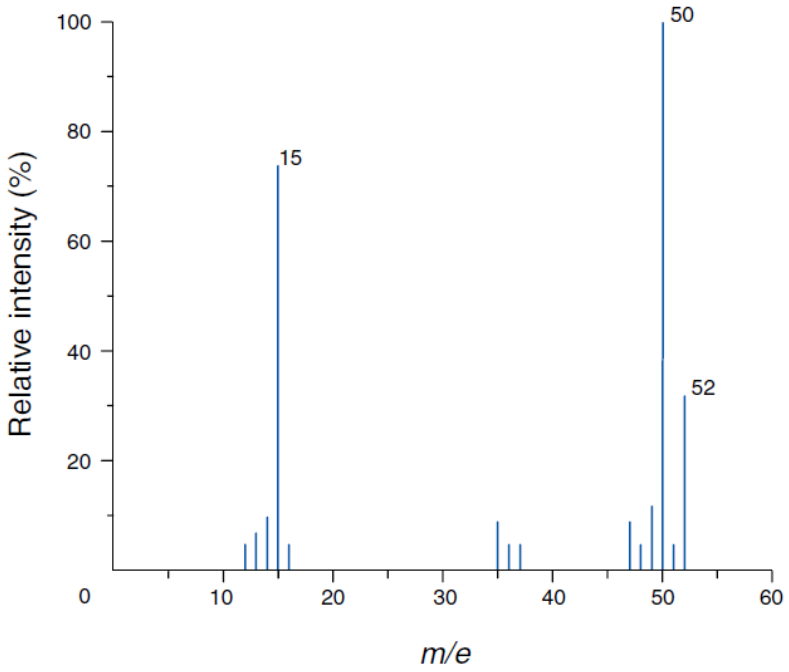
Quiz (Mass Spectrometry)

1. A mass spectrum of chloromethane is shown below.

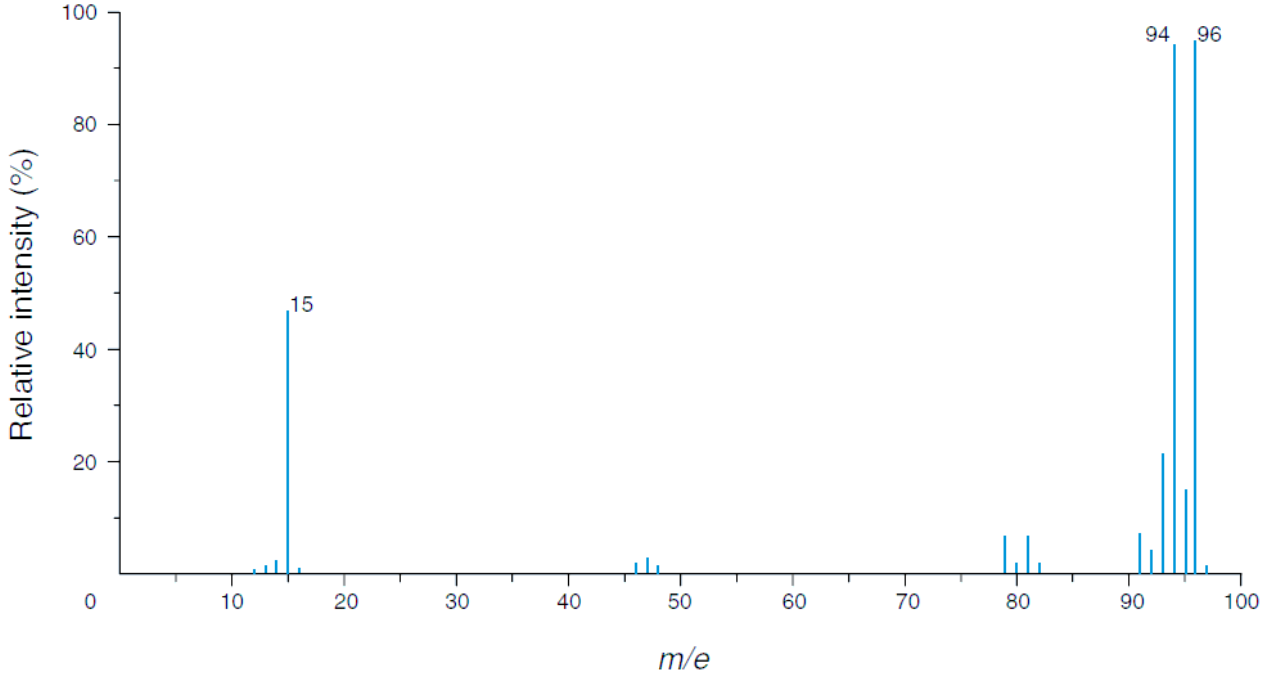


(a) Suggest one chemical species corresponding to each of the peaks at *m/e* = 52, *m/e* = 50 and *m/e* = 15 in the mass spectrum.

(b) It is found that the peak heights of the peaks at *m/e* = 52 and *m/e* = 50 are in the ratio of 1 : 3. What does this information indicate about the relative abundance of the two isotopes ^{37}Cl and ^{35}Cl?

(c) By using the information given in the mass spectrum, calculate the relative molecular mass of CH_3Cl.

2. The mass spectrum of bromomethane is shown below.



(a) What are the ions that account for the peaks at *m/e* = 15, *m/e* = 94 and *m/e* = 96 respectively in the mass spectrum?

