# "*Across the spectrum*"

**Y13 UNIT 4 TEST 7**

**4.10 ORGANIC SYNTHESIS AND ANALYSIS**
**4.11 STRUCTURE DETERMINATION**

**Answer all questions**

# GOOD LUCK!

Answer all questions
Total 54 marks

**Name:……**

**Mark for Section A……./39**

**Mark for section B……. /15**

**Total: …… /54**

**Grade……..**

## SECTION A

**1.** 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

.....

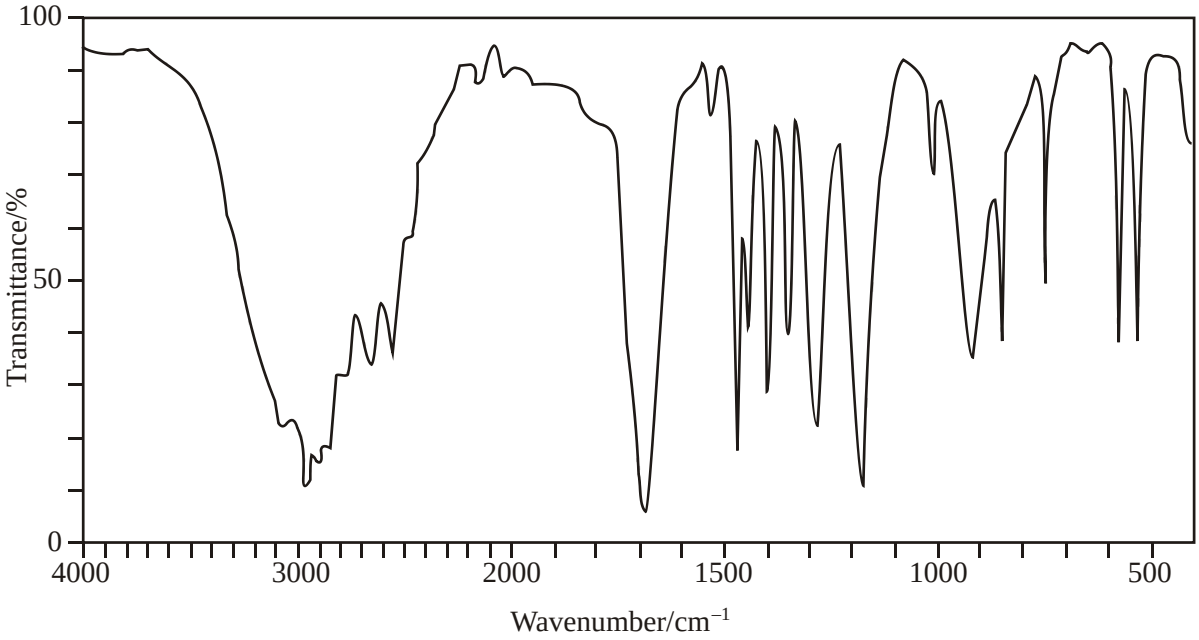
(iii) Two triplet peaks.

.....

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

**(4)**

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



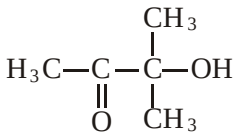

(i) What can be deduced from the broad absorption centred on 3000 cm$^{-1}$ in the infra-red spectrum of **X**?

.....

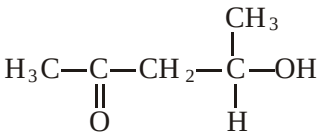
(ii) Given that the proton n.m.r. spectrum of **X** contains only two peaks with the integration ratio 9:1, deduce the structure of **X**.

**(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* .....

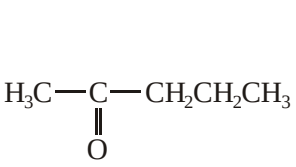
*Observation with **Y*** .....

*Observation with **Z*** .....

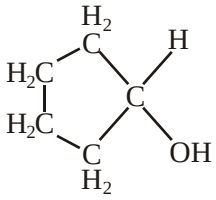
**(3)**

**(Total 9 marks)**

**2.** Compounds **C** and **D**, shown below, are isomers of $C_5H_{10}O$



C



D

(a) Name compound **C**.

.....

**(1)**

(b) Use **Table 2** on the Data Sheet to help you to answer this question.

