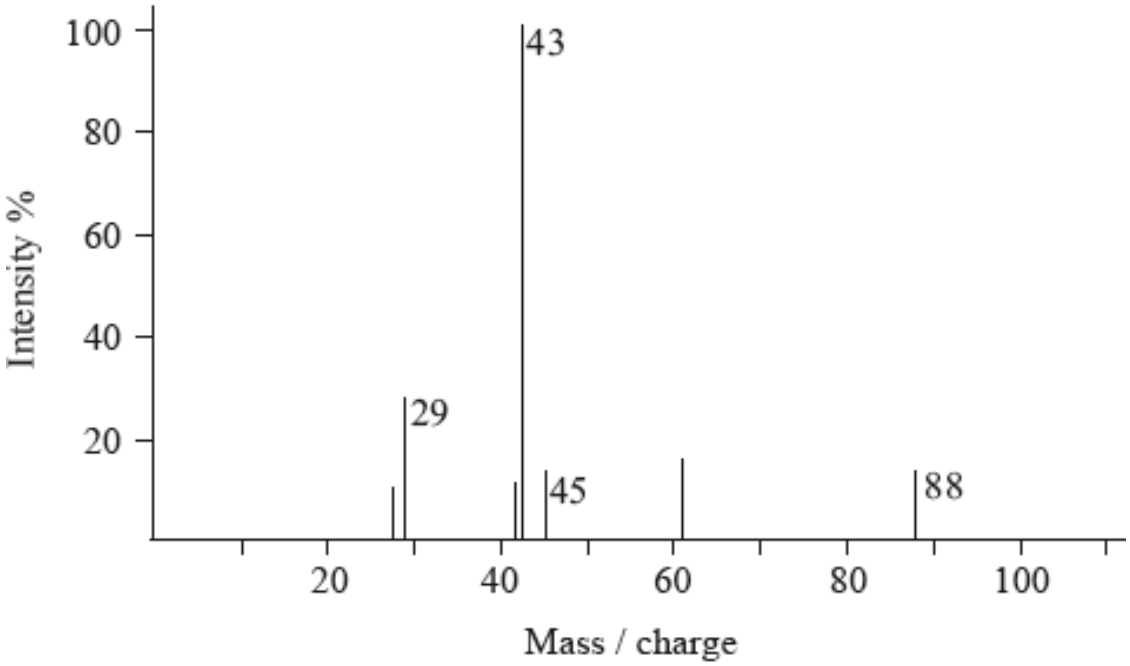
11.3 Spectroscopic Determination of Organic Compounds

Past Exam Questions (Paper 2)

1a. *[2 marks]*

The mass spectrum of an unknown compound, **X**, of empirical formula C_2H_4O is shown below.



[Source: Cleapss Guides: L202 Spectra (Cleapss School Science Service), Sept 2000.]

Determine the relative molecular mass of **X** from the mass spectrum and deduce the formula of the molecular ion.

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1b. *[1 mark]*

Identify a fragment which gives rise to the peak at *m/z* = 29.

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1c. *[1 mark]*

Comment on the absence of a peak at m/z = 59.

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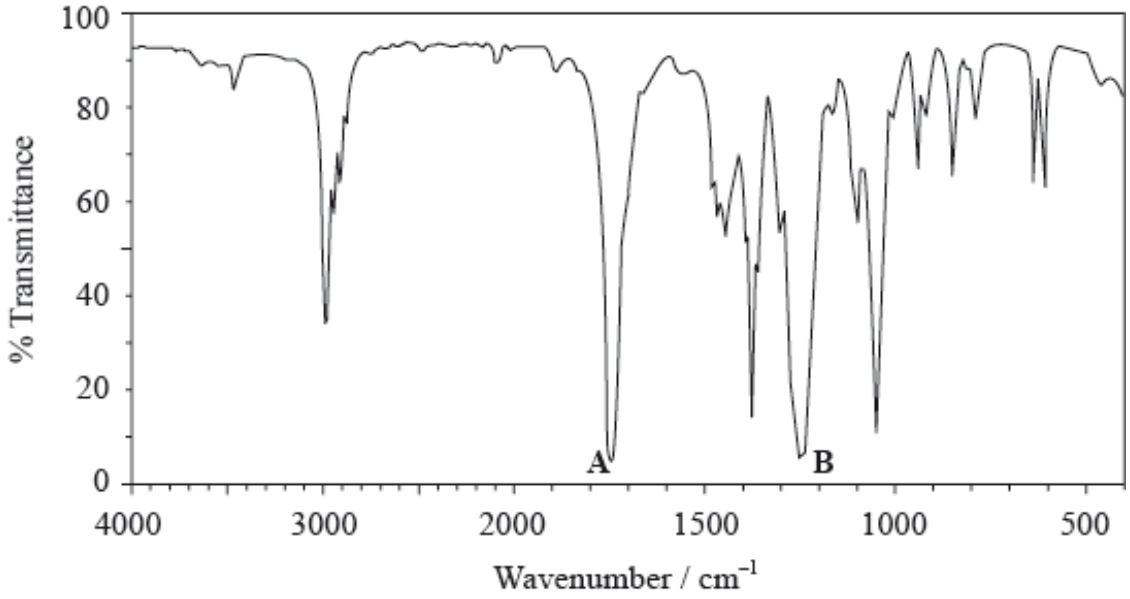
1d. *[1 mark]*

The IR spectrum of **X** is shown below.



[Source: http://modbo1.ibase.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng]

Use Table 17 of the Data Booklet to identify the bonds which correspond to the absorptions **A** and **B**.

A:

B:

1e. *[1 mark]*

Deduce the name of the functional group present in **X**.

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1f. *[1 mark]*

The $^{1}H\ NMR$ spectrum of **X** shows three peaks. State the information that can be obtained from the number of peaks.

