Empirical Formula

1. The manufacturer of the soft drink referred to in question 39 also produces a diet version of the drink, containing artificial sweetener. The quality assurance procedures of the soft drink manufacturer require that incoming batches of the artificial sweetener be analysed to ensure compliance with standards. A combustion analysis of a 1.021 g sample of sweetener produced 1.715 g CO2, 0.2521 g H2O, 0.2558 g NO2 and 0.3568 g SO2. The sweetener contains the elements C, H, O, N and S. Determine its empirical formula.

The manufacturer of the soft drink referred to in question 39 also produces a diet version of the drink, containing artificial sweetener. The quality assurance procedures of the soft drink manufacturer require that incoming batches of the artificial sweetener be analysed to ensure compliance with standards. A combustion analysis of a 1.021 g sample of sweetener produced 1.715 g CO_2, 0.2521 g H_2O, 0.2558 g NO_2 and 0.3568 g SO_2. The sweetener contains the elements C, H, O, N and S. Determine its empirical formula.

$$n(C) = n(CO_2) = \frac{1.715\text{g}}{44.01\text{ g mol}^{-1}} = 3.8968\times10^{-2}\text{ mol}$$

$$n(H) = 2\times n(H_2O) = 2\times\frac{0.2521\text{ g}}{18.016\text{ g mol}^{-1}} = 2.799\times10^{-2}\text{ mol}$$

$$n(N) = n(NO_2) = \frac{0.2558\text{g}}{46.01\text{ g mol}^{-1}} = 5.5597\times10^{-3}\text{ mol}$$

$$n(S) = n(SO_2)\ \frac{0.3568\text{g}}{64.06\text{ g mol}^{-1}} = 5.5698\times10^{-3}\text{ mol}$$

$m(C) = 4.680 \times 10^{-1}$ g

$m(H) = 2.821 \times 10^{-2}$ g

$m(N) = 7.7891 \times 10^{-2}$ g

$m(S) = 1.786 \times 10^{-1}$ g

$m(O) = 1.021 - (4.680\times10^{-1} + 2.821\times10^{-2} + 7.7891\times10^{-2} + 1.786\times10^{-1})\text{ g} = 0.2685\text{ g}$

$$n(O) = \frac{0.2685\text{ g}}{16.00\text{ g mol}^{-1}} = 1.6781\times10^{-2}\text{ mol}$$

Element	C	H	O	N	S
No. mol	3.868×10^{-2}	2.799×10^{-2}	1.6787×10^{-2}	5.560×10^{-3}	5.574×10^{-3}
Mole ratio	$\frac{3.868\times10^{-2}}{5.560\times10^{-3}}$	$\frac{2.799\times10^{-2}}{5.560\times10^{-3}}$	$\frac{1.6781\times10^{-2}}{5.560\times10^{-3}}$	$\frac{5.560\times10^{-3}}{5.560\times10^{-3}}$	$\frac{5.574\times10^{-3}}{5.560\times10^{-3}}$
	6.99	5.02	3.01	0.997	1
Round	7	5	3	1	1

Empirical formula is $C_7H_5O_3NS$

Fast mark

Description	Marks
Empirical formula = $C_7H_5O_3NS$ Full marks for any valid method of determining the empirical formula.	13
Question incorrectly answered or not attempted.	0
Total	**13**

Part mark

Description	Cumulative marks
1 mark each for number of moles of C (**3.868×10^{-2}**), H (**2.799×10^{-2}**), N (**5.560×10^{-3}**) and S (**5.574×10^{-3}**);	1-4
1 mark each for mass of C (**4.680×10^{-1} g**), H (**2.821×10^{-2} g**), N (**7.7891×10^{-2} g**), S (**1.786×10^{-1} g**) and O (**2.6846×10^{-1} g**);	5-9
1 mark for n(O) = **1.6787×10^{-2}**	10
1 mark for ratio	11
1 mark for rounding	12
1 mark for empirical formula	13
Total	**13**

2. Sevoflurane is a gaseous compound (at room temperature) used for inducing and maintaining general anaesthesia. It contains carbon, hydrogen, oxygen and fluorine. Analysis of a 1.6328 g sample of sevoflurane yielded, on combustion, 866.0 mL of carbon dioxide at 50°C and 101.3 kPa and 0.220 g of water. The fluorine was released as hydrogen fluoride and absorbed by alkaline solution, revealing 5.71 × 10–2 mole of hydrogen fluoride. Determine the empirical formula of sevoflurane

