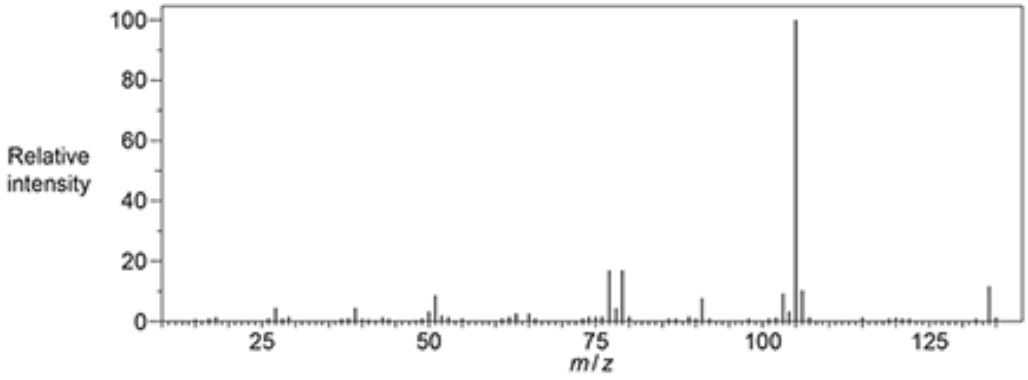
1. Analysis of an unknown organic compound **J** produces the following results.

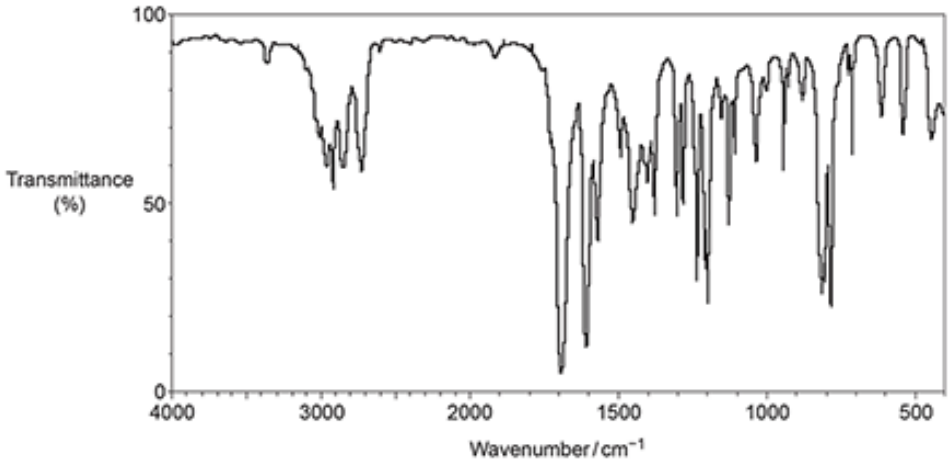
Elemental analysis by mass of compound J

