

Q1. It is necessary to use several analytical techniques to determine the structure of an unknown compound.

An analytical chemist was asked to determine the structure of compound **Q** which was found in a waste tank in a mixture of volatile liquids.

Compound **Q** has the molecular formula C_4H_7ClO . It is a volatile liquid which does not produce misty fumes when added to water.

(a) Suggest how the chemist could obtain a sample of **Q** for analysis from the mixture of volatile liquids.

.....

(1)

(b) The infra-red spectrum of **Q** contains a major absorption at 1724 cm^{-1} . Identify the bond which causes this absorption.

.....

(1)

(c) The mass spectrum of **Q** contains two molecular ion peaks at $m/z = 106$ and $m/z = 108$. It also has a major peak at $m/z = 43$.

(i) Suggest why there are two molecular ion peaks.

.....

(ii) A fragment ion produced from **Q** has $m/z = 43$ and contains atoms of **three** different elements. Identify this fragment ion and write an equation showing its formation from the molecular ion of **Q**.

Fragment ion

Equation

(3)

(d) The proton n.m.r. spectrum of **Q** was recorded.

(i) Suggest a suitable solvent for use in recording this spectrum of **Q**.

-
- (ii) Give the formula of the standard reference compound used in recording proton n.m.r. spectra.
-

(2)

- (e) The proton n.m.r. spectrum of Q shows 3 peaks. Complete the table below to show the number of adjacent, non-equivalent protons responsible for the splitting patterns.

	Peak 1	Peak 2	Peak 3
Integration value	3	3	1
Splitting pattern	doublet	singlet	quartet
Number of adjacent, non-equivalent protons	1		

(1)

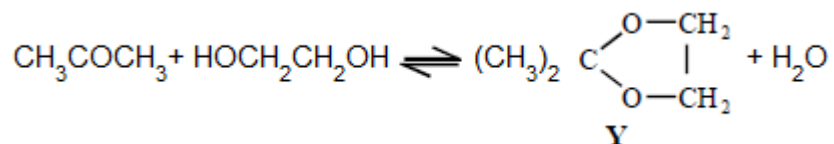
- (f) Using the information in parts (a), (b) and (d) deduce the structure of compound Q.

(1)

- (g) A structural isomer of Q reacts with cold water to produce misty fumes. Suggest a structure for this isomer.

(1)
(Total 10 marks)

Q2. This question is about the reaction between propanone and an excess of ethane-1,2-diol, the equation for which is given below.



In a typical procedure, a mixture of 1.00 g of propanone, 5.00 g of ethane-1,2-diol and 0.100 g of benzenesulphonic acid, $\text{C}_6\text{H}_5\text{SO}_3\text{H}$, is heated under reflux in an inert solvent. Benzenesulphonic acid is a strong acid.

The products would **not** have an absorption in the infra-red at

- A** 1050 cm^{-1}
- B** 1720 cm^{-1}
- C** 2950 cm^{-1}
- D** 3400 cm^{-1}

(Total 1 mark)

Q3. 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)

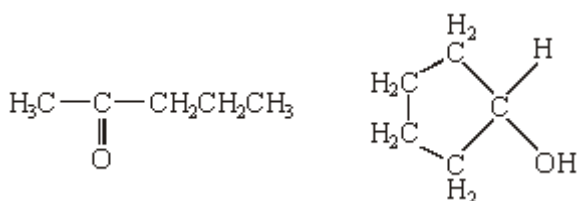
(e) Compounds **I** and **J** have the molecular formula C_6H_{12}

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)

Q4. 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**, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO}$, is also an isomer of $\text{C}_5\text{H}_{10}\text{O}$

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.

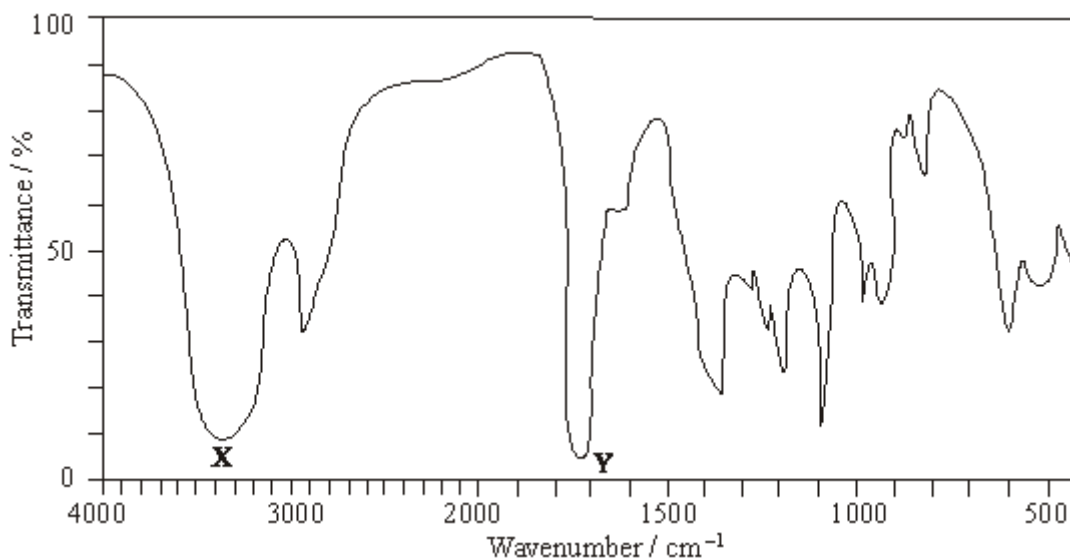
Reagent

Observation with E

(2)

(Total 9 marks)

- Q5.** (a) The infra-red spectrum of compound **A**, $\text{C}_3\text{H}_6\text{O}_2$, is shown below.



Identify the functional groups which cause the absorptions labelled X and Y.

Using this information draw the structures of the three possible structural isomers for **A**.

Label as **A** the structure which represents a pair of optical isomers.

(6)

- (b) Draw the structures of the three **branched-chain** alkenes with molecular formula C_5H_{10}

Draw the structures of the three dibromoalkanes, $C_5H_{10}Br_2$, formed when these three alkenes react with bromine.

One of these dibromoalkanes has only three peaks in its proton n.m.r. spectrum. Deduce the integration ratio and the splitting patterns of these three peaks.

(10)

(Total 16 marks)