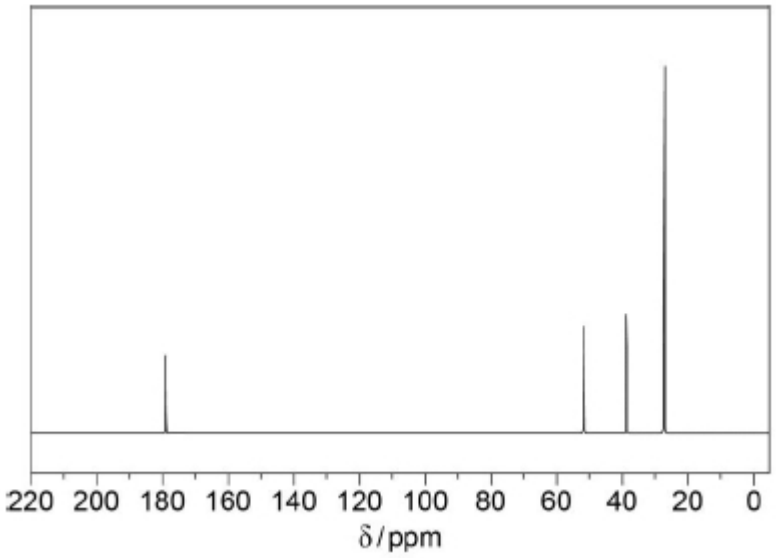
**S**

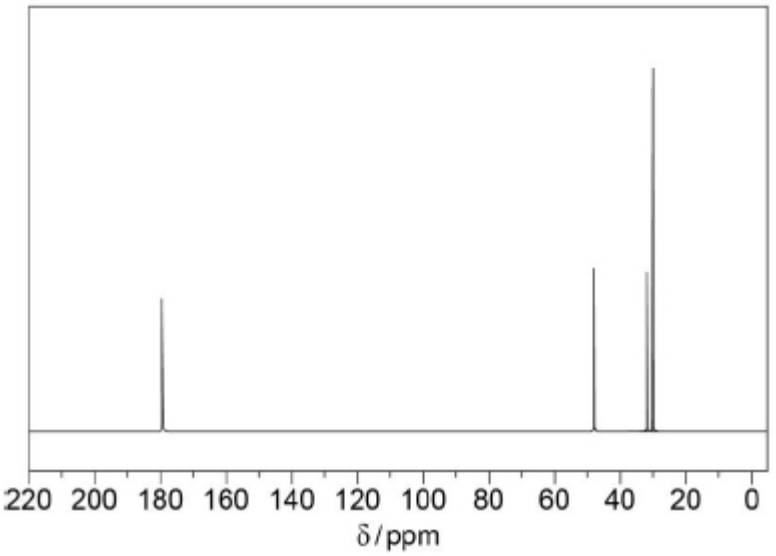
The $^{13}C$ NMR spectra of three of these isomers are shown in **Figure 2**.

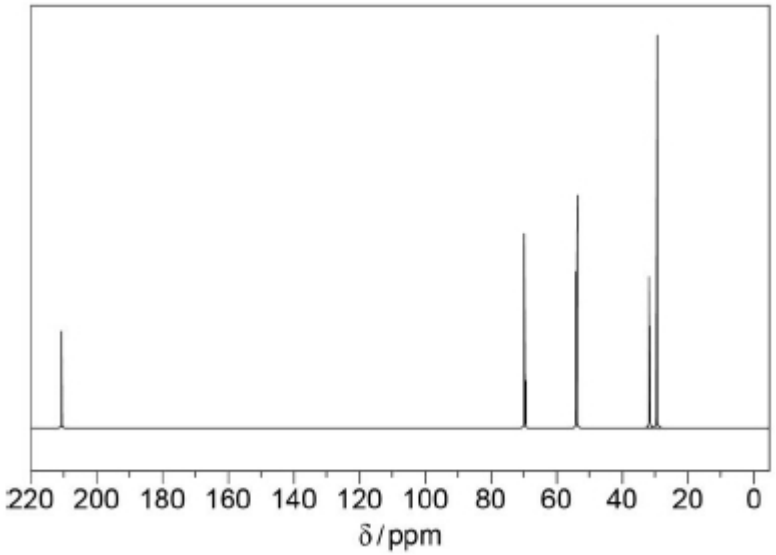
Use **Table C** in the Data Booklet to help you to identify which isomer produces each spectrum.

