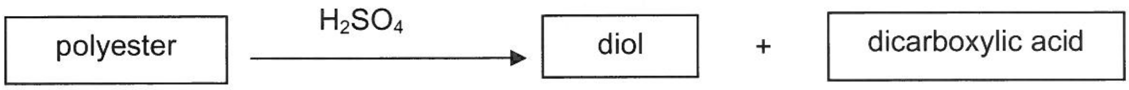
Chapter 14A Calculations: Organic

1. **[11 marks]** *(2009:03)*

A polyester polymer was analysed to determine its empirical formula. Combustion of a 9.76 g sample of the polyester in excess oxygen produced 17.9 g of carbon dioxide and 4.88 g of water.

(a) Calculate the empirical formula of the polyester.

The polymer was then hydrolysed using sulfuric acid to split it into the diol and dicarboxylic acid monomers used in its preparation. The flow diagram below illustrates this.



2.20 g of the dicarboxylic acid monomer was isolated and dissolved in 250.0 mL of distilled water. 50.0 mL of the diacid solution required 15.3 mL of 0.487 mol L^{-1} sodium hydroxide solution for complete neutralisation.

(b) Calculate the molar mass of the dicarboxylic acid monomer.

(c) Draw a possible structure of the dicarboxylic acid that is consistent with your answer to part (b).

2. **[13 marks]** *(2010:40)*

A manufacturer of soft drink produces a diet version 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.

3. [10 marks] *(2011:36)*

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.

4. [18 marks] *(2012:39)*

Qualitative analysis of an organic compound showed that it contained only carbon, hydrogen and oxygen. 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. [10]

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(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]

(c) When the original 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]

Name: ______________________________

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

5. **[7 marks]** *(2013:35)*

A white solid is analysed and found to have the empirical formula CHO and a molar mass of 116 g mol^{-1}.

(a) Determine the molecular formula of the compound. Justify your answer. *4.9* [2]

(b) Two tests were conducted on the white 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. *4.3* [2]

Test	**Observation**	**Possible functional group**
Water solubility	788 g L^{-1}	
Add to bromine water	Bromine water decolourises rapidly	

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(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. *4.9* [3]

6. **[14 marks]** *(2014:39)*

An organic compound that contains only carbon, hydrogen, oxygen and bromine was analysed to determine its empirical formula. A combustion analysis of 1.50 g of the compound produced 1.58 g of carbon dioxide and 0.563 g water.

On treatment of 1.75 g of the compound to convert the bromine in the compound to bromide ions and further reaction with silver nitrate, 1.97 g of silver bromide was precipitated.

(a) Determine the empirical formula of the compound. [10]

CONTINUED NEXT PAGE

(b) 1.95 g of the compound was vaporised and was found to occupy 0.387 L at 95.0 kPa and 105°C. Determine the molecular formula of the compound. [2]

(c) Further analysis of the organic compound revealed that it had a carboxylic acid functional group. Draw a possible structural formula of the organic compound. [2]

7. [14 marks] *4.9 (2016:38)*

A hydrolysis reaction is one that involves water being consumed as a reactant. Hydrolysis reactions can be represented by the following general equation.

$$A-B + H_2O \rightarrow A-OH + H-B$$

Many processes within the human body involve hydrolysis reactions. These hydrolysis reactions usually require a catalyst; in living organisms that catalyst is an enzyme.

(a) What type of organic compound is an enzyme? [1]

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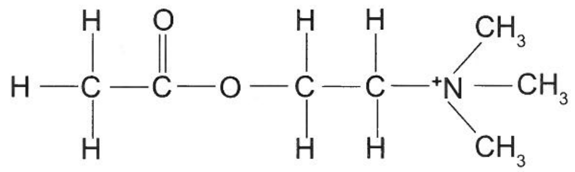
Acetylcholinesterase is an enzyme that is used in the hydrolysis of acetylcholine, a neurotransmitter in the brain.

The structure of acetylcholine is drawn below.



(b) Two products are formed when acetylcholine undergoes hydrolysis in the presence of the enzyme acetylcholinesterase; one of these is a charged molecule called choline and the other is a carboxylic acid. Draw structures of these **two** products. [2]

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A catalyst is said to be **active** if it is working to form the desired products. To ensure the acetylcholinesterase is **active** and so catalysing the hydrolysis of acetylcholine, the charged compound found in the reacting vessel is separated and analysed using a combustion reaction to determine its empirical formula.