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1g. *[2 marks]*

The $^{1}H\ NMR$ spectrum of **X** includes peaks at 2.0 and 4.1 ppm. Use the Data Booklet to suggest the chemical shift of the third peak and state its relative peak area. Show your answers in the table below.

Peak	Chemical shift / ppm	Relative peak area
First	2.0	3
Second	4.1	2
Third		

1h. *[1 mark]*

Deduce a possible structure for **X** that is consistent with the mass, IR and $^{1}H\ NMR$ spectra.

2a. *[3 marks]*

Explain what occurs at a molecular level during the absorption of infrared (IR) radiation by the sulfur dioxide molecule, SO_2.

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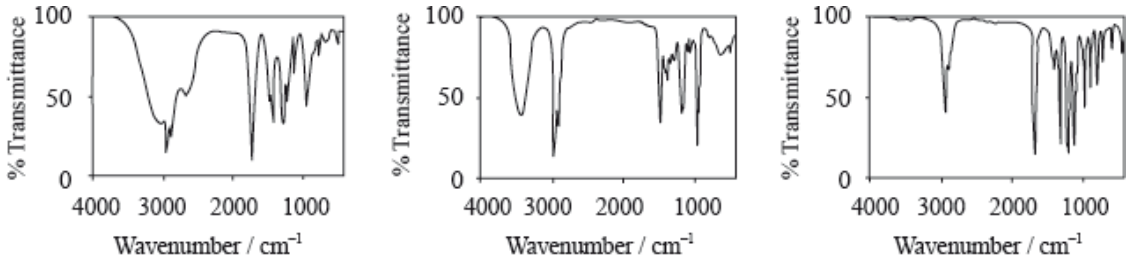
2b. *[5 marks]*

Consider the IR spectra of the following three compounds.

$$A = CH_3(CH_2)_3COOH \; B = CH_3COOC(CH_3)_3 \; C = (CH_3CH_2)_3COH$$



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Determine which IR spectrum corresponds to each compound A, B and C. Explain your reasoning. IR data can be found in Table 17 of the Data Booklet.

Compound	Spectrum	Reason
A	....	....
B	....	....
C	....	....

3a. *[1 mark]*

Compound **P** contains a carbonyl group (C=O) and has the molecular formula C_3H_6O.

Draw the **two** possible structures of compound **P**.

3b. *[1 mark]*

Explain why the infrared spectra of the structures in (a) are very similar.

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3c. *[2 marks]*

Explain how the mass spectra of the structures in (a) can be used to distinguish between them.

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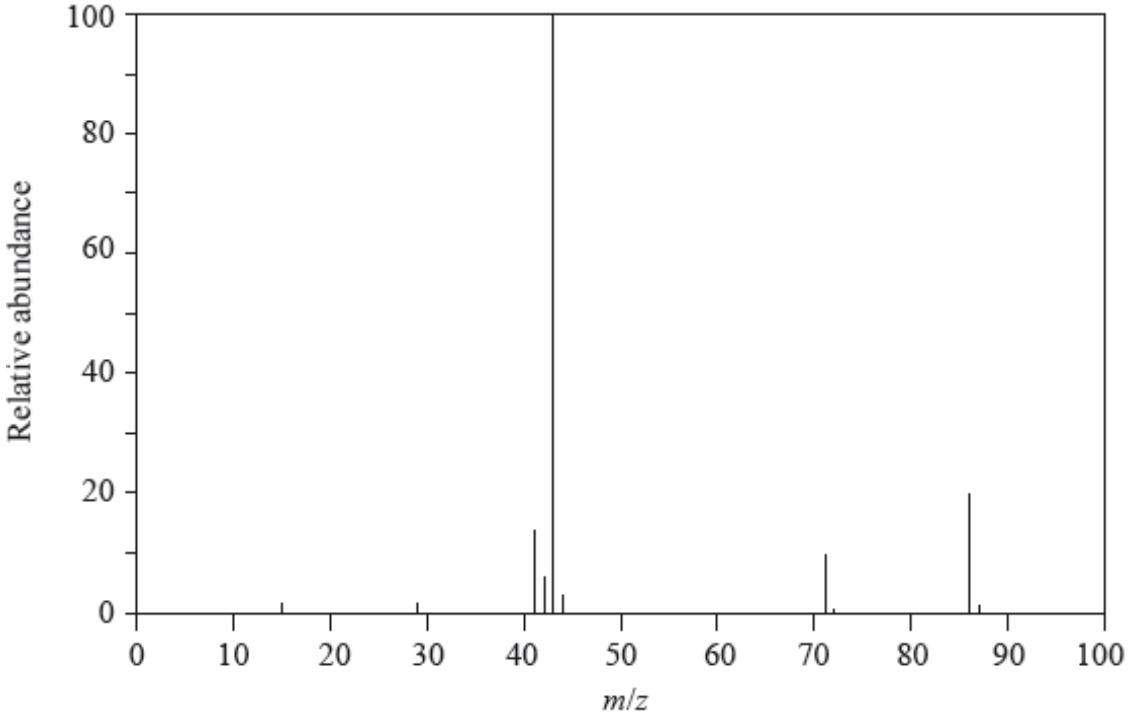
3d. *[3 marks]*

Pentan-2-one has the following mass spectrum.



Deduce the formulas of the species with the m/z values at 86, 71 and 43.

$m/z = 86$:

$m/z = 71$:

$m/z = 43$:

3e. *[1 mark]*

Suggest a reason for the peak at m/z = 43 having an exceptionally high relative abundance.