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

**Figure 2**


220 200 180 160 140 120 100 80 60 40 20 0
δ / ppm

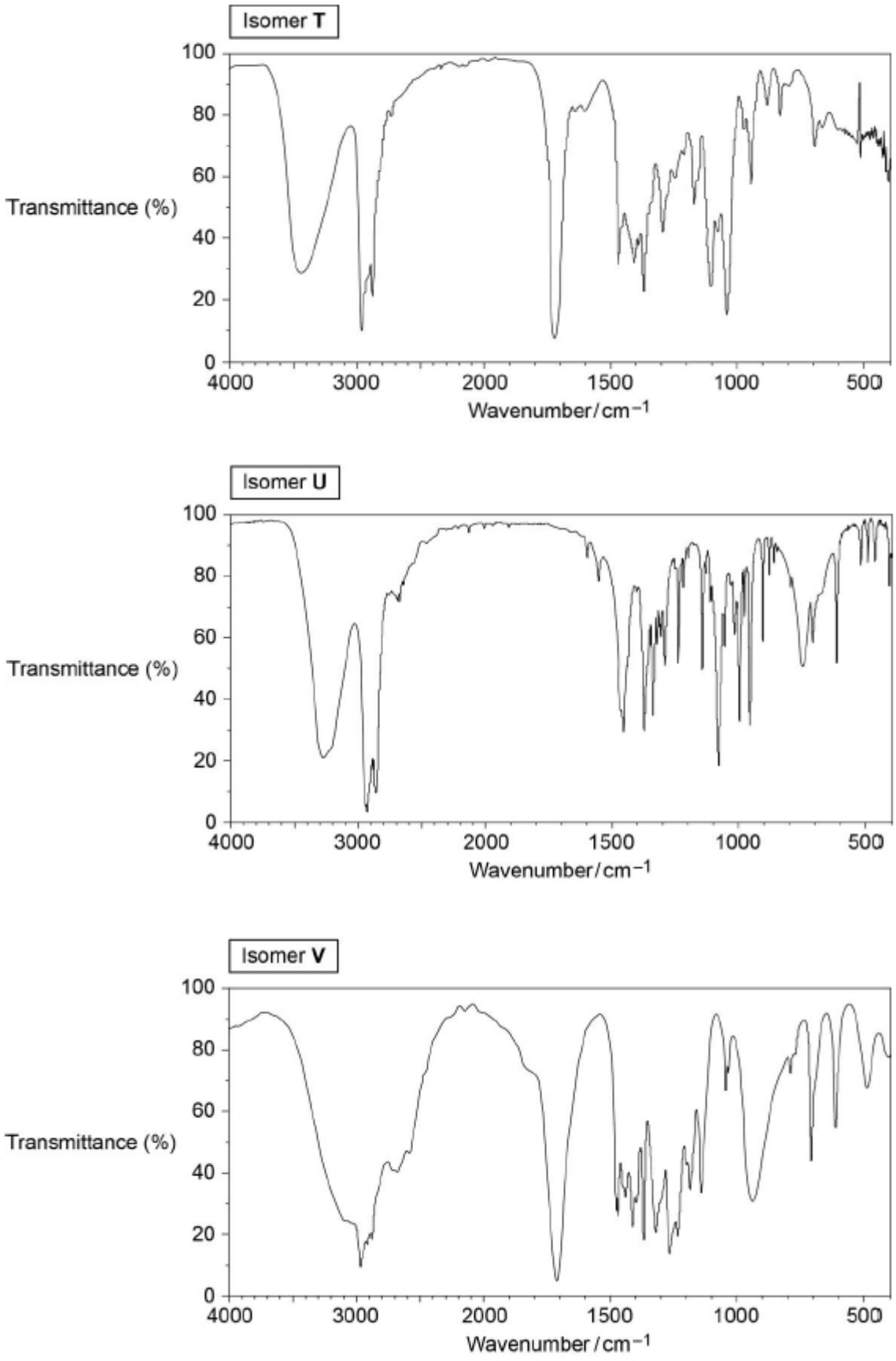

220 200 180 160 140 120 100 80 60 40 20 0
δ / ppm




**(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 $^1H$ 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.

_____

_____

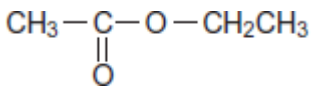
_____

_____

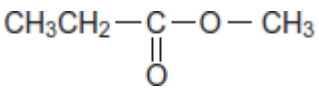
**(2)**

**(Total 17 marks)**

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

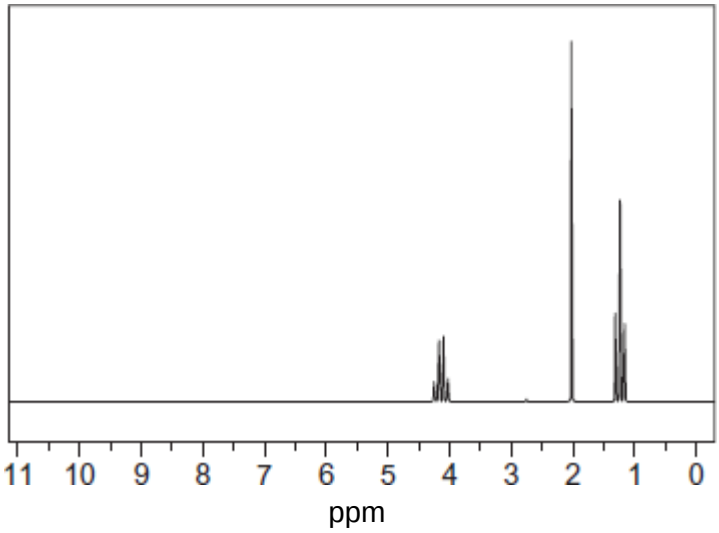


**Ester 1**



**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.

**(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.

**(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.

**(3)**

**(Total 11 marks)**

**4.** When the molecular formula of a compound is known, spectroscopic and other analytical techniques can be used to distinguish between possible structural isomers.

Draw **one** possible structure for each of the compounds described in parts (a) to (d).

(a) Compounds **F** and **G** have the molecular formula $C_6H_4N_2O_4$ and both are dinitrobenzenes.
**F** has two peaks in its $^{13}C$ n.m.r. spectrum.
**G** has three peaks in its $^{13}C$ n.m.r. spectrum.

**F** **G**

**(2)**

(b) Compounds **H** and **J** have the molecular formula $C_6H_{12}$.
Both have only one peak in their $^{1}H$ n.m.r. spectra.
**H** reacts with aqueous bromine but **J** does not.

**H** **J**

**(2)**

(c) **K** and **L** are cyclic compounds with the molecular formula $C_6H_{10}O$.
Both have four peaks in their $^{13}C$ n.m.r. spectra.
**K** is a ketone and **L** is an aldehyde.