A 4.270 g sample was combusted in the presence of pure oxygen until no solid remained. 9.020 g of carbon dioxide, 5.169 g of water and 1.886 g of nitrogen dioxide were produced.

(c) Calculate the empirical formula of the combusted sample. [9]

(d) Use your calculated empirical formula to demonstrate that the enzyme is **active**. [2]

c) Calculation of the average titre of NaOH solution:

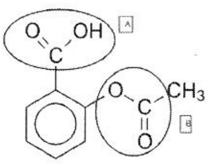
Final volume (mL)	25.30	23.55	22.40	22.25
Initial volume (mL)	3.50	2.70	1.50	1.30
Titre (mL)	21.80	20.85	20.90	20.95

Discarding the first titre of 21.80 mL, the average titre of NaOH = **20.90 mL**

d) Determining the percentage composition of citric acid by mass.
Volume of the cleaner liquid taken = 10.0 mL
Volume of the stock solution made by dilution = 100.0 mL
Volume of the aliquot used for titration = 20.0 mL
Citric acid is a triprotic acid. This means that one mole of citric acid requires 3 mols of NaOH for complete neutralisation.
n (NaOH) = (c × v) = (0.0916 mol L^{-1} × 0.02090 L) = 1.91444 × 10^{-3} mol
Therefore n (citric acid in 20.0 ml dilute) = (1.91444 × 10^{-3} ÷ 3) = 6.3815 × 10^{-4} mol
Therefore, 100.0 mL dilute stock solution contains
= [(6.3815 × 10^{-4} ÷ 20) × 100] = 3.19073 × 10^{-3} mol of citric acid.
Therefore, the mass of citric acid in 10.0 mL of the original solution = (n × M) = 3.19073 × 10^{-3} × 192.184) = 0.6130 g
Therefore, the mass of citric acid in the original undiluted solution is 0.6130 g.
Since the mass of the 10.0 mL of the original solution is 10.4 g,
% by mass of citric acid in the cleaner = [(0.6130 ÷ 10.4) × 100] = **5.89%**

e) Since citric acid is a weak acid and NaOH is a strong base, the equivalence point occurs on the basic side of the pH scale which is between 8 and 10. The hydrolysis of citrate ion will produce OH^- ions according to the equation, $C_6H_5O_7^{3-}(aq)$ + 3 $H_2O(\ell)$ → $C_6H_8O_7(aq)$ + 3 $OH^-(aq)$. The most suitable indicator from the given list is 'thymol blue' (pH = 8.00 to 9.6).

6.(2015:36) a) i)



ii) Group A: carboxylic acid, Group B: ester
b) i) At the equivalence point the Na^+ and $C\ell^-$ ions are neutral. The carboxylate ions react with water to form the carboxylic acid and hydroxide ions

$RCOO^-(aq) + H_2O(\ell) \rightarrow RCOOH(aq) + OH^-(aq)$

The basic solution means that it is necessary to use an indicator that changes colour higher than 7.
ii) $n(H^+)$ = cv = 0.125 × 0.01789 = 2.236 × 10^{-3} mol
$n(OH^-)_{excess}$ in 20 mL = $n(H^+)$ = 2.236 × 10^{-3} mol
$n(OH^-)_{excess}$ in 100 mL = 2.236 x 10^{-3} × 5 = 1.118 × 10^{-2} mol
$n(OH^-)_{initially}$ in 100 mL = cv = 0.204 × 0.1 = 0.0204 mol
$n(OH^-)_{reacting\ with\ aspirin}$ = 0.0204 – 0.01118 = 0.00921 or 9.21 × 10^{-3}mol
iii) $n_{(aspirin)}$ = ½ $n(OH^-)$ = ½ × 0.00921 = 0.00461 mol
$m_{(aspirin)}$ = 0.00461 × 180.154 = 0.8304 g
$m_{(aspirin)}$ in 1 tablet = 0.8304 ÷ 3 = 0.2768 g
% aspirin in 1 tablet = 0.2768/0.3 × 100 = 92.3%
c)

	Description	
Washing procedure	**Effect on the volume of hydrochloric acid used**	**Effect on the % of aspirin calculated**
The conical flask was washed with distilled water	No effect	No effect
The burette was washed with distilled water	Increase	decrease