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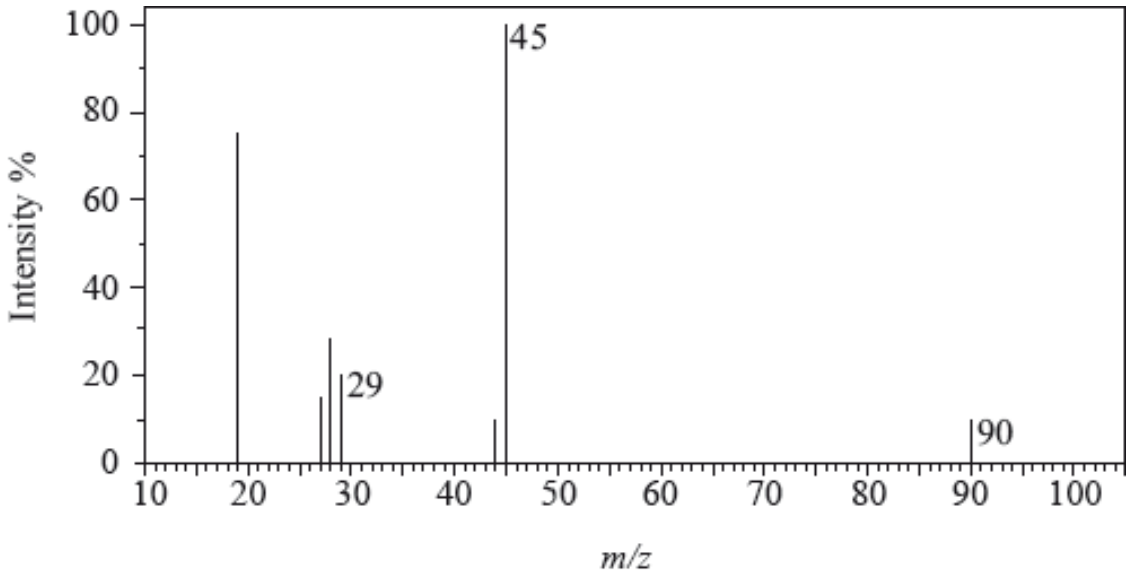
4a. *[2 marks]*

The mass spectrum of an unknown acidic compound, **X**, with empirical formula CH_2O, is shown below.



Determine the relative molecular mass, to the nearest integer, of the compound from the mass spectrum and deduce the formula of the molecular ion.

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4b. *[1 mark]*

Deduce the formula of the fragment responsible for the peak at 45.

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4c. *[1 mark]*

Deduce the formula of the fragment responsible for the peak at 29.

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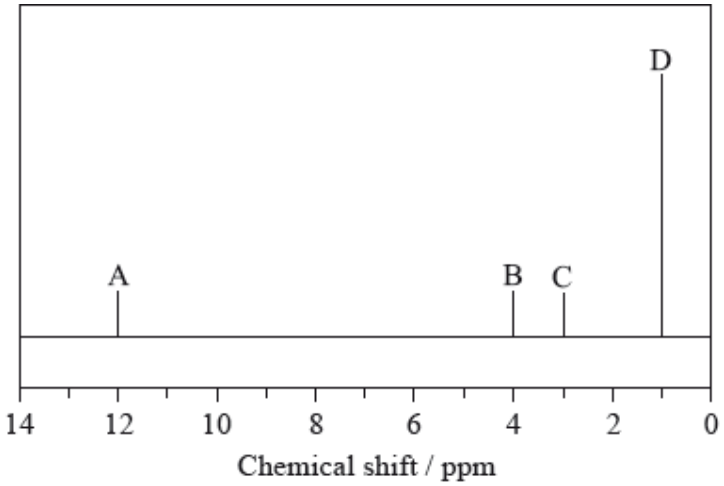
4d. *[1 mark]*

The low-resolution $^{1}H\ NMR$ spectrum of **X** shows four peaks. A simplified representation is shown alongside a table with relative peak areas.



Peak	Relative peak area
A	1
B	1
C	1
D	3

Identify the group responsible for the peak at **D**.

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4e. *[1 mark]*

Suggest a possible structure for **X**.

5a. *[1 mark]*

Mass spectrometry is a powerful analytical technique used in the identification of organic compounds. The mass spectrum of a compound with empirical formula CH_2O displays peaks at *m/z* 15, 45 and 60.

Determine the molecular formula of the compound.

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5b. *[2 marks]*

Identify the fragments responsible for the peaks at

m/z = 15

m/z = 45

5c. *[1 mark]*

Identify a compound that could produce this spectrum.

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6a. *[3 marks]*

Infrared (IR) spectroscopy is widely used as a technique in analytical chemistry.

Explain what happens at a molecular level during the absorption of IR radiation by carbon dioxide, CO_2.

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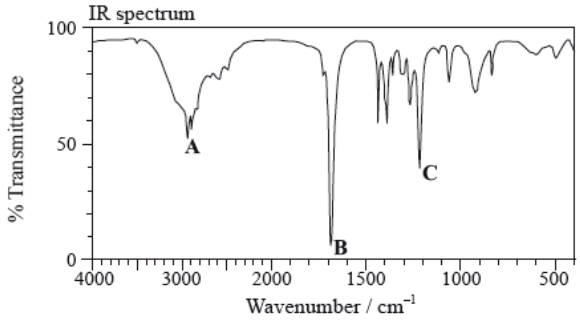
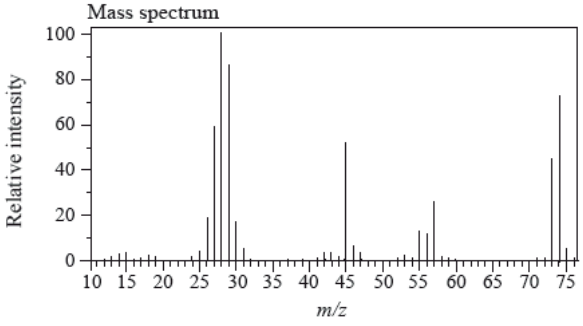
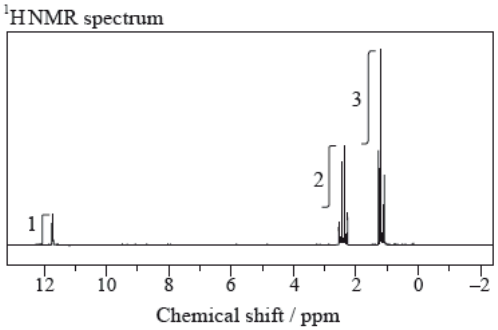
6b. *[7 marks]*