Description	Marks
$n(C) = n(CO_2) = \frac{PV}{RT} = \frac{101.3 \times 0.866}{8.315 \times 323} = 3.266 \times 10^{-2}\,mol$	1
$m(C) = 12.01 \times 3.266 \times 10^{-2} = 0.3923\ g$	1
$n(H) = 2 \times n(H_2O) = 2 \times \frac{0.220}{18.016} = 2.44 \times 10^{-2}\,mol$	1
$m(H) = 1.008 \times 2.44 \times 10^{-2} = 2.462 \times 10^{-2}\ g$	1
$m(F) = 19.00 \times 5.71 \times 10^{-2} = 1.085\ g$	1
$m(O) = 1.6328 - (0.3923 + 2.462 \times 10^{-2} + 1.085) = 0.13099\ g$	1
$n(O) = \frac{0.13099}{16.00} = 8.187 \times 10^{-3}\,mol$	1
÷ by smallest: C: $\frac{0.03266}{0.008187} = 3.99 = 4$; H: $\frac{0.0244}{0.008187} = 2.98 = 3$; O: $\frac{0.008187}{0.008187} = 1 = 1$; F: $\frac{0.0571}{0.008187} = 6.97 = 7$ 1 mark for ÷ by smallest; 1 mark for rounding	1–2
Thus EF is $C_4H_3OF_7$	1
Question incorrectly answered	0
Question not attempted	–
Total	**10**

N.B.: Any appropriate logic leading to the correct answer is acceptable.
N.B.: $C_7H_{18}OF_{12}$ = rounding error (9 marks)
If reasonable attempt to produce whole numbers from EF developed from H from water and HF then full marks

3. Qualitative analysis of an organic compound showed that it contained carbon, hydrogen and oxygen only. A quantitative study of the same compound was performed, in which a 0.5096 g sample was burnt in excess oxygen to produce 0.4160 g of water and 700.7 mL of carbon dioxide, collected at 100.0°C and 102.8 kPa.
   (a) Determine the empirical formula of the compound
   (b) A second 0.4832 g sample of the compound was heated to 261°C. The vaporised sample was found to exert a pressure of 241 kPa in a 100.0 mL container. Use this information to determine the molecular formula of the compound. (4 marks)
   (c) When the compound was reacted with acidified ethanol it produced a fruity smelling liquid. Infer the structure of the original compound, and draw its structure in the box below. Name the original compound
   (d) Describe briefly and give observations for an additional chemical test to confirm the identity of the functional group in the original compound. (2 marks)

(a) Determine the empirical formula of the compound. (10 marks)

Description	Marks
$n(C)=n(CO_2)=\frac{PV}{RT}=\frac{102.8\times0.7007}{8.314\times373.15}=2.3218\times10^{-2}\text{mol}$	1
$m(C) = 12.01 \times 2.3216 \times 10^{-2} = 0.27885$ g	1
$n(H_2O) = \frac{0.416}{18.016} = 2.3090586 \times 10^{-2}\text{mol}$	1
$n(H) = 2 \times 2.3090586 \times 10^{-2} = 4.6181 \times 10^{-2}$ mol	1
$m(H) = 1.008 \times 4.6181 \times 10^{-2} = 4.655 \times 10^{-2}$ g	1
$m(O) = 0.5096 - (0.27885 + 4.655 \times 10^{-2}) = 0.18423$ g	1
$n(O) = \frac{0.18423}{16.00} = 1.1514 \times 10^{-2}\text{mol}$	1
C H O 0.02319 0.04618 0.011514 ÷ by smallest $\frac{0.02319}{0.011514}$ $\frac{0.04618}{0.011514}$ 1.000 2.014 4.011 1.000 2 4 1 1 mark for ÷ by smallest; 1 mark for rounding	1–2
Thus EF is C_2H_4O	1
Total	**10**

Note:
If students don't multiply H × 2
Ratio 1.79 1.79 1
EF is C_2H_2O 8 marks
$C_9H_9O_5$ 9 marks