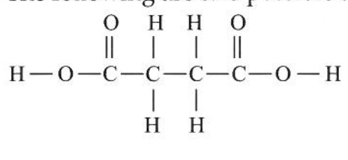
Chapter 14A: Calculations: Organic

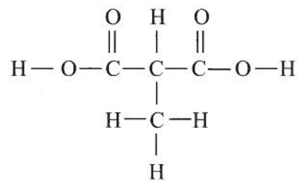
1.(2009:03) a) Calculating the empirical formula:
mass of the sample = 9.76 g; mass of carbon dioxide = 17.9 g; mass of water = 4.88 g.
m (C) = [17.9 × (12.01 ÷ 44.01)] = 4.88 g.
m (H) = [4.88 × (2.016 ÷ 18.016)] = 0.546 g.
Therefore m (O) = [9.76 – (4.88 + 0.546)] = 4.33 g.

	C	H	O
Mass ratio (g)	4.88	0.546	4.38
Mole ratio	4.88 ÷ 12.01	0.546 ÷ 1.008	4.33 ÷ 16.00
	0.406	0.542	0.271
Simple ratio	0.406 ÷ 0.271	0.542 ÷ 0.271	0.271 ÷ 0.271
Simple ratio	1.5	2.00	1.00
Empirical ratio	3	4	2

Therefore the empirical formula is **$C_3H_4O_2$**

b) Calculating the molar mass of the dicarboxylic acid monomer:
n (NaOH) = c × v = 0.487 × 0.0153 = 7.451 × 10^{-3} mol
n (acid) in 0.050 L =($\frac{1}{2}$ × 7.451 × 10^{-3} mol) = 3.725 × 10^{-3} mol
n (acid) in 0.250 L = [3.725 × 10^{-3} × (0.250 ÷ 0.050)] = 1.863 × 10^{-2} mol
Therefore the molar mass of the acid = (m ÷ n) = (2.20 ÷ 1.863 × 10^{-2}) = **118.1 g mol^{-1}**
c) A possible structure for the dicarboxylic acid:
The monomer has four oxygen atoms as it has two 'COOH' groups in it. Taking away the mass of the four oxygen atoms from the molar mass of 118, the residual mass is (118 – 64) 54 which is shared by 4 carbon atoms and 6 hydrogen atoms. This gives a molecular formula of $C_4H_6O_4$.
The following are two possible structures:





2.(2010:40)

m (sample sweetener) = 1.021 g; m (CO_2) = 1.715 g, m (H_2O) = 0.2521 g; m (NO_2) = 0.2558 g; m (SO_2) = 0.3568 g

m (C) = [1.715 × (12.01 ÷ 44.01)] = 0.4680 g
Therefore, n (C) = (0.4680 ÷ 12.01) = *0.03897*

m (H) = [0.2521 × (2.016 ÷ 18.016)] = 0.02821 g
Therefore, n (H) = (0.02821 ÷ 1.008) = *0.02799*

m (N) = [0.2558 × (14.01 ÷ 46.01)] = 0.07789 g
Therefore, n (N) = (0.07789 ÷ 14.01) = *0.00556*

m (S) = [(0.3568 × (32.06 ÷ 64.06)] = 0.17857 g
Therefore, n (S) = (0.17857 ÷ 32.06) = *0.00557*

Therefore, m (O) = [1.021 – (0.4680 + 0.02821 + 0.07789 + 0.17857)] = 0.2683 g
n (O) = (0.2683 ÷ 16.0) = *0.01677*

	C	H	N	S	O
Mole ratio	0.03897	0.02799	0.00556	0.00557	0.01677
Dividing each by the smallest mole of 0.00556					
Simple ratio	6.959	4.998	1.000	1.002	3.016
	7	5	1	1	3

Therefore, the empirical formula is **$C_7H_5NSO_3$**

3.(2011:36) This is an empirical-molecular formula calculation in which gas volume calculation steps are involved. The compound contains carbon, hydrogen, oxygen and fluorine.