**K** **L**

**(2)**

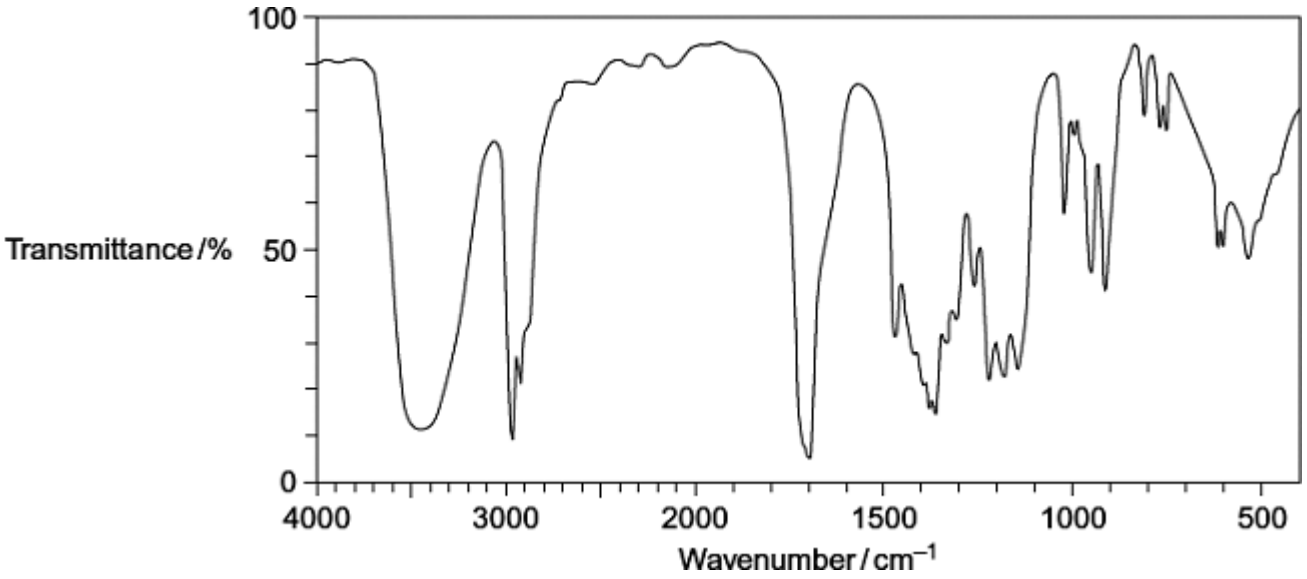
(d) Compounds **M** and **N** have the molecular formula $C_6H_{15}N$.
**M** is a tertiary amine with only two peaks in its $^{1}H$ n.m.r. spectrum.
**N** is a secondary amine with only three peaks in its $^{1}H$ n.m.r. spectrum.

**M** **N**

**(2)**
**(Total 8 marks)**

**5.** Compound **X** ($C_6H_{12}O_2$) was analysed by infrared spectroscopy and by proton nuclear magnetic resonance spectroscopy.

(a) The infrared spectrum of **X** is shown below.
Use **Table 1** on the Data Sheet to help you answer the question.




Identify the functional group that causes the absorption at 3450cm$^{-1}$ in the spectrum.

_____

**(1)**

(b) The proton n.m.r. spectrum of **X** consists of 4 singlet peaks.

The table below gives the chemical shift for each of these peaks, together with their integration values.

| δ /ppm | 1.2 | 2.2 | 2.6 | 3.8 |
|---|---|---|---|---|
| Integration value | 6 | 3 | 2 | 1 |

Use **Table 2** on the Data Sheet to help you answer the following questions.

Use the chemical shift and the integration data to show what can be deduced about the structure of **X** from the presence of the following in its proton n.m.r. spectrum.

(i) The peak at δ = 2.6

_____

**(1)**

(ii) The peak at δ = 2.2

_____

**(1)**

(iii) The peak at δ = 1.2

_____

**(1)**

(iv) Deduce the structure of **X** ($C_6H_{12}O_2$)

**(1)**

**(Total 5 marks)**

**6.** This question concerns four isomers, **W**, **X**, **Y** and **Z**, with the molecular formula $C_5H_{10}O_2$

(a) The proton n.m.r. spectrum of **W** shows 4 peaks.
The table below gives the chemical shifts, δ values, for each of these peaks, together with their splitting patterns and integration values.

| δ/ppm | 2.18 | 2.59 | 3.33 | 3.64 |
|---|---|---|---|---|
| Splitting pattern | singlet | triplet | singlet | triplet |
| Integration value | 3 | 2 | 3 | 2 |

State what can be deduced about the structure of **W** from the presence of the following in its n.m.r. spectrum.

