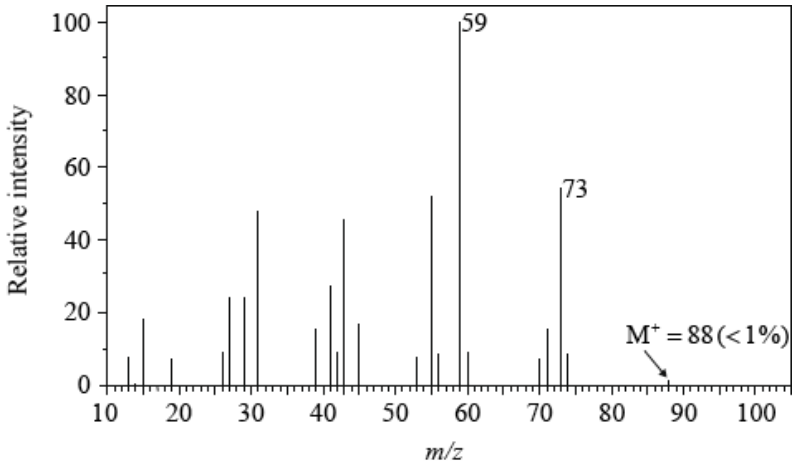
HL Paper 3

Organic compound X is 68.11% carbon, 13.74% hydrogen and 18.15 % oxygen by mass.

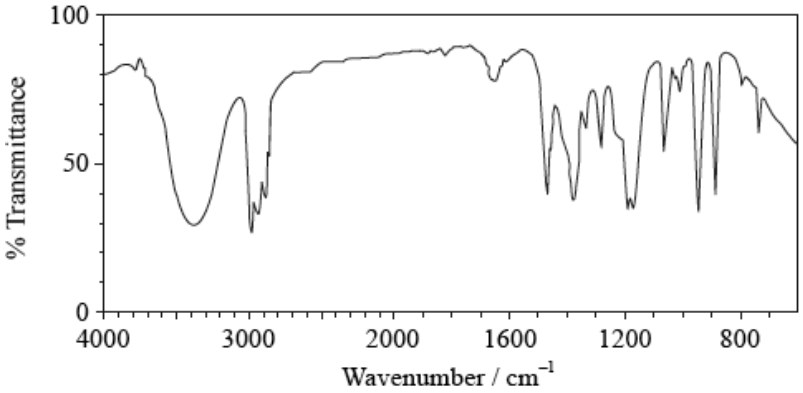
a. Show that the empirical formula of compound **X** is $C_5H_{12}O$. [1]

b. The mass spectrum, infrared spectrum and details of the $^1H\,NMR$ spectrum of compound **X** are given below. [11]

Mass spectrum:



Infrared spectrum:



$^1H\,NMR$ spectrum:

Peak with splitting	Integration trace (area under peak)
Singlet	1
Singlet	6
Triplet	3
Quartet	2

Analyse these three spectra and, using relevant information, deduce the identity of the compound.

Mass spectrum:

Infrared spectrum:

$^1\mathrm{H\ NMR}$ spectrum:

Identity of X:

Markscheme

a.

Element	Amount / mol	Simplest ratio
carbon	$\frac{68.11}{12.01} = 5.671$	5
hydrogen	$\frac{13.74}{1.01} = 13.60$	12
oxygen	$\frac{18.15}{16.00} = 1.134$	1

/ OWTTE;

Accept mass of $C_5H_{12}O$ = 88.17 so % of $C = \left(\frac{60.05}{88.17}\right) \times 100 = 68.11$,

% of $H = \left(\frac{12.12}{88.17}\right) \times 100 = 13.75$ *and % of* $O = \left(\frac{16.00}{88.17}\right) \times 100 = 18.15$.

Allow integer values for atomic masses.

b. *Mass spectrum:*

molecular ion peak at $88/\mathrm{M}^+ = 88$ shows molecular formula is $\mathrm{C_5H_{12}O}$;

absorption at 73 due to $(\mathrm{M–CH_3})^+$ / **X** contains a methyl group as peak at M–15 / *OWTTE*;

absorption at 59 due to $(\mathrm{M–C_2H_5})^+$ / **X** contains an ethyl group as peak at M–29;

Penalise once only if + charge omitted.

*Accept that **X** contains a CHO group due to M–29 but in fact it cannot as there are too many hydrogen atoms in the compound for it to be an aldehyde.*

Infrared spectrum:

peak in range at 3200–3600 cm^{-1} shows it contains an OH group / *OWTTE*;

(sharp) peaks just below $3000\ \mathrm{cm}^{-1}$/in range 2850–3100 cm^{-1} due to C–H

absorptions;

lack of peak at approximately $1700\ \mathrm{cm}^{-1}$ shows it does not contain C=O;

absorption between 1050 and $1410\ \mathrm{cm}^{-1}$ due to C–O;

Allow "due to alcohol" instead of due to C–O.