C, 80.60%; H, 7.46%; O, 11.94%

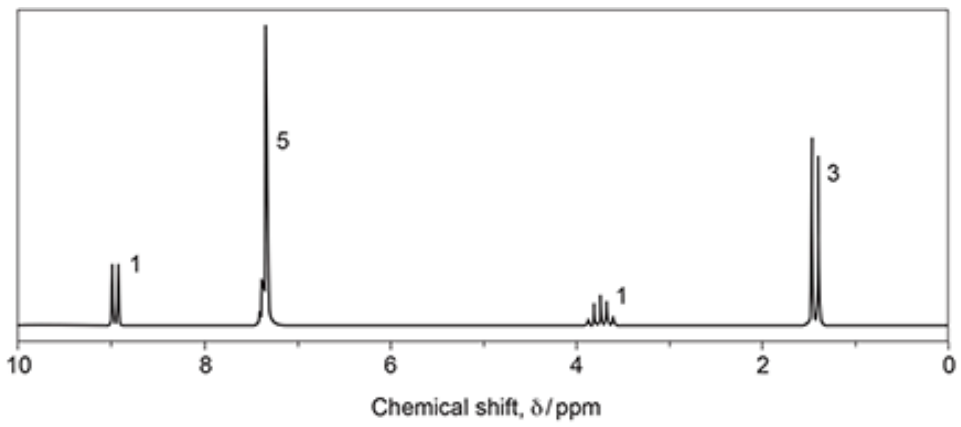
Mass spectrum of compound J



IR spectrum of compound J



Proton NMR spectrum of compound J

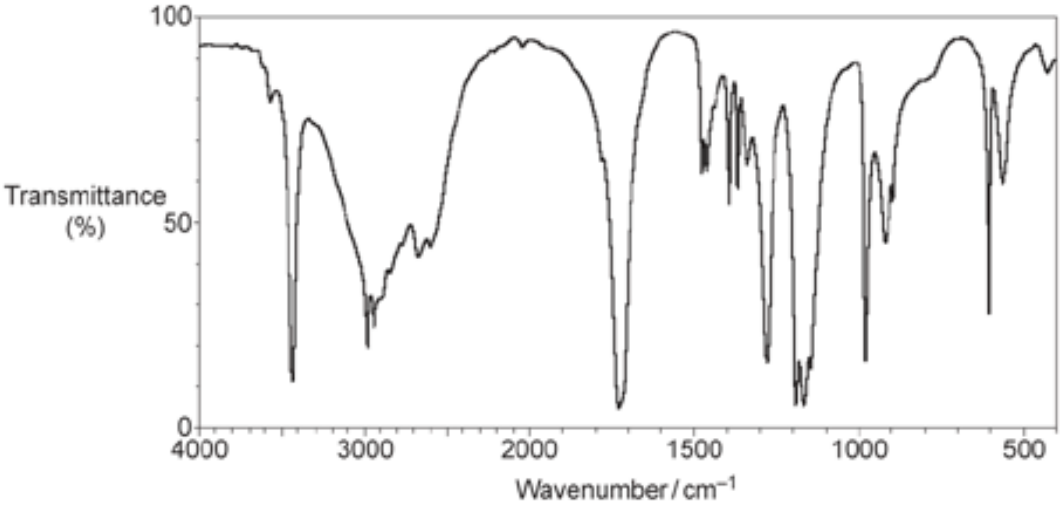


The numbers by the peaks are the relative peak areas.

Determine the structure of compound **J**, showing **all** your reasoning.

[6]

2. Which compound could have produced the IR spectrum shown below?



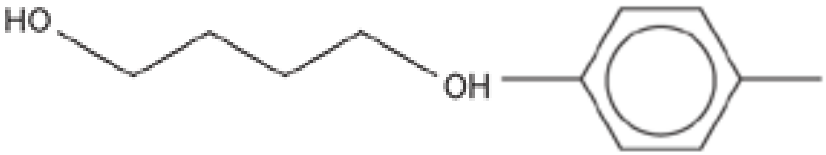
A $HOCH_2CHO$
B CH_3CH_2COOH
C $CH_3CH_2COOCH_3$
D $(CH_3)_2C(OH)COOH$

Your answer ☐ **[1]**

3. The structures of 3 compounds, **1**, **2** and **3**, are shown below.

Which compound(s) would produce a carbon-13 NMR spectrum with 2 peaks?

1



2 **3**

A 1, 2 and 3
B Only 1 and 2
C Only 2 and 3
D Only 1

Your answer ☐ **[1]**

4. There are 4 structural isomers of $C_4H_{10}O$ that are alcohols.

A student predicts that these structural isomers could be distinguished using carbon-13 NMR spectroscopy.

Explain whether the student is correct.

In your answer, show how the peaks in the carbon-13 NMR spectra are linked to the structure of each alcohol isomer.