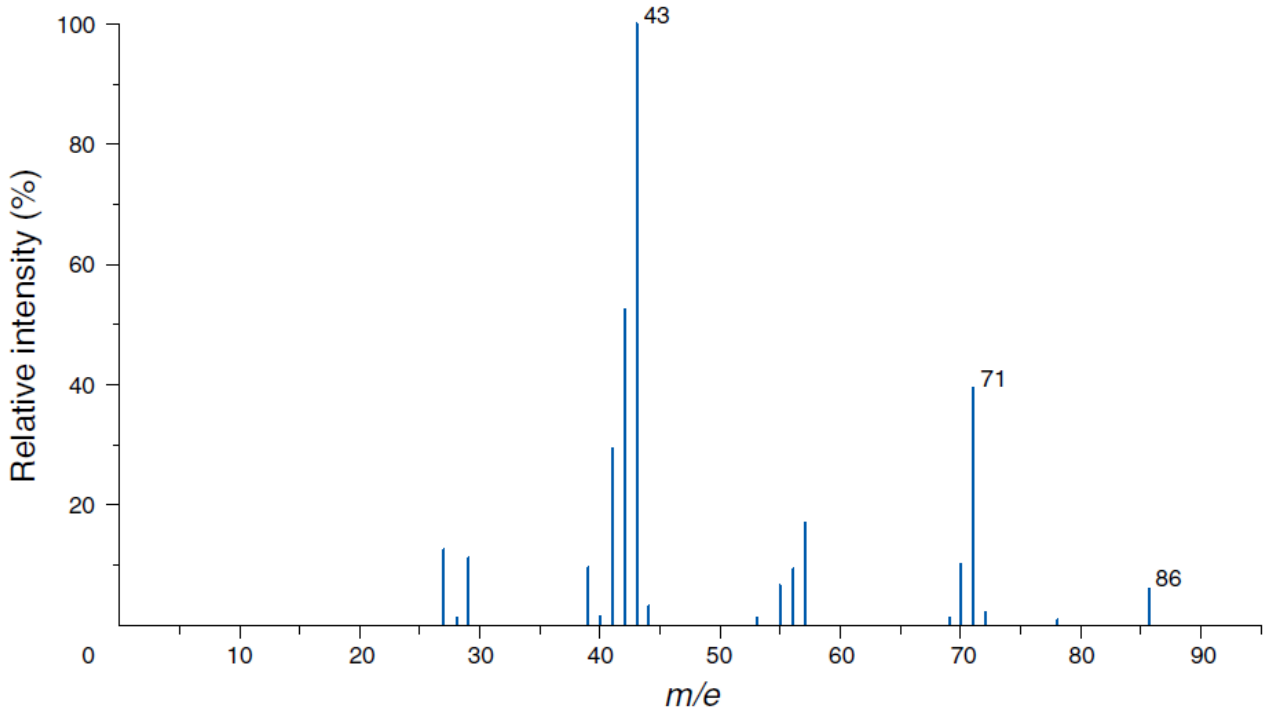
(b) (i) What is the ratio of the heights of the peaks at *m/e* = 94 and *m/e* = 96?
(ii) What does this information indicate?

(c) By using the information given in the mass spectrum, calculate the relative molecular mass of CH_3Br.

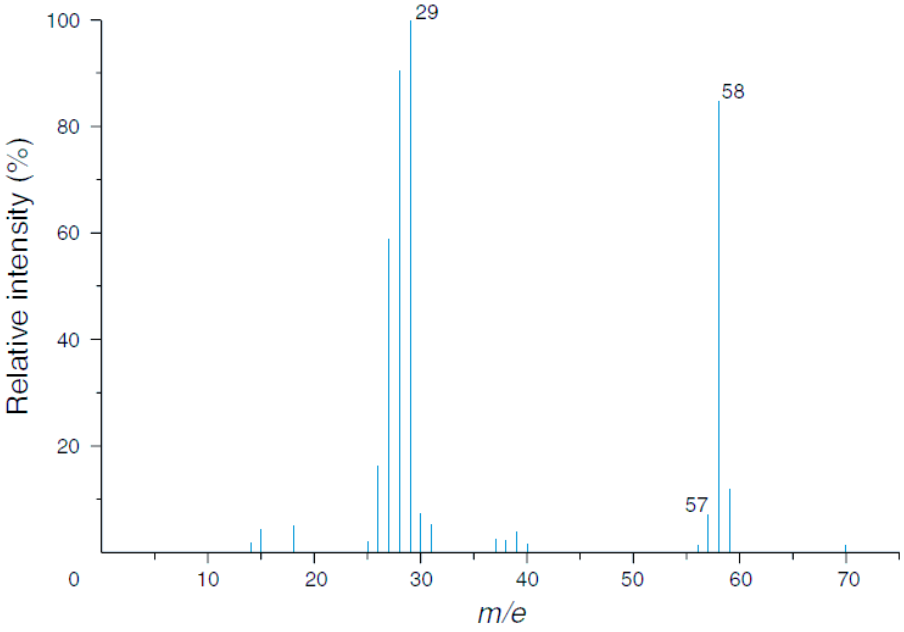
3. (a) Identify the molecular ion peak in the mass spectrum of 2-methylpentane.

(b) Hence, or otherwise, determine the relative molecular mass of 2-methylpentane.