The IR spectrum, mass spectrum and $^1H\ NMR$ spectrum of an unknown compound, **X**, of molecular formula $C_3H_6O_2$ are as follows.







(i) Identify the bonds responsible for the peaks **A**, **B** and **C** in the IR spectrum of **X**.

A:

B:

C:

(ii) In the mass spectrum of **X**, deduce which ions the *m/z* values at 74, 45 and 29 correspond to.

m/z = 74:

m/z = 45:

m/z = 29:

(iii) Identify the peak at 11.73 ppm in the $^{1}H\ NMR$ spectrum.

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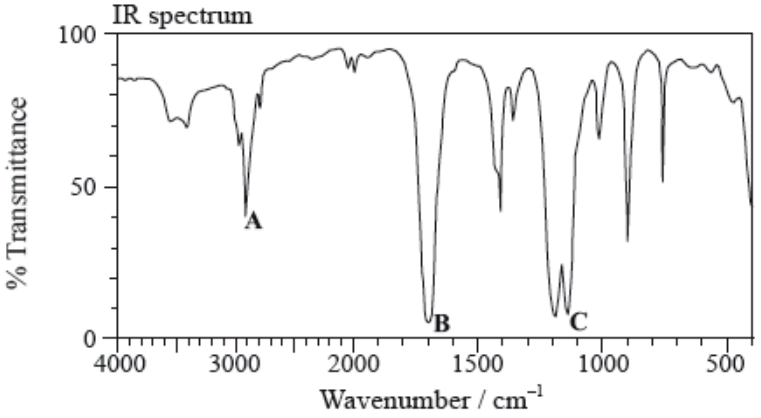
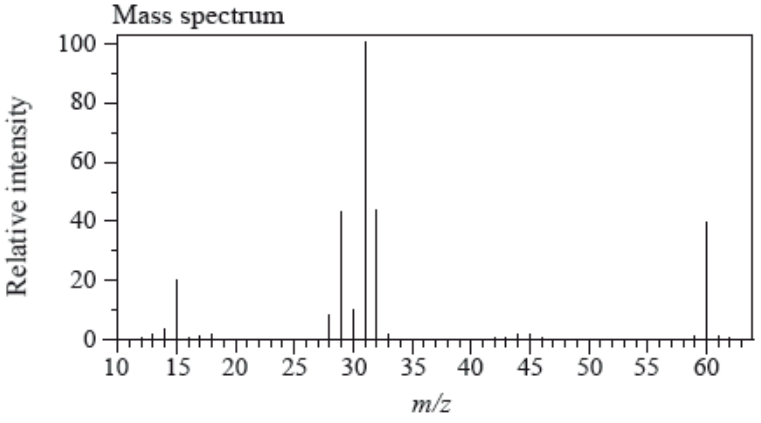
(iv) Deduce the structure of **X**.

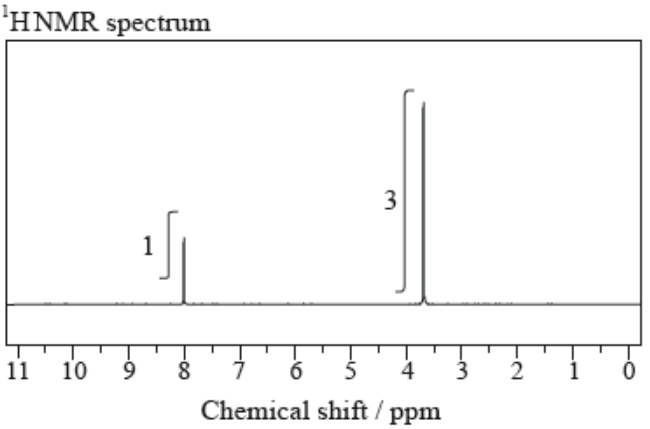
7. *[9 marks]*

Infrared (IR) spectroscopy is widely used as a technique in analytical chemistry.

The IR spectrum, mass spectrum and $^1H\ NMR$ spectrum of an unknown compound, **Y**, of molecular formula $C_2H_4O_2$ are as follows.







[Source: SDBSWeb: http://riodb01.ibase.aist.go.jp/sdbs/ (National Institute of Advanced Industrial Science and Technology)]

(i) Identify the bonds responsible for the peaks **A**, **B** and **C** in the IR spectrum of **Y**.

A:

B:

C:

(ii) In the mass spectrum of **Y**, deduce which ions the *m/z* values at 31 and 29 correspond to.

m/z = 31:

m/z = 29:

(iii) Identify the peaks at 3.76 and 8.07 ppm in the $^{1}H\ NMR$ spectrum.

3.76 ppm:

8.07 ppm:

(iv) State what information can be obtained from the integration trace about the hydrogen atoms responsible for the peak at 3.76 ppm in the $^{1}H\ NMR$ spectrum.

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(v) Deduce the structure of **Y**.

(vi) Explain why tetramethylsilane (TMS) is suitable as a reference standard.