[5]

5. An unknown organic compound is analysed.

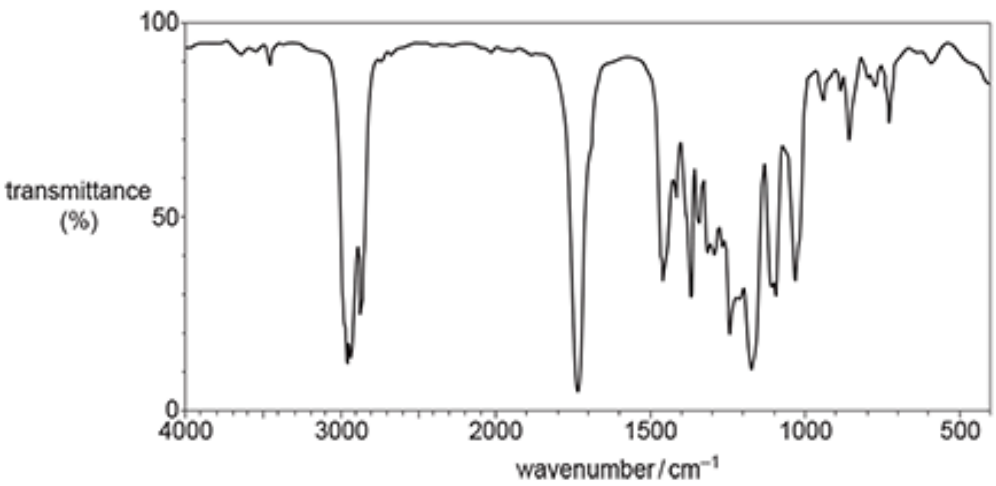
The results are shown below.

Addition of 2,4-DNP
No visible change

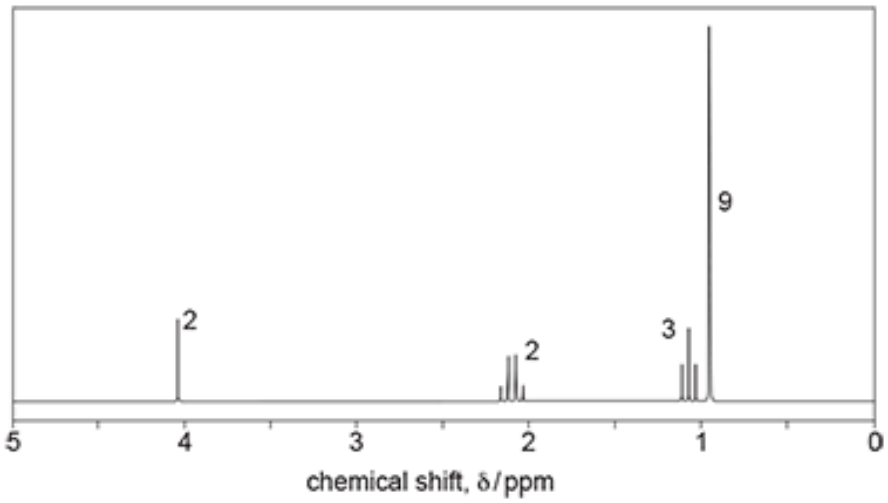
Elemental analysis by mass
C, 66.63%; H, 11.18%; O, 22.19%

Mass spectrum
Molecular ion peak at *m / z* = 144.0

IR spectrum



Proton NMR spectrum
The numbers by each peak are the relative peak areas.

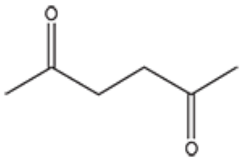
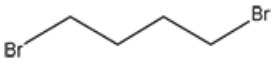
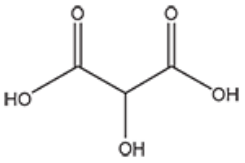
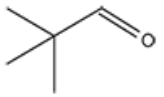


Use the information to identify the organic compound.

Show **all** your reasoning.