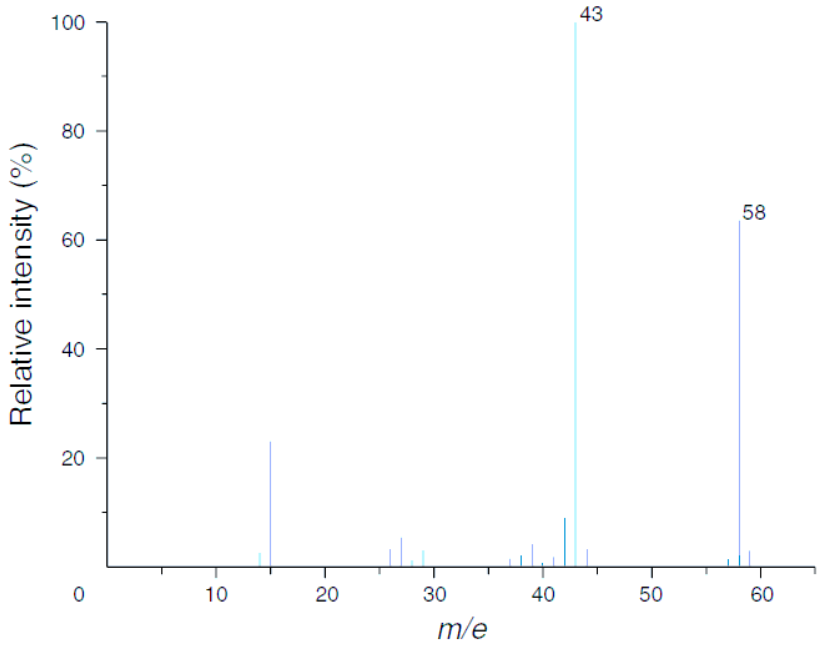
(c) Show the fragmentation patterns that account for the peaks at *m/e* = 71 and *m/e* = 43 in the mass spectrum.



4. The following shows the mass spectra of two isomers: propanal and propanone. Identify the spectrum of each isomer and explain briefly.