Accept "absorption between 1050 and 1410 cm^{-1} due to ether or ester" although it cannot be either as there is only one O atom and it has been identified as bonded to H.

fingerprint region specific to compound but needs to be compared with library / *OWTTE*;

^{1}H NMR spectrum:

(12 protons are in) four different chemical environments (in the ratio 1:2:6:3);

singlet (with integration trace of 1) due to OH proton;

singlet (with integration trace of 6) suggests (two $\mathrm{CH_3}$) groups attached to a carbon atom with no Hs attached to it;

quartet (with integration trace of 2) due to $\mathrm{CH_2}$ next to $\mathrm{CH_3}$;

triplet (with integration trace of 3) due to $\mathrm{CH_3}$ next to $\mathrm{CH_2}$;

Reference must be made to the association of the splitting pattern (singlet, triplet etc.) to the specific carbon fragments.

(**X** is) 2-methylbutan-2-ol/$\mathrm{CH_3CH_2C(CH_3)_2OH}$;

No ECF throughout 2(b).

Examiners report

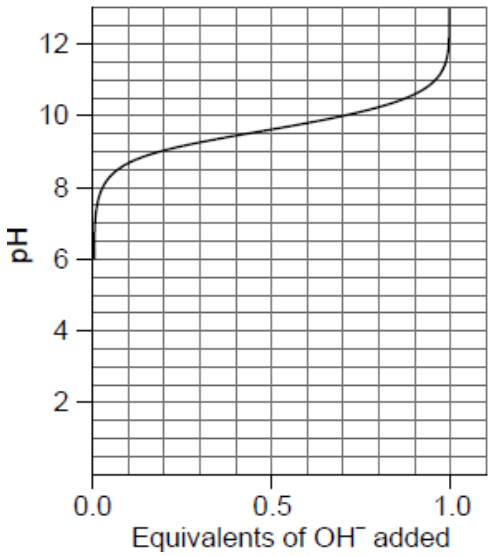
a. The question on empirical formula in (a) posed no difficulty and even the weaker candidates scored the mark. In the spectroscopy question in (b), some of the better candidates managed to score all 11 marks assigned to this extended response type question. In the MS, + was often omitted. Many students could not distinguish between observed ions and lost fragments. Only one candidate mentioned the "fingerprint" region of IR but did not refer to the need to compare with library spectral data. For the IR the majority of candidates scored all three marks, though the weaker candidates frequently suggested NH bonds and CF bonds even though neither nitrogen nor fluorine are part of the empirical formula given in the stem of the question. Discussion of the $^1\mathrm{H\ NMR}$ spectrum proved the most challenging and many candidates did not relate the splitting pattern to the specific carbon fragments. It was disappointing at HL seeing a number of candidates not including hydrogens in their final answer for the structural formula of 2-methylbutan-2-ol.

b. The question on empirical formula in (a) posed no difficulty and even the weaker candidates scored the mark. In the spectroscopy question in (b), some of the better candidates managed to score all 11 marks assigned to this extended response type question. In the MS, + was often omitted. Many students could not distinguish between observed ions and lost fragments. Only one candidate mentioned the "fingerprint" region of IR but did not refer to the need to compare with library spectral data. For the IR the majority of candidates scored all three marks, though the weaker candidates frequently suggested NH bonds and CF bonds even though neither nitrogen nor fluorine are part of the empirical formula given in the

stem of the question. Discussion of the $^1\text{H NMR}$ spectrum proved the most challenging and many candidates did not relate the splitting pattern to the specific carbon fragments. It was disappointing at HL seeing a number of candidates not including hydrogens in their final answer for the structural formula of 2-methylbutan-2-ol.

Analysis of amino acid and protein concentration is a key area of biological research.

The titration curve of aqueous glycine zwitterions with aqueous sodium hydroxide is shown from pH 6.0 to 13.0. Refer to section 33 of the data booklet.



a. Deduce the pH range in which glycine is an effective buffer in basic solution. [1]

b. Enzymes are biological catalysts. [1]

The data shows the effect of substrate concentration, [S], on the rate, *v*, of an enzyme-catalysed reaction.

[S] / mmol dm^{-3}	*v* / mmol dm^{-3} min^{-1}
0.0	0.00
0.67	0.40
1.5	0.60
2.0	0.68
4.0	0.78
6.0	0.80
8.0	0.80
10.0	0.80

Determine the value of the Michaelis constant (K_m) from the data. A graph is not required.

c. Outline the action of a non-competitive inhibitor on the enzyme-catalysed reaction. [2]

d. The sequence of nitrogenous bases in DNA determines hereditary characteristics. [2]

Calculate the mole percentages of cytosine, guanine and thymine in a double helical DNA structure if it contains 17% adenine by mole.

Cytosine:

. . . . . .

. . . . . .

Guanine:

. . . . . .

. . . . . .

Thymine:

. . . . . .

. . . . . .

Markscheme

a. «pH range» 8.6–10.6

Accept any value between 8.2 and 11.0.

[1 mark]

b. «K_m =» 0.67 «mmol dm^{-3}»

Do not penalize if a graph is drawn to determine the value.

[1 mark]

c. does not compete for active site

OR

binds to allosteric site/away from «enzyme» active site

OR

alters shape of enzyme

reduces rate/V_{max}

[2 marks]

d. «% cytosine + % guanine = 100% – 17% – 17% = 66%»

Cytosine: 33 «%» ***AND*** Guanine: 33 «%»

Thymine: 17 «%»

[2 marks]

Examiners report

a. [N/A]
[N/A]

b. [N/A]
d. [N/A]