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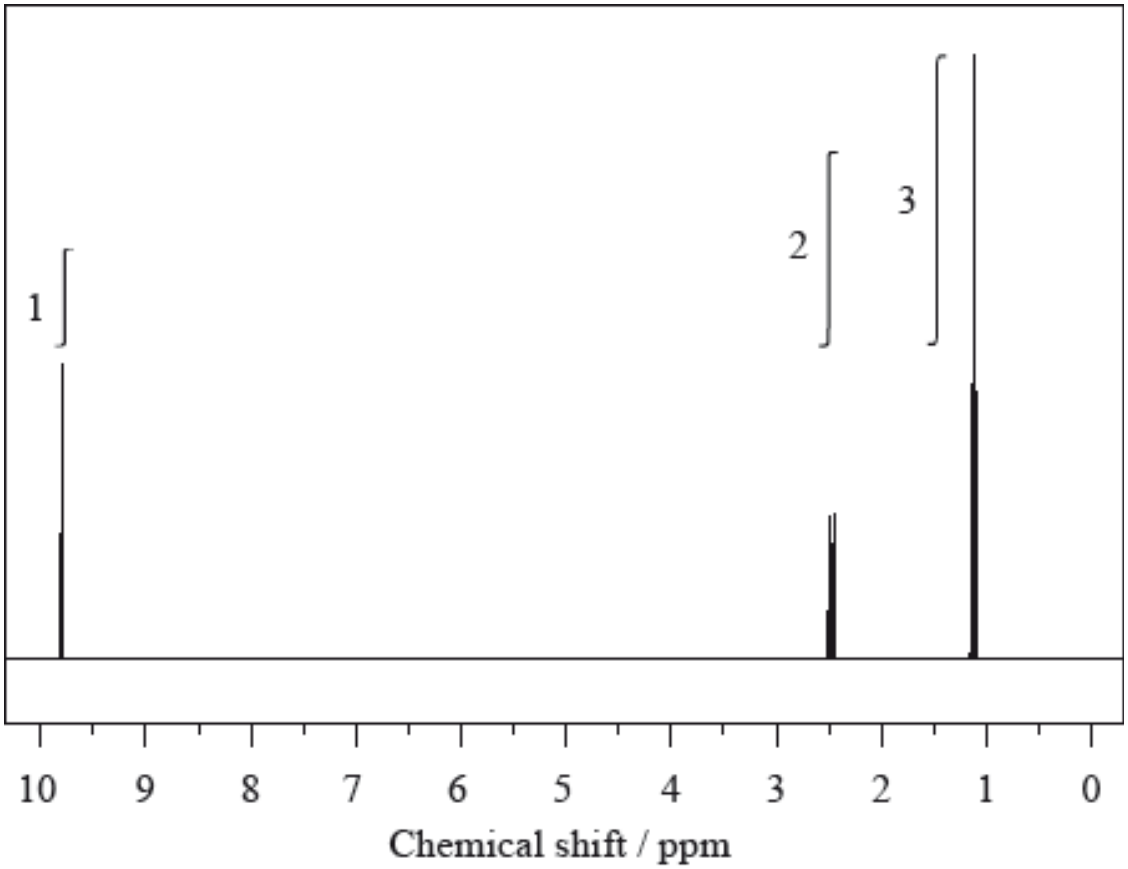
8a. *[2 marks]*

The $^{1}H\ NMR$ spectrum of **X** with molecular formula C_3H_6O is shown below.



Deduce which of the following compounds is **X** and explain your answer.

CH_3–CO–CH_3 CH_3–CH_2–CHO CH_2–CH–CH_2OH

Compound:

Explanation:

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8b. *[2 marks]*

Deduce which one of the peaks in the $^{1}H\ NMR$ spectrum of **X** would also occur in the spectrum of one of the other isomers, giving your reasoning.

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8c. *[1 mark]*

The infrared and mass spectra for **X** were also recorded.

Apart from absorptions due to C–C and C–H bonds, suggest **one** absorption, in wavenumbers, that would be present in the infrared spectrum.

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8d. *[1 mark]*

Apart from absorptions due to C–C and C–H bonds, suggest **one** absorption, in wavenumbers, absent in this infrared spectrum but present in one of the other compounds shown in part (c).

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8e. *[2 marks]*

Suggest the formulas and m/z values of **two** species that would be detected in the mass spectrum.

Species:

m/z:

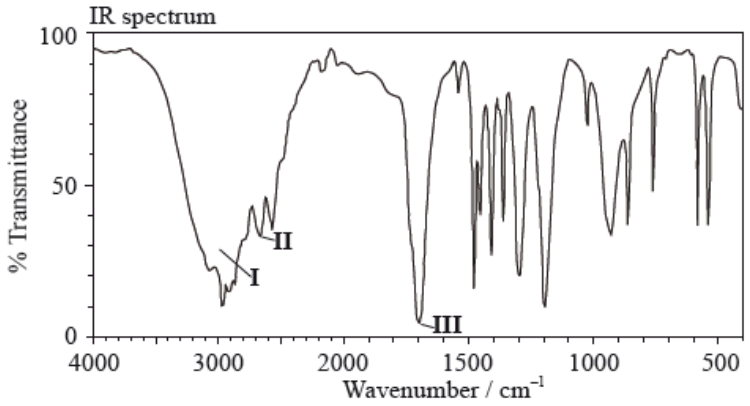
Species:

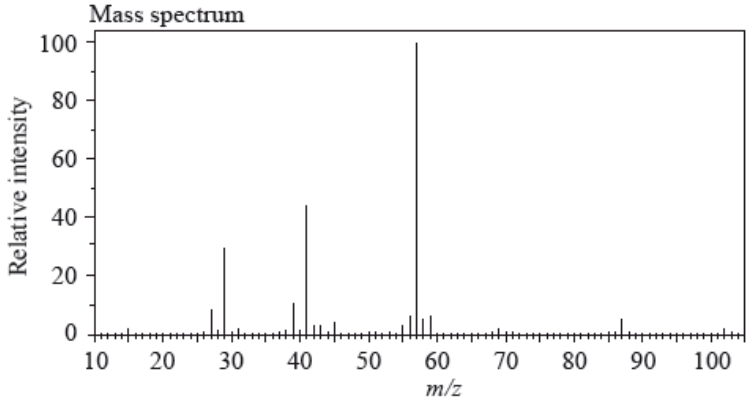
m/z:

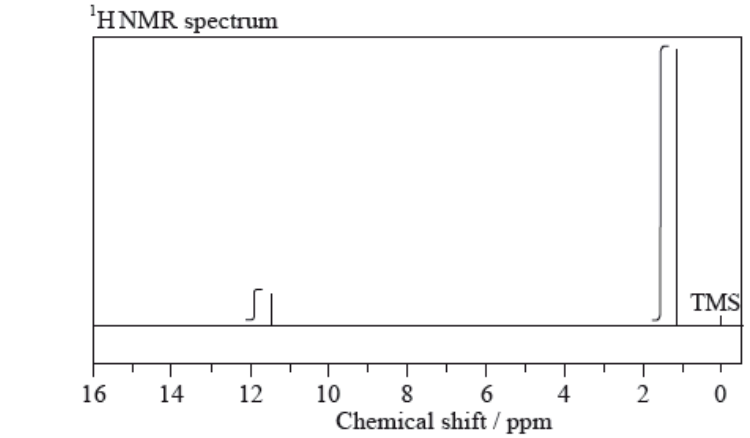
9a. *[3 marks]*

Infrared spectroscopy is commonly used as an analytical technique by inorganic, physical and organic chemists.

The IR spectrum, mass spectrum and $^1H\ NMR$ spectrum of an unknown compound, **X**, of molecular formula $C_5H_{10}O_2$, are as follows.







[Source: SDBSWeb:http://riod01.ibase.aist.go.jp/sdbs/(National Institute of Advanced Industrial Science and Technology)]

In the IR spectrum, identify the bond responsible for each of the absorptions labelled **I**, **II** and **III**.

I:

II:

III:

9b. *[3 marks]*

In the mass spectrum, deduce which fragments the *m/z* values at 102, 57 and 45 correspond to.

m/z =102:

m/z = 57:

m/z = 45:

9c. *[1 mark]*

Identify the peak at 11.5 ppm in the $^{1}H\ NMR$ spectrum.

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9d. *[1 mark]*

State what information can be obtained from the integration traces in the $^{1}H\ NMR$ spectrum about the hydrogen atoms responsible for the peak at 1.2 ppm.

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9e. *[1 mark]*

Deduce the structure of **X**.

9f. *[2 marks]*

$CH_3COOCH_2CH_2CH_3$ is an isomer of **X**. Deduce **two** differences between the $^1H\ NMR$ spectrum of this isomer and that of **X**.

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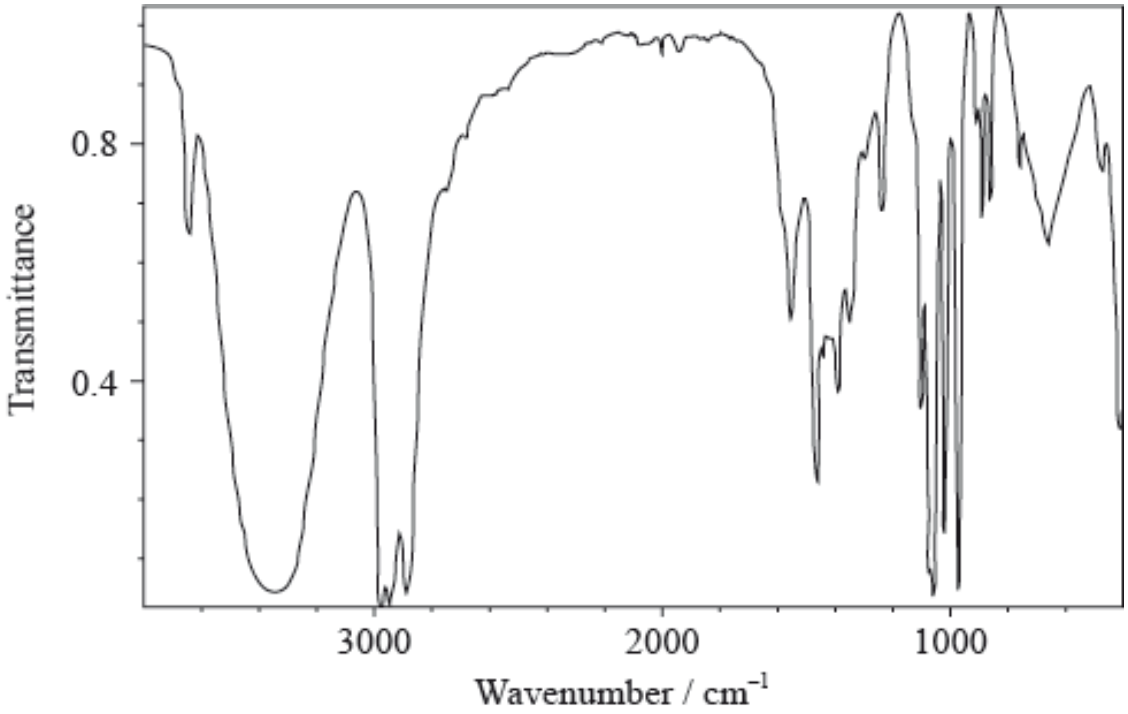
10a. *[1 mark]*

The IR spectrum below represents one of the three organic compounds: propan-1-ol ($CH_3CH_2CH_2OH$), propanal (CH_3CH_2CHO) or propanoic acid (CH_3CH_2COOH).