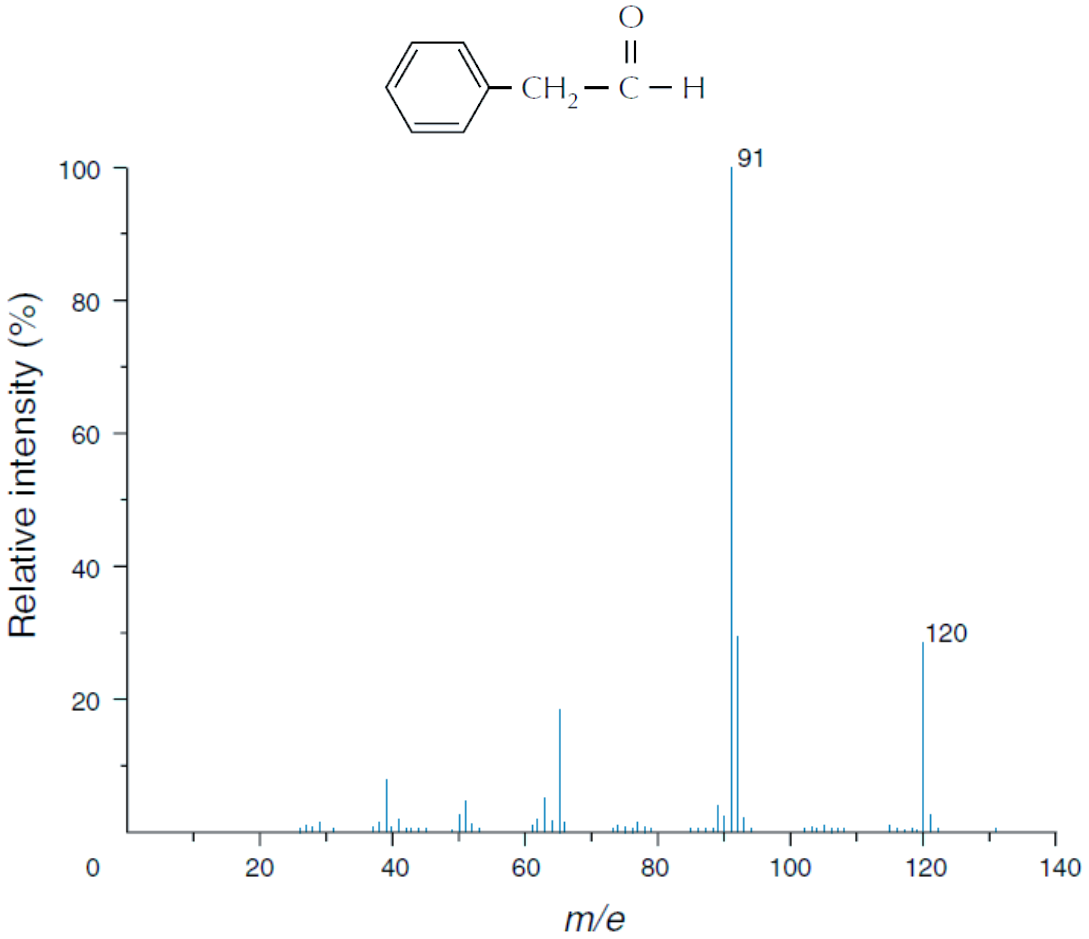


Mass spectrum *P*



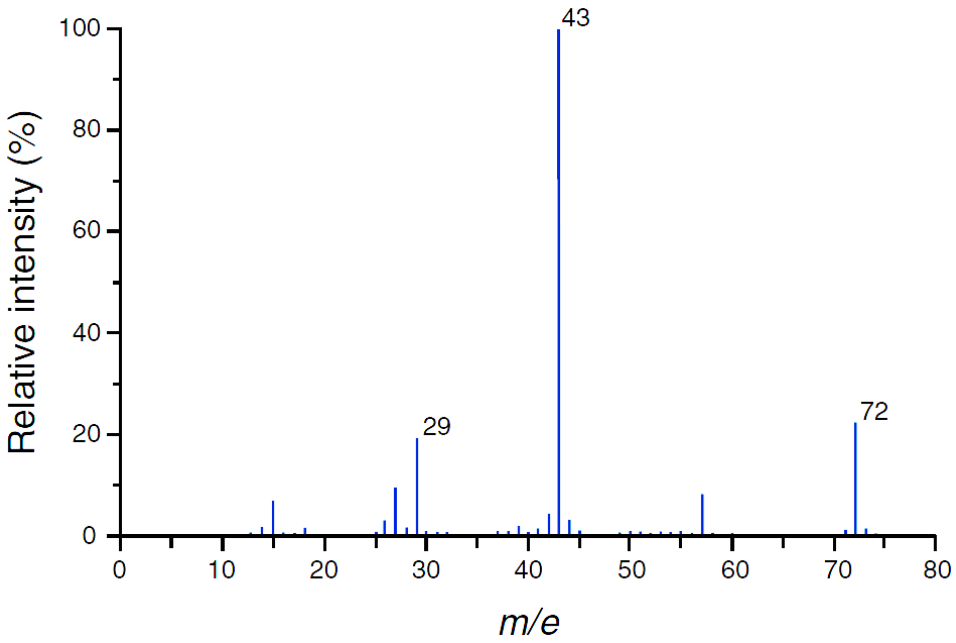
Mass spectrum *Q*

5. The structural formula of a carbon compound and its mass spectrum are shown below:



What ions do the peaks at *m/e* = 120 and 91 represent? Explain your answer briefly.

6. An organic compound *Y* has the following percentage composition by mass: 66.7% carbon, 11.1% hydrogen and 22.2% oxygen. Its mass spectrum is shown below:



It is known that compound *Y* reacts with 2,4-dinitrophenylhydrazine to form an orange precipitate but does not form a silver mirror with Tollens' reagent.
(Relative atomic masses: H = 1.0, C = 12.0, O = 16.0)

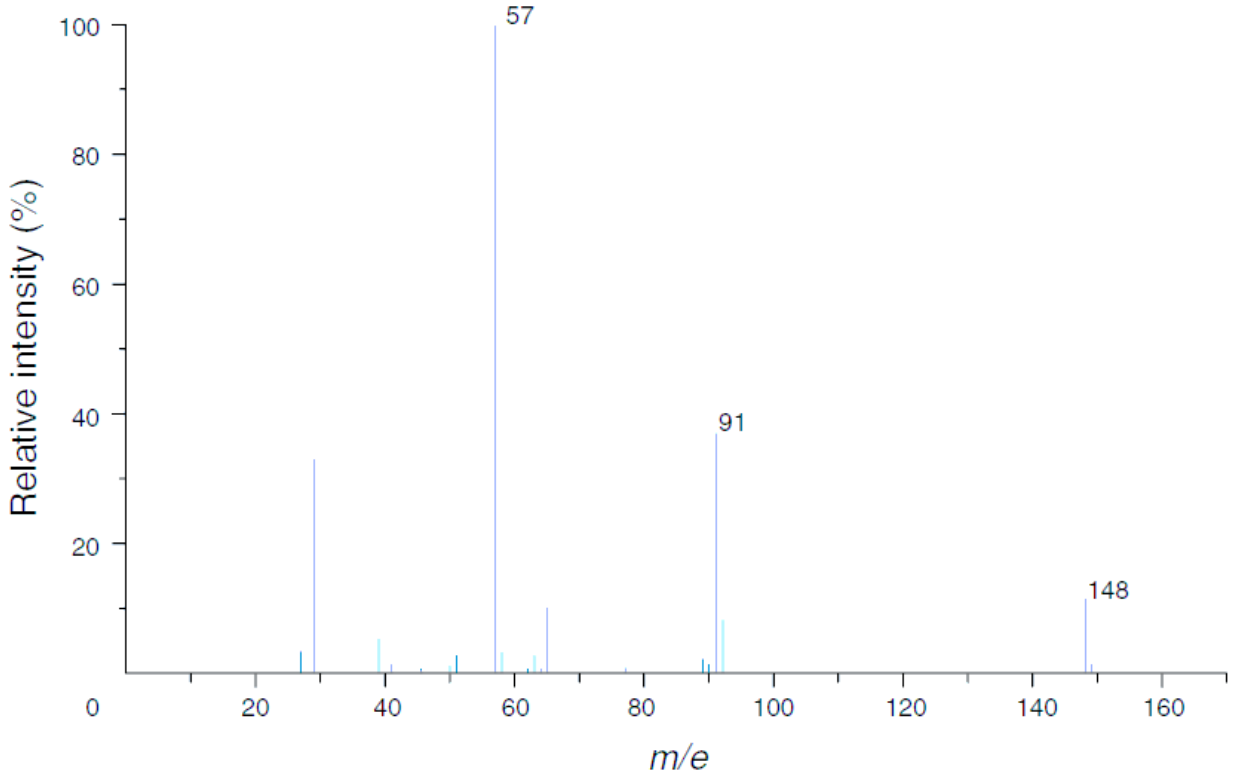
(a) Deduce the empirical formula of compound *Y*.

(b) Deduce the molecular formula of compound *Y* using the information from the mass spectrum.

(c) Suggest one chemical species corresponding to each of the peaks at *m/e* = 43 and *m/e* = 29.

(d) Deduce the possible structure of compound *Y*.