[6]

6. Which compound has the greatest number of peaks in its proton NMR spectrum?

A	
B	
C	
D	

Your answer ☐ **[1]**

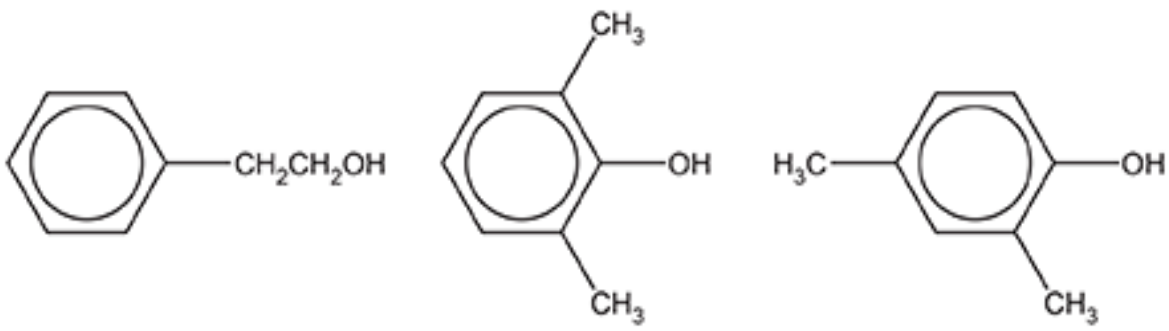
7. Which compound is used for proton exchange in NMR spectroscopy?

A CCl_4
B $CDCl_3$
C D_2O
D $Si(CH_3)_4$

Your answer ☐ **[1]**

8. This question is about the chemistry of aromatic compounds.

Compounds **J**, **K** and **L**, shown below, are structural isomers.



Compound J **Compound K** **Compound L**

i. What chemical test(s) could be used to confirm the presence of the phenol group in compounds **K** and **L**?

[1]

ii. A student thought that ^{13}C NMR spectroscopy could be used to distinguish between compounds **J**, **K** and **L**.

Explain, with reasoning, whether the student is correct.

[3]

iii. Compound **J** is substituted at the 2- and 4- positions by chlorine in the presence of a catalyst.

Outline the mechanism for the 4 substitution of compound **J** by chlorine in the presence of a catalyst.

Show the role of the catalyst.

[4]

9. Which compound produces two triplets in its ^{1}H NMR spectrum?

A $CH_3CH_2COOCH_2CH_3$
B $CH_3CH_2COCH_2CH_3$
C $HOOCCH_2CH_2COOH$
D $HOOCCH_2CH_2CH_2COOH$

Your answer ☐ **[1]**

10. Which isomer(s) of C_5H12O has/have 4 peaks in its/their ^{13}C NMR spectrum?

1 3-methylbutan-2-ol
2 2-methylbutan-2-ol
3 2-methylbutan-1-ol

A 1, 2 and 3
B Only 1 and 2
C Only 2 and 3
D Only 1

Your answer ☐ **[1]**

11. This question is about unsaturated hydrocarbons.

Compounds **B** and **C** are **branched** hydrocarbons that are structural isomers of C_6H_{12}.

Compounds **B** and **C** both have stereoisomers.

• Compound **B** has *cis* and *trans* isomers but does **not** have optical isomers.

• Compound **C** has optical isomers but does **not** have *cis* and *trans* isomers.

i. What is meant by the term **structural isomers**?

_____

_____

[1]

ii. What is meant by the term **stereoisomers**?

_____

_____

[1]

iii. Draw structures for the *cis* and *trans* isomers of the branched hydrocarbon **B**.

***cis* isomer**	***trans* isomer**

[2]

iv. Draw 3D structures for the optical isomers of compound **C**.

Optical isomers	

[2]

v. Compounds **D** and **E** are two more structural isomers of C_6H_{12}.

Compounds **D** and **E** do **not** show stereoisomerism.

Table 16.1 shows NMR and infrared (IR) spectral data for **D** and **E**.