The mass spectrum of the same compound contains strong peaks of $(M_r - 15)^+$ and $(M_r - 17)^+$ ions. The first signal corresponds to the loss of a methyl group, CH_3, from the molecule. Deduce which fragment is lost to produce the second peak.

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10b. *[1 mark]*

Using the information above, deduce the identity of the organic compound.

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10c. *[1 mark]*

Predict the number of peaks in the $^{1}H\ NMR$ spectrum of this compound.

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11a. *[1 mark]*

Analytical techniques are very useful in determining molecular structures. A compound, **X**, has the empirical formula C_2H_4O.

Identify the analytical technique that would most readily provide the additional data required to calculate the molecular formula of **X**.

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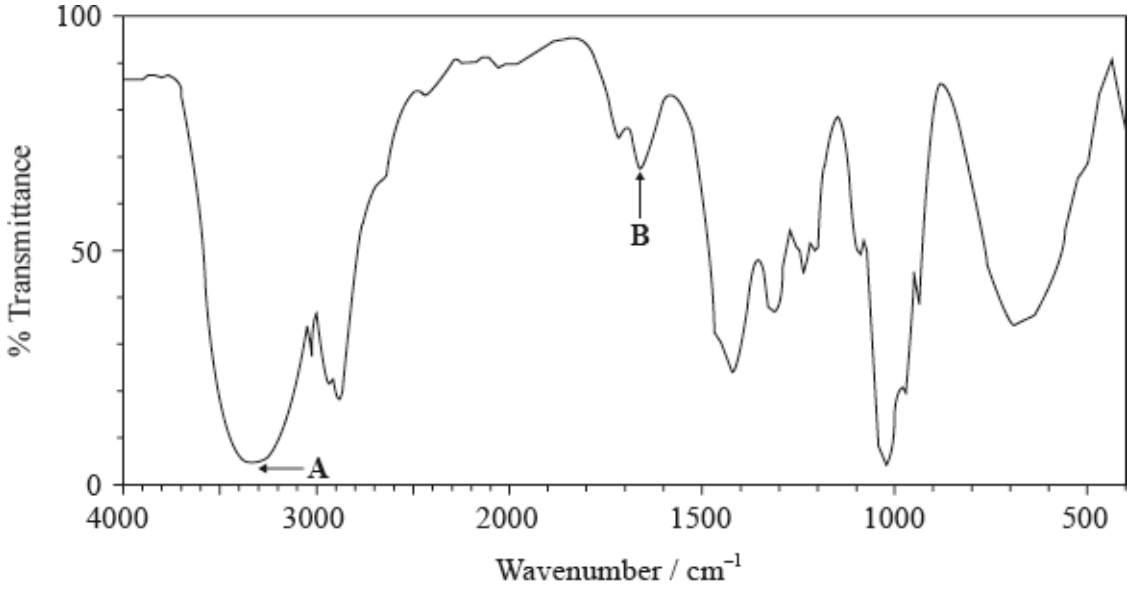
11b. *[4 marks]*

The molecular formula of **X** is $C_4H_8O_2$. The information in the IR spectrum below can be used to help determine the structure of **X**.



(i) State what information about a molecule can be obtained from its IR spectrum.

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(ii) Deduce the information obtained from absorptions **A** and **B**.

A:

B:

(iii) Comment on the absence of any major absorption in the region 1700–1750 cm^{-1}.

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11c. *[4 marks]*

The $^{1}H\ NMR$ spectrum of **X** shows three peaks with relative areas of 2:1:1.

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(i) Deduce what information can be obtained from these data.

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(ii) Deduce the structure of **X**.

12a. *[3 marks]*

Deduce the number of peaks in the $^{1}H\ NMR$ spectra of 1-bromobutane and 2-bromobutane. Explain how the integration trace can be used to distinguish between the two compounds.

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12b. *[2 marks]*

Compare the $^{1}H\ NMR$ spectrum of 1-bromo-2-methylpropane with the two spectra considered in (a). Include the number of peaks and the integration trace.

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13a. *[1 mark]*

$^{1}H\ NMR$ and IR spectroscopy both involve the absorption of electromagnetic radiation.

Identify the region of the electromagnetic spectrum used in $^{1}H\ NMR$ spectroscopy.

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13b. *[1 mark]*

Identify which of these two techniques involves higher energy radiation.

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14. *[4 marks]*

Distinguish between the $^{1}H\ NMR$ spectra of 1-bromopropane and 2-bromopropane (splitting patterns are not required).

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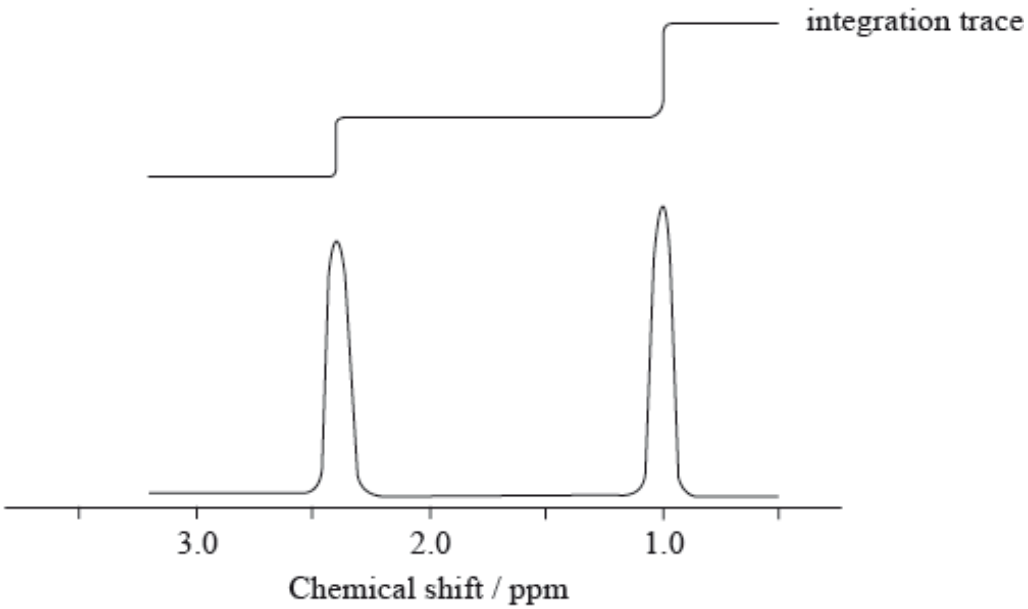
15a. *[1 mark]*