7. A student converts compound *A* ($C_{10}H_{14}O$) to compound *B* ($C_{10}H_{12}O$) by heating compound *A* with acidified potassium dichromate solution.
The mass spectrum of compound *B* is shown below:



It is known that compound *B* reacts with 2,4-dinitrophenylhydrazine to form an orange precipitate.

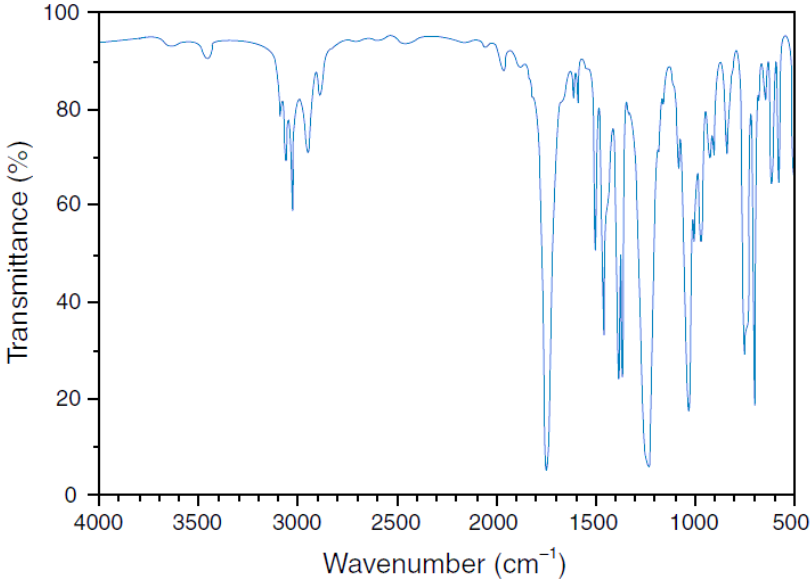
(a) What information could be obtained from the chemical test on compound *B*?

(b) Suggest one chemical species corresponding to each of the peaks at *m/e* = 57 and *m/e* = 91.

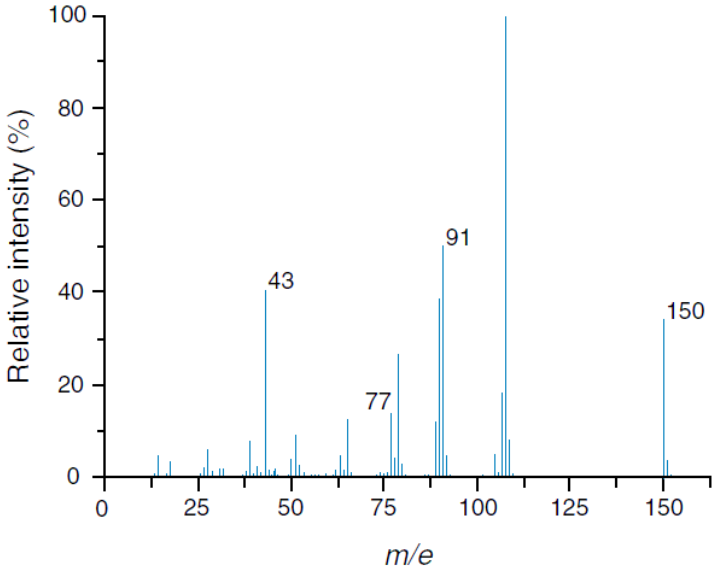
(c) Deduce the possible structure of compound *B*.

8. Compound *A* has a molecular formula of $C_9H_{10}O_2$ and is found naturally in flowers like jasmine. It can also be made by reacting compound *B* (C_7H_8O) with compound *C* ($C_2H_4O_2$) in laboratories. The infrared spectrum and mass spectrum of compound *A* are shown below:

Infrared spectrum



Mass spectrum



(a) From the infrared spectrum, suggest ONE functional group present in compound *A*.

(b) Suggest one chemical species corresponding to each of the peaks at *m/e* = 150, 91 and 43 respectively in the mass spectrum.

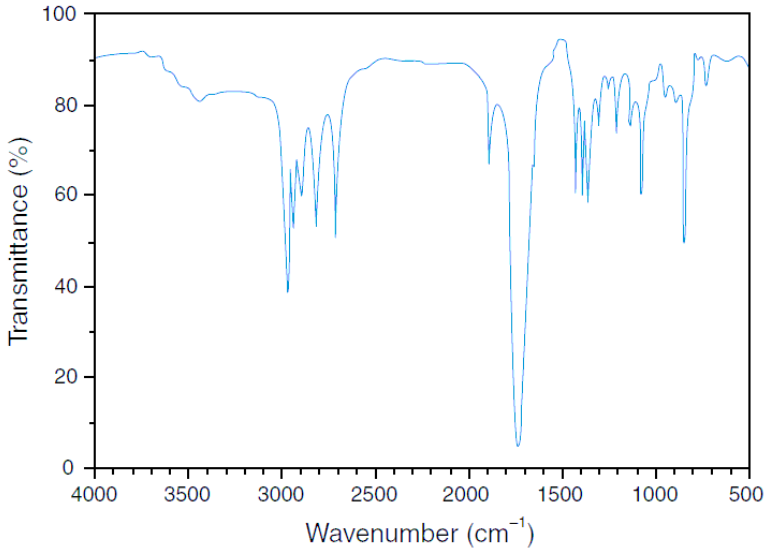
(c) Deduce the possible structure of compound *A*.

(d) Hence, deduce the possible structures of compounds *B* and *C*.