(i) The singlet peak at δ = 2.18

_____

(ii) The singlet peak at δ = 3.33

_____

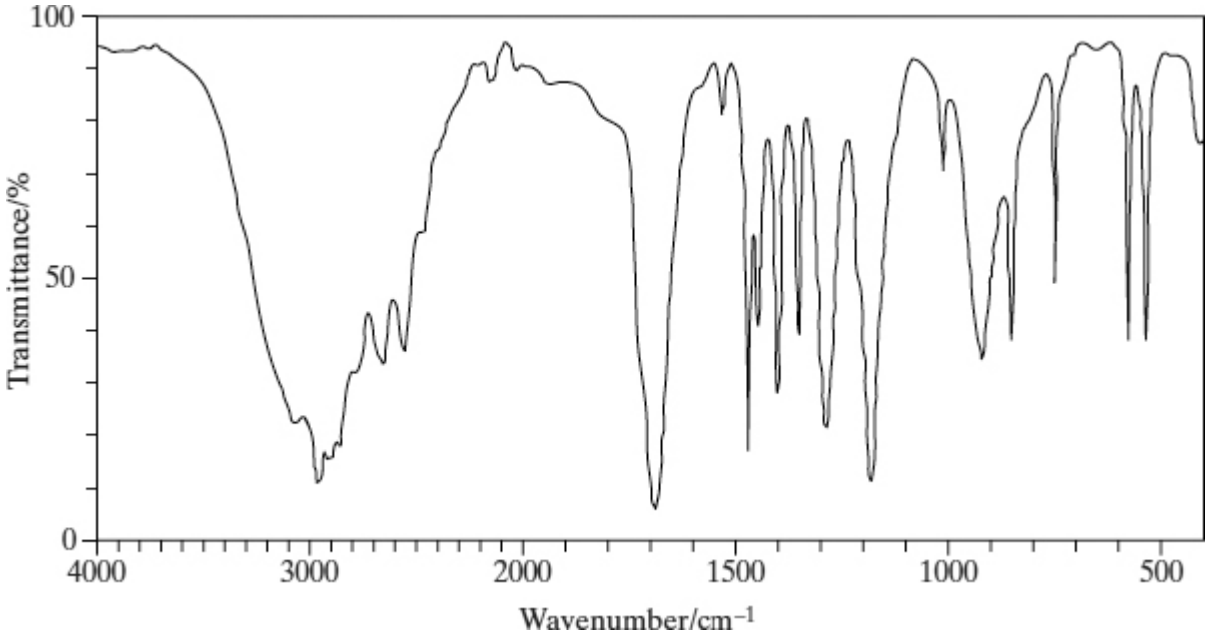
(iii) Two triplet peaks.

_____

(iv) Hence, deduce the structure of **W**.

**(4)**

(b) The infra-red spectrum of **X** is shown below.



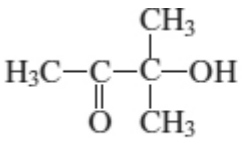

(i) What can be deduced from the broad absorption centred on 3000 $cm^{-1}$ in the infra-red spectrum of **X**?

_____

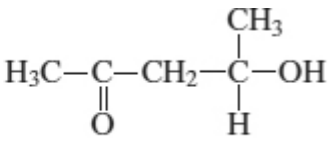
(ii) Given that the proton n.m.r. spectrum of **X** contains only two peaks with the integration ratio 9:1, deduce the structure of **X**.

**(2)**

(c) Isomers **Y** and **Z** have the structures shown below.



**Y**



**Z**

Identify the two reagents you could use in a simple chemical test to distinguish between **Y** and **Z**. State what you would observe when each of **Y** and **Z** is tested with a mixture of these two reagents.

*Reagents* _____

*Observation with **Y*** _____

*Observation with **Z*** _____

**(3)**

**(Total 9 marks)**