	Number of peaks in ^{1}H NMR spectrum	**Number of peaks in ^{13}C NMR spectrum**	**IR peak at 1620–1680 cm^{-1}**
D	1	1	No
E	1	2	Yes

Table 16.1

Draw the structures of **D** and **E** and explain how the spectral data in **Table 16.1** provides evidence for the structures.

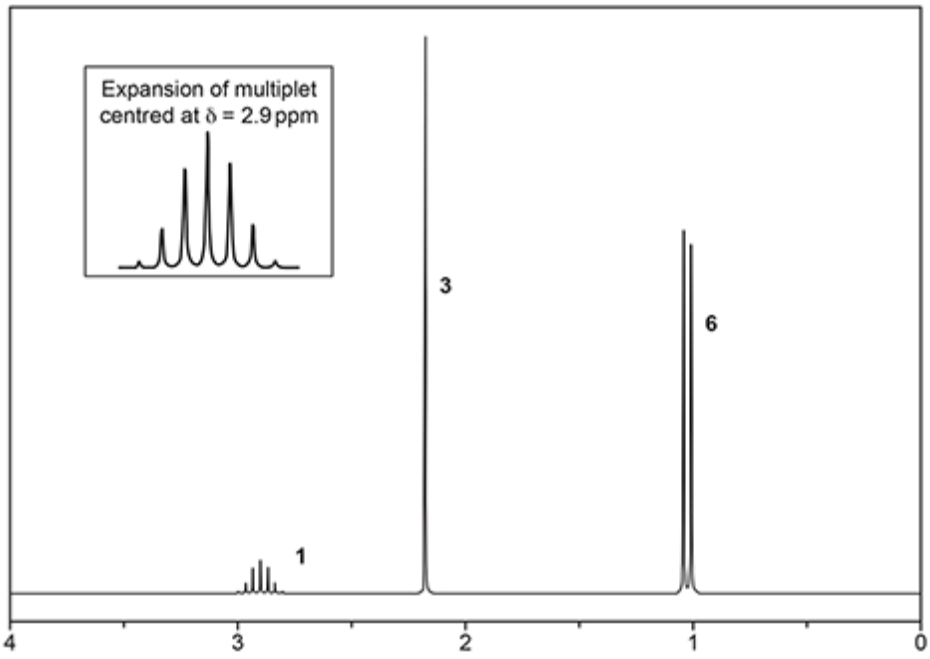
D	**E**

[4]

12. The organic compound **H** contains carbon, hydrogen and oxygen only and has an M_r of 114.0.

Compound **H** has two carbonyl groups and no other functional groups.

The ^{1}H NMR spectrum of organic compound **H** is shown below.



chemical shift, δ /ppm

The numbers by the peaks are the relative peak areas.

Analyse the spectrum to suggest a possible structure for compound **H**.

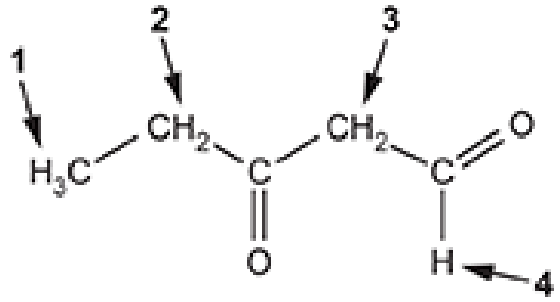
Show all your reasoning.

Compound H

[4]

13. The structure of an organic compound is shown below.

The protons are in four different environments, which are labelled **1**-**4**.



i. Fill in the table to predict the splitting patterns in the **proton** NMR spectrum of the organic compound.

Proton environment	Splitting pattern
1	
2	
3	
4	

[2]

ii. The table shows the chemical shifts for the peaks in the **proton** NMR spectrum at proton environments **2** and **3**.

Proton environment	2	3
Chemical shift, δ	2.5 ppm	3.6 ppm

Suggest why the peaks for proton environments **2** and **3** have the chemical shifts which are shown in the table.

[2]

END OF QUESTION PAPER