(i) Suggest the wavenumber of an absorption which is present in the infra-red spectrum of **C** but not in that of **D**.

.....

(ii) Suggest the wavenumber of an absorption which is present in the infra-red spectrum of **D** but not in that of **C**.

.....

**(2)**

(c) Deduce the number of peaks in the proton n.m.r. spectrum of **C**.

.....

**(1)**

(d) Identify a reagent that you could use to distinguish between **C** and **D**. For each of **C** and **D**, state what you would observe when the compound is treated with this reagent.

*Reagent* ……..……..

*Observation with* **C** ……..

*Observation with* **D** ……..

**(3)**

(e) Compound **E**, $CH_3CH_2CH_2CH_2CHO$, is also an isomer of $C_5H_{10}O$

Identify a reagent which will react with **E** but not with **C** or **D**. State what you would observe when **E** is treated with this reagent.

*Reagent* ……..……..

*Observation with* **E** ……..

**(2)**

**(Total 9 marks)**

**3.** Each of the parts (a) to (e) below concerns a different pair of isomers.

Draw one possible structure for each of the species **A** to **J**, using Table 2 on the Data Sheet where appropriate.

(a) Compounds **A** and **B** have the molecular formula $C_5H_{10}$
**A** decolourises bromine water but **B** does not.

**A** **B**

**(2)**

(b) Compounds **C** and **D** have the molecular formula $C_2H_4O_2$

Each has an absorption in its infra-red spectrum at about 1700 $cm^{-1}$ but only **D** has a broad absorption at 3350 $cm^{-1}$

**C** **D**

**(2)**

(c) Compounds **E** and **F** are esters with the molecular formula $C_5H_{10}O_2$

The proton n.m.r. spectrum of **E** consists of two singlets only whereas that of **F** consists of two quartets and two triplets.

**E** **F**

**(2)**

(d) Compounds **G** and **H** have the molecular formula $C_3H_6Cl_2$
**G** shows optical activity but **H** does not.

**G** **H**

**(2)**

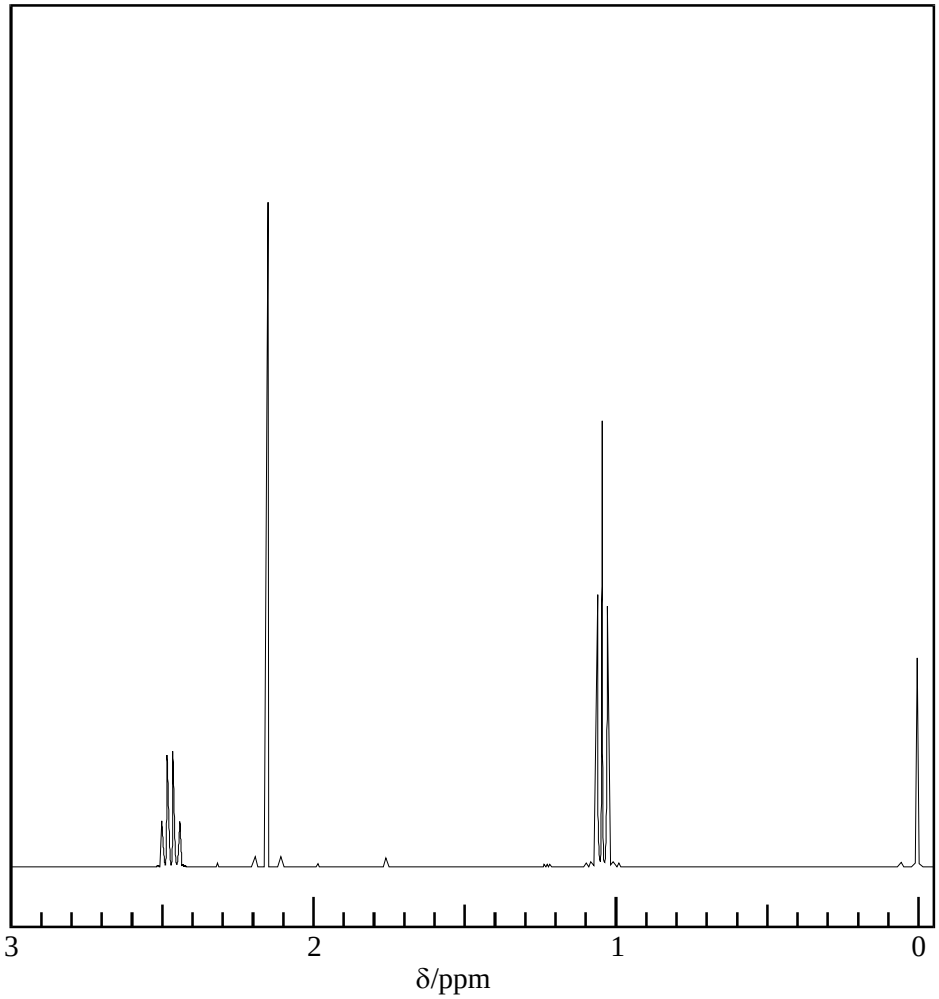
(e) Compounds **I** and **J** have the molecular formula $C_6H_{12}$