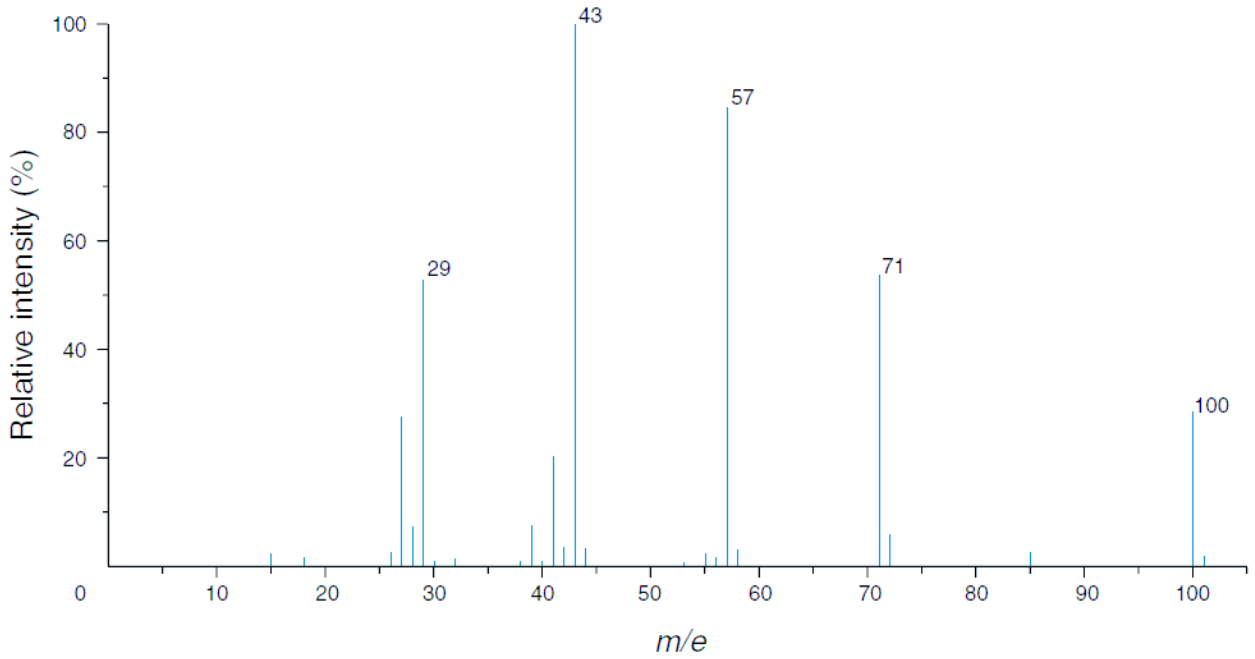
9. An unknown compound *X* has the following composition by mass: 72.0% carbon, 12.0% hydrogen and 16.0% oxygen.
(Relative atomic masses: H = 1.0; C = 12.0; O = 16.0)

The infrared and mass spectra of compound *X* are shown below.

Infrared spectrum



Mass spectrum



(a) Determine the empirical formula of compound *X*.

(b) By analysing the mass spectrum, determine the relative molecular mass of compound *X*.

(c) By analysing both the mass and infrared spectra, determine the possible structure for compound *X*.

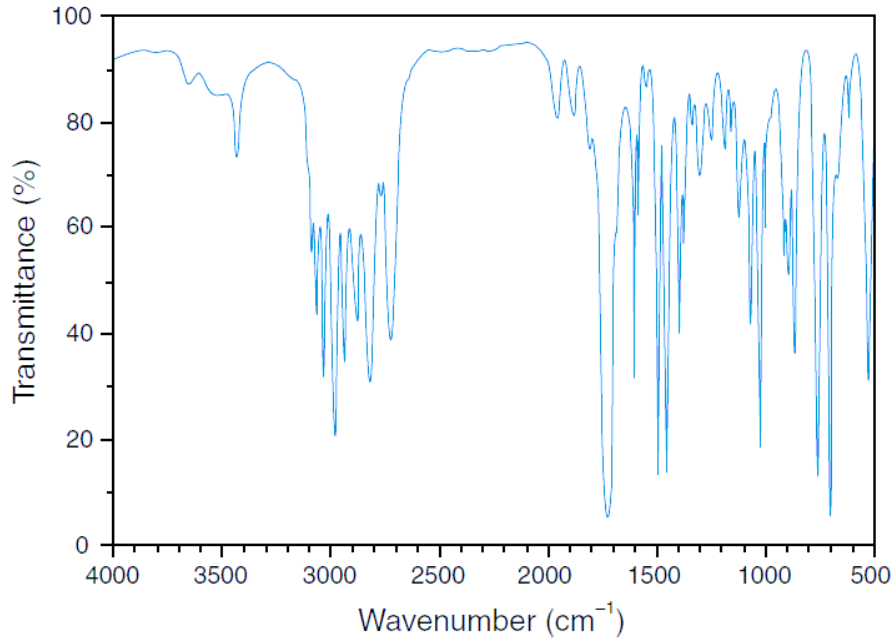
10. Compound *Z* is an aromatic compound with molecular formula of $C_9H_{10}O$. Two chemical tests are performed on compound *Z* and the results are as follows:

    Test (1): Compound *Z* turns acidified potassium dichromate solution from orange to green.