m (sample) = 1.6328 g.
The volume of CO_2 produced at 50°C and 101.3 kPa = 0.866 L.
Since, PV = nRT, n = (PV ÷ RT),
n = [(101.3 × 0.866) ÷ (8.315 × 323)] = 0.03266 mol
Therefore, n (C) = **0.03266 mol** and, m (C) = n × M = 0.03266 × 12.01 = **0.3923 g**

m (H_2O) = 0.220 g; n (H_2O) = (0.220 ÷ 18.016) = 0.0122 mol
Therefore, n (H) = 2 × 0.0122 = **0.02442 mol** and, m (H) = 0.02442 × 1.008 = **0.02462 g**

n (HF) = 0.0571 mol
Therefore, n (F) = **0.0571 mol** and, m (F) = 0.0571 × 19.00 = **1.0849 g**

m (O) = [1.638 –(0.3923 + 0.02462 + 1.0849)] = **0.131 g**
Therefore, n (O) = (0.131 ÷ 16.0) = **0.008188 mol**

	C	H	O	F
Mass ratio	0.3923	0.02462	0.131	1.0849
Mole ratio	0.03266	0.0244	0.008188	0.0571
Simple ratio	÷ 0.008188	÷ 0.008188	÷ 0.008188	÷ 0.008188
	3.989	2.98	1	6.97
Whole No. ratio	4	3	1	7

Empirical Formula = $\mathbf{C_4H_3OF_7}$

Alternative Method using the percentage composition

% C = [(0.0923 ÷ 1.6328) × 100] = 24.03%; Mol ratio = (24.03 ÷ 12.01) = 2.00
% H = [(0.02462 ÷ 1.632) × 100] = 1.51%; Mol ratio = (1.51 ÷ 1.008) = 1.50
% O = [(0.131 ÷ 1.632) × 100] = 8.03%; Mol ratio = (8.03 ÷ 16.00) = 0.50
% F = [(1.0849 ÷ 1.632) × 100] = 66.48%; Mol ratio = (66.48 ÷ 19.00) = 3.5

Fractional mole ratio of the elements in the compound: C = 2.00, H = 1.50; O = 0.50 and F = 3.5
Multiplying this ratio throughout by 2, in order to get whole numbers,
we get the empirical formula: $\mathbf{C_4H_3OF_7}$

4.(2012:39)

a) The compound contains carbon, hydrogen and oxygen only.
m (sample) = 0.5096 g
n (H_2O) = 0.4160 g
n (H_2O) = 0.4160 ÷ 18.016 = 0.0231 mol
n (H) = 2 × 0.0231 = 0.0462 mol
m (H) = n × M = 0.0462 × 1.008 = 0.04655 g

V (CO_2 - 100°C & 102.8 kPa) = 0.7007 L
Using the equation, PV = nRT
n = (PV ÷ RT) = [(102.8 × 0.7007) ÷ (8.314 × 373.15)] = 0.02322 mol of CO_2
Therefore, n (C) = n (CO_2) = 0.02322 mol
Therefore, m (C) = n × M = 0.02322 × 12.01 = 0.2789 g

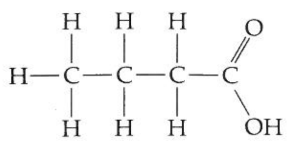
Therefore, m (O) = [0.5096 g – (0.04655 g + 0.2789 g)] = 0.1842 g
Therefore, n (O) = (m ÷ M) = (0.1842 ÷ 16) = 0.01151 mol

	C	H	O
Mass ratio	0.2789 g	0.04655 g	0.1842 g
Mole ratio	0.2789 ÷ 12.01	0.04655 ÷ 1.008	0.01842 ÷ 16
	0.02322	0.04618	0.01151
Dividing by the smallest mole of 0.01151,			
Simple ratio	0.02322 ÷ 0.01151	0.04618 ÷ 0.01151	0.01151 ÷ 0.01151
	2.017	4.012	1
Rounded mole ratio	2	4	1
Empirical Formula:	$\mathbf{C_2H_4O}$	(Empirical Mass = 44.052 g)	

b) Determining the molecular mass.
m (second sample) = 0.4832 g
This sample at 261°C, has a pressure of 241 kPa in a 100.0 mL container.
Using the relationship, PV = nRT, and, n = PV ÷ RT,
n = [(241 × 0.100) ÷ (8.314 × 534.15)] = 5.4268×10^{-3} mol
Since, 5.4268×10^{-3} mol has a mass of 0.4832 g
One mole has a mass = [(1 × 0.4832) ÷ (5.4268×10^{-3})] = 89.04 g mol^{-1}.
The ratio of molecular mass ÷ empirical mass = (89.04 ÷ 44.052) = Nearly 2.
Therefore, the **molecular formula** = 2 × C_2H_4O = $\mathbf{C_4H_8O_2}$

c) Since a fruity smell is characteristic of an ester and the ester is the product of an alcohol and a carboxylic acid, this compound is most likely to be butanoic acid with the following Lewis structure.