Each has an absorption in its infra-red spectrum at about 1650 $cm^{-1}$ and neither shows geometrical isomerism. The proton n.m.r. spectrum of **I** consists of a singlet only whereas that of **J** consists of a singlet, a triplet and a quartet.

**I** **J**

**(2)**
**(Total 10 marks)**

**4.** The proton n.m.r. spectrum of an organic compound **F,** $C_4H_8O$, is shown below.




The measured integration trace gives the ratio 0.5 to 0.75 to 0.75 for the peaks at δ 2.47, 2.15 and 1.05, respectively. The infra-red spectrum of compound **F** has an intense band at 1715 $cm^{-1}$. In the mass spectrum of **F,** dominant fragmentation peaks appear at $m/z$ = 43 and $m/z$ = 57.

(a) Give the structural formula of the compound responsible for the signal at δ 0.00 in the n.m.r. spectrum.

**(1)**

(b) How many different types of proton are present in compound **F**?

.....

**(1)**

(c) What is the ratio of the numbers of each type of proton?

.....

**(1)**

(d) Which alkyl group is responsible for the signal at δ 2.15 in the n.m.r. spectrum?

.....

**(1)**

(e) The peaks at ä 2.47 and ä 1.05 arise from one group in compound **F.** Identify this group and explain the appearance of the splitting pattern shown in the n.m.r. spectrum.

*Group*.....

*Explanation* .....

.....

.....

**(3)**

(f) Which group is responsible for the band at 1715 $cm^{-1}$ in the infra-red spectrum of compound **F**?

.....

**(1)**

(g) Give the structures of the species responsible for the peaks at m/z values of 43 and 57 in the mass spectrum.

*Peak at m/z = 43*.....

*Peak at m/z = 57*.....

**(2)**

(h) Give the structure of compound **F.**

.....

**(1)**

**(Total 11 marks)**

## SECTION B

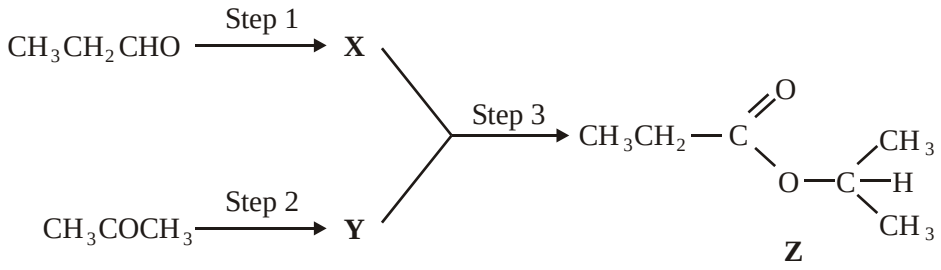
**5.** (a) Describe how propanal, $CH_3CH_2CHO$, and propanone, $CH_3COCH_3$, can be distinguished using

(i) a chemical test and

(ii) the number of peaks in their proton n.m.r. spectra.

**(5)**

(b) Compound **Z** can be produced by the reaction of compound **X** with compound **Y** as shown in the synthesis outlined below.




Identify compounds **X** and **Y**.
For each of the three steps in the synthesis, name the type of reaction involved and give reagents and conditions. Equations are **not** required.

**(10)**
**(Total 15 marks)**

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