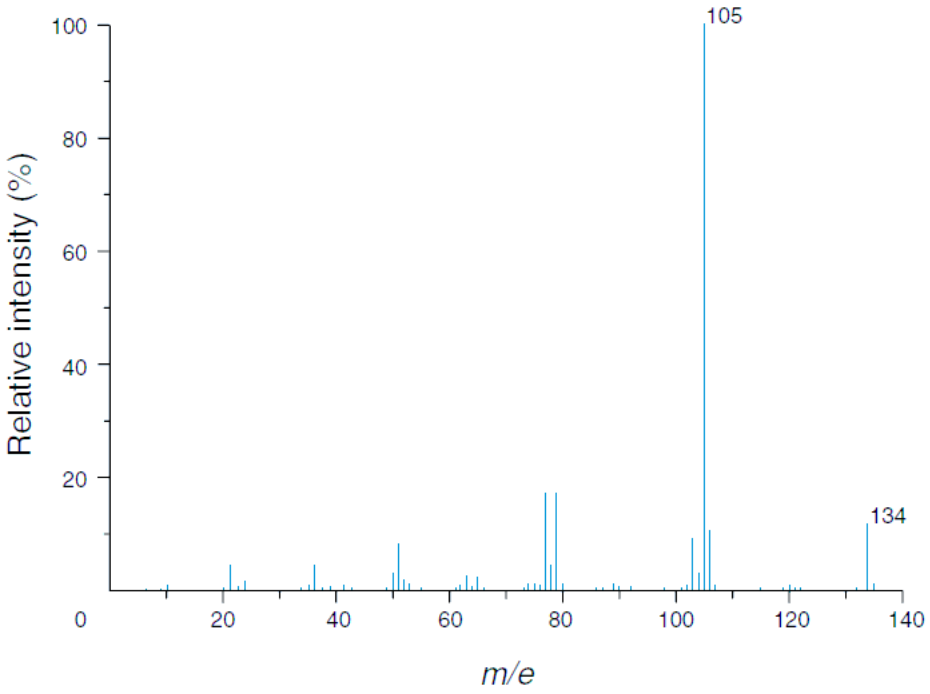
    Test (2): Compound *Z* forms a silver mirror inside the test tube when Tollens' reagent is added.

    The infrared and mass spectra of compound *Z* are shown below:

Infrared spectrum



Mass spectrum



(a) (i) With reference to the result of test (1), suggest the functional group(s) that compound *Z* may contain.

(ii) With reference to the result of test (2), suggest the functional group(s) that compound *Z* may contain.

(b) From the infrared spectrum, suggest ONE functional group present in compound *Z*.

(c) Suggest one chemical species corresponding to each of the peaks at *m/e* = 134 and 105 respectively in the mass spectrum.

(d) Draw a possible structure of compound *Z*.

Suggested Answer

1. (a) The peaks at *m/e* = 52 and *m/e* = 50 are due to the molecular ions $CH_3{}^{37}Cl^+$ and $CH_3{}^{35}Cl^+$ respectively.
The peak at *m/e* = 15 is due to the ion CH_3^+.

   (b) The relative abundance of ^{37}Cl and ^{35}Cl is in the ratio of 1 : 3.

   (c) Relative molecular mass of CH_3Cl
   = relative molecular mass of $CH_3{}^{37}Cl$ × percentage abundance + relative molecular mass of $CH_3{}^{35}Cl$ × percentage abundance
   = 52 × 25% + 50 × 75%
   = 50.5

2. (a) The peaks at *m/e* = 15, *m/e* = 94 and *m/e* = 96 are due to the ions CH_3^+, $CH_3{}^{79}Br^+$ and $CH_3{}^{81}Br^+$ respectively.

   (b) (i) 1 : 1
   (ii) The relative abundance of ^{79}Br and ^{81}Br is in the ratio of 1 : 1.

   (c) Relative molecular mass of CH_3Br
   = 94 x 50% + 96 x 50%
   = 95

3. (a) The molecular ion peak is at *m/e* = 86.

   (b) The relative molecular mass of 2-methylpentane is 86.

   (c) The fragmentation patterns that produce the peaks at *m/e* = 71 and 43 respectively are shown below.

   - The peak at *m/e* = 71 is due to the cation $(CH_3{-}CH_2{-}CH_2{-}\overset{\overset{CH_3}{|}}{C}H^+)$ formed from the molecular ion by stripping off a $-CH_3$ group $(CH_3{-}CH_2{-}CH_2{-}\overset{\overset{CH_3}{|}}{C}H{-}CH_3^+)$.
   - The peak at *m/e* = 43 is due to the cation $(CH_3{-}\overset{\overset{CH_3}{|}}{C}H^+)$ formed from the molecular ion by stripping off a $CH_3{-}CH_2{-}CH_2{-}$ group $(CH_3{-}CH_2{-}CH_2{-}\overset{\overset{CH_3}{|}}{C}H{-}CH_3^+)$.

4. Interpretation of prominent peaks in the mass spectrum P:

m/e	Ion
58	$CH_3CH_2CHO^+$
57	$CH_3CH_2CO^+$
29	$CH_3CH_2^+$ OR CHO^+

The absence of peak at m/e = 43 indicates that no CH_3CO^+ ion forms during fragmentation. Hence, mass spectrum P belongs to propanal.

Interpretation of prominent peaks in the mass spectrum Q:

m/e	Ion
58	$CH_3COCH_3^+$
43	CH_3CO^+

The presence of peak at m/e = 43 corresponds to the CH_3CO^+ ion. Hence, mass spectrum Q belongs to propanone.

5. The peak at m/e = 120 corresponds to the molecular ion $C_6H_5CH_2CHO^+$. The peak at m/e = 91 is due to the cation ($C_6H_5CH_2^+$) formed from the molecular ion by stripping off a —CHO group ($C_6H_5CH_2$—**CHO**$^+$).