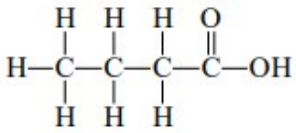
If students divide H by 2
EF is $C_7H_6O_5$ 9 marks
$C_4H_2O_5$ 9 marks

(b) A second 0.4832 g sample of the compound was heated to 261°C. The vaporised sample was found to exert a pressure of 241 kPa in a 100.0 mL container. Use this information to determine the molecular formula of the compound. (4 marks)

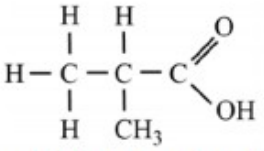
Description	Marks
$n(\text{sample}) = \frac{PV}{RT} = \frac{241 \times 0.100}{8.314 \times 534.15} = 5.4268 \times 10^{-3}\,\text{mol}$	1
$m(\text{sample}) = \frac{m}{n} = \frac{0.4832}{5.4268 \times 10^{-3}} = 89.04\,\text{gmol}^{-1}$	1
Since Empirical formula mass = 44.052 Then MF is 2 × EF = $C_4H_8O_2$	1 1
Total	**4**

Note: If E.F. is incorrect max 3 marks.

(c) When the compound was reacted with acidified ethanol it produced a fruity smelling liquid. Infer the structure of the original compound, and draw its structure in the box below. Name the original compound. (2 marks)



butanoic acid



methylpropanoic acid

Description	Marks
Correct structure	1
Correct name	1
Total	**2**

Note: Award one mark for correct name for incorrect structure, or incorrect name for correct structure. Must be carboxylic acid structure.

(d) Describe briefly and give observations for an additional chemical test to confirm the identity of the functional group in the original compound. (2 marks)

e.g. Test: reaction with a carbonate or Mg or Na
Observation: effervescence

Description	Marks
Any correct chemical test. e.g. react with acid suitable indicator that changes colour at appropriate pH (e.g. Universal Indicator, but not phenolphthalein)	1
Any correct observation	1
Total	**2**

Note: addiction of MnO_4^- and 'no reaction', is not acceptable

4. (a) A white solid is analysed and found to have the empirical formula CHO and a molar mass of 116 g mol−1
(b) Two tests were conducted on the solid, as shown in the table below. Complete the table by drawing a possible functional group that is consistent with the finding of each of the tests. (2 marks)
(c) A further 2.32 g sample of the white solid was analysed and shown to release 0.0400 mol of H+ ions. Use this information and your answers to (a) and (b) to determine the structural formula of the white solid, and draw it in the box below. Show all atoms in your structure.

(a) Determine the molecular formula of the compound. Justify your answer. (2 marks)

Empirical mass = 12.01 + 1.008 + 16.00 = 29.018 g

$$\frac{\text{Molar mass}}{\text{Empirical mass}} = \frac{116}{29.018} \cong 4$$

Thus molecular formula is $C_4H_4O_4$

Description	Marks
Ratio of molar mass to empirical mass	1
Molecular formula	1
Total	**2**

(b)

Test	Observation	Possible functional group
Water solubility	788 g L^{-1}	Diagram of alcohol or carboxylic acid (R)—OH **or** (R)—C(=O)OH
Add to bromine water	Bromine water decolourises rapidly	Diagram of alkene or alkyne C=C **or** —C≡C—

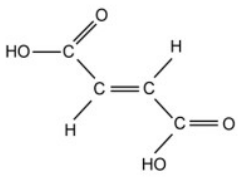
Description	Marks
1 for each functional group correctly drawn	1–2
Total	**2**

(c) A further 2.32 g sample of the white solid was analysed and shown to release 0.0400 mol of H^+ ions. Use this information and your answers to (a) and (b) to determine the structural formula of the white solid, and draw it in the box below. Show **all** atoms in your structure.

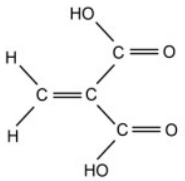
(3 marks)

$$n(X) = \frac{2.32}{116} = 0.0200 \text{ mol}$$

n(x) : $n(H^+)$ = 1:2, thus the substance is a diprotic acid



cis or *trans* acceptable.



also acceptable

Description	Marks
moles of X = 0.0200 mol	1
Recognition that X is diprotic	1
Structure of X with all atoms shown	1
Total	**3**