The low resolution $^1H\ NMR$ spectrum of compound **Q** is shown.



Identify what information from the spectrum allows the determination of the relative numbers of hydrogen atoms producing each peak.

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15b. *[1 mark]*

Deduce which of the following compounds is **Q**.

$CH_3CH_2CH_3$ $CH_3CH_2COCH_2CH_3$ CH_3CH_2OH

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15c. *[1 mark]*

Identify the wavenumbers of **two** peaks in the infrared spectrum of compound **Q**, using the Data Booklet.

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16a. *[3 marks]*

Nuclear magnetic resonance (NMR) and mass spectrometry are diagnostic techniques often used in the identification of organic compounds.

Deduce **two similarities** and **one difference** in the $^1H\ NMR$ spectra of the two isomers CH_3COOH, a carboxylic acid, and $HCOOCH_3$, an ester. $^1H\ NMR$ data are given in the Data Booklet

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16b. *[2 marks]*

The mass spectrum of one of the two isomers above has significant peaks at mass to charge ratios of 15, 45 and 60, while the other isomer has peaks at 15, 29, 31 and 60. Analyse these fragmentation patterns in the two mass spectra in order to distinguish between the two isomers.

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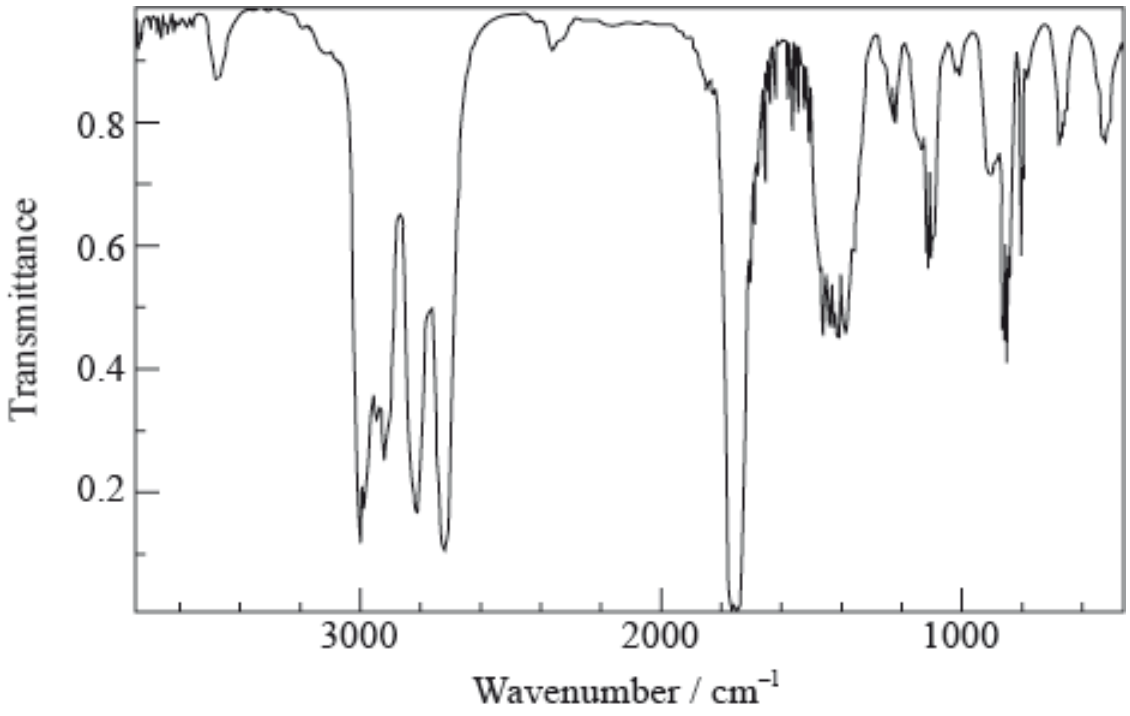
17a. *[2 marks]*

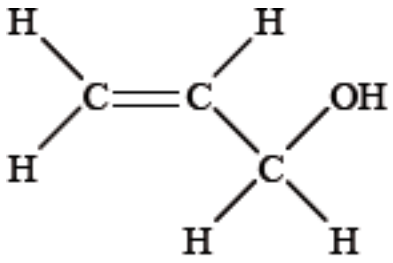
Infrared spectroscopy is an analytical technique that uses electromagnetic radiation.

The infrared spectrum of a substance, X, with empirical formula C_3H_6O is given below.



[Source: NIST http://webbook.nist.gov/chemistry]

Explain why the structural formula of X **cannot** be:



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17b. *[2 marks]*

The $^{1}H\ NMR$ spectrum of X consists of three peaks. Deduce the structural formula of X and the relative areas under each peak.

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