6. (a) Let the mass of compound *Y* be 100 g,
Thus, the mass of carbon in the compound = 66.7 g
the mass of hydrogen in the compound = 11.1 g
the mass of oxygen in the compound = 22.2 g

	Carbon	**Hydrogen**	**Oxygen**
Mass (g)	66.7	11.1	22.2
Number of moles (mol)	66.7 / 12.0 = 5.56	11.1 / 1.0 = 11.1	22.2 / 16.0 = 1.39
Mole ratio	5.56 / 1.39 = 4	11.1 / 1.39 = 8	1.39 / 1.39 = 1

$\therefore$ the empirical formula of compound *Y* is C_4H_8O.

(b) From the mass spectrum, the highest *m/e* value occurs at 72. Therefore, the relative molecular mass of compound *Y* is 72. Let the molecular formula of the compound be $(C_4H_8O)_n$.

Relative molecular mass of $(C_4H_8O)_n$ = 72
$n \times (12.0 \times 4 + 1.0 \times 8 + 16.0) = 72$
$\Rightarrow$ n = 1

$\therefore$ the molecular formula of compound *Y* is C_4H_8O.

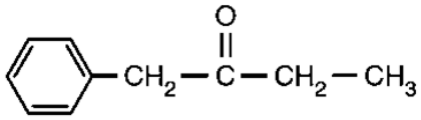
(c) Compound *Y* reacts with 2,4-dinitrophenylhydrazine. It contains carbonyl group C=O.
m/e = 43 suggests the presence of CH_3CO^+.
m/e = 29 suggests the presence of $CH_3CH_2^+$.

(d) Compound *Y* has a molecular formula of C_4H_8O and has a carbonyl group. It should not be an aldehyde because it does not form a silver mirror with Tollens' reagent. Therefore, compound *Y* is a ketone. Its possible structure is:

7. (a) Compound B should contain a carbonyl group.

(b) The peaks at *m/e* = 57 and 91 correspond to the ion $CH_3CH_2CO^+$ and $C_6H_5CH_2^+$ respectively.

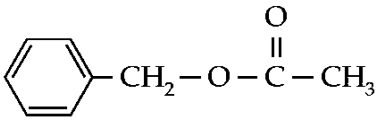
(c) As compound B contains a carbonyl group, it should be an aldehyde or a ketone. Compound B has 10 carbon atoms and it produces fragment ions of $CH_3CH_2CO^+$ and $C_6H_5CH_2^+$ during fragmentation. Therefore, compound B is a ketone. Its possible structure is:



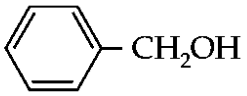
8. (a) The absorption peak at 1700 cm^{-1} corresponds to the presence of C=O bond. Compound *A* contains C=O group.

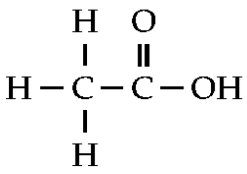
(b) *m/e* = 150 is due to the molecular ion $C_9H_{10}O_2^+$.
m/e = 91 suggests the presence of $C_6H_5CH_2^+$.
m/e = 43 suggests the presence of CH_3CO^+.

(c) The peak at *m/e* = 77 in the mass spectrum shows that compound *A* consists of a benzene ring (*m/e* = 77 for $C_6H_5^+$).
Besides, the absence of broad absorption peak at about 2500–3300 cm–1 in the IR spectrum indicates that the compound does not contain –OH group of carboxylic acid. Hence, compound *A* is not a carboxylic acid. It is likely to be an ester.
Referring to the fragmentation patterns found in the mass spectrum, compound *A* has the possible structure:



(d) Compound *A* is an ester made by the reaction between an alcohol and a carboxylic acid. Therefore, compounds *B* and *C* have the possible structures:

Compound *B*: 

Compound *C*: 

9. (a) Let the mass of compound *X* be 100 g,
Thus, the mass of carbon in the compound = 72.0 g
the mass of hydrogen in the compound = 12.0 g
the mass of oxygen in the compound = 16.0 g

	Carbon	**Hydrogen**	**Oxygen**
Mass (g)	72.0	12.0	16.0
Number of moles (mol)	72.0 / 12.0 = 6	12.0 / 1.0 = 12	16.0 / 16.0 = 1
Mole ratio	6	12	1

$\therefore$ the empirical formula of compound *X* is $C_6H_{12}O$.

(b) From the mass spectrum, the peak at *m/e* = 100 corresponds to the molecular ion. Hence, the relative molecular mass of compound *X* is 100.

(c) Let the molecular formula of compound X be $(C_6H_{12}O)_n$.
$n \times (12.0 \times 6 + 1.0 \times 12 + 16.0) = 100$
$\Rightarrow$ $n = 1$
$\therefore$ the molecular formula of compound *X* is $C_6H_{12}O$.

From the IR spectrum, there is a strong absorption peak at 1750 cm^{-1}. This indicates the presence of the C=O bond. The compound may be hexanal, hexan-2-one or hexan-3-one.

Interpretation of prominent peaks in the mass spectrum:

m/e	Ion
100	$CH_3CH_2CH_2COCH_2CH_3^+$
71	$CH_3CH_2CH_2CO^+$
57	$CH_3CH_2CO^+$

$\therefore$ Compound X is hexan-3-one.

10. (a) (i) The compound should contain a hydroxyl group or an aldehyde group.
(ii) The compound should contain an aldehyde group.

(b) The strong absorption peak at 1720 cm^{-1} corresponds to the presence of C=O bond. Compound Z contains a carbonyl group.

(c) m/e = 134 is due to the molecular ion $C_6H_5CH_2CH_2CHO^+$.
m/e = 105 is due to the fragment ion $C_6H_5CH_2CH_2^+$.

(d)