Structure of butanoic acid



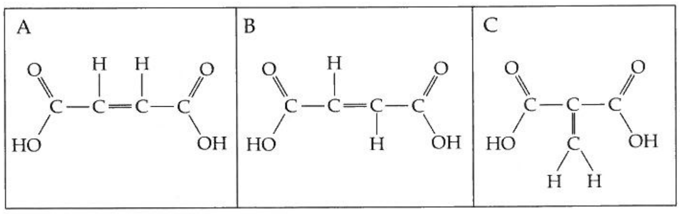
d) Additional chemical tests for butanoic acid:
i) Reaction with metallic carbonates such as $CaCO_3$ would produce a colourless, odourless gas and the test tube (if the reaction is carried out in a test tube) will get warm.
$CaCO_3(s) + CH_3CH_2CH_2COOH(\ell) \rightarrow Ca(CH_3CH_2CH_2COO)_2(aq) + CO_2(g) + H_2O(\ell)$
Other minor tests for consideration:
ii) Litmus test: acids turn litmus red. This confirms that the compound is an acid.
A large amount of heat is produced when butanoic acid is mixed with water.

5.(2013:35) a) Empirical formula = CHO
Empirical mass = 12.01 + 1.008 + 16.00 = 29.018
Molecular mass = 116 g mol^{-1}
Molecular mass to empirical mass ratio = 116 ÷ 29.018 = 3.9975 ≈ 4
Molecular formula = Empirical formula × 4 = CHO × 4 = **$C_4H_4O_4$**
b)

Test	Observation	Possible functional group
Water solubility	788 g L^{-1}	R–COOH = carboxylic acid or, R–OH = alcohol
Add to bromine water	Bromine water decolourises rapidly	Can be a double bond or a triple bond.

c) m (sample of the white solid) = 2.32 g
n (H^+) ions in the above sample = 0.0400 mol
n (in 2.32 g sample) = (2.32 ÷ 116) = 0.0200 mol
Therefore, the ratio of the moles of the compound to the moles of hydrogen = 0.0200 ÷ 0.0400
= 1:2

Therefore, the substance is a diprotic acid
Three possible structures are shown below:



6.(2014:39) This is a straightforward empirical-molecular formula calculation.
a) The organic compound contains C, H, O and Br. The mass of the sample is 1.50 g.
m (CO_2) produced on combustion = 1.58 g
n (CO_2) produced = (1.58 ÷ 44.01) = 0.03590 mol
Therefore, n (C) = n (CO_2) = 0.03590 mol
Therefore, m (C) = 0.03590 × 12.01 = 0.4312 g. Therefore, carbon is **28.7%** of the compound.

m (H_2O) produced on combustion = 0.563 g.
n (H_2O) produced = (0.563 ÷ 18.016) = 0.03125 mol
Therefore n (H) produced = 2 × 0.03125 = 0.0625 mol
Therefore, m (H) produced = 0.0625 × 1.008 = 0.0630 g. Therefore, hydrogen is **4.2%** of the compound.

Another sample of mass 1.75 g results in 1.97 g of AgBr.
Therefore, the original mass, 1.50 g sample would have produced, [(1.50 × 1.97) ÷ 1.75] = 1.6886 g of AgBr.
Therefore, n (Br) = n (AgBr) = 1.6886 ÷ (107.9 + 79.90) = 0.008991 mol.
Therefore, m (Br) produced = 0.008991 × 79.90 = 0.7184 g. Therefore, bromine is **47.9%** of the compound.

Therefore, the mass of oxygen in the compound is = [1.50 – (0.4313 + 0.0630 + 0.7184)] = 0.2874 g. Oxygen is **19.2%** of the compound.
n (O) = (0.2874 ÷ 16.0) = 0.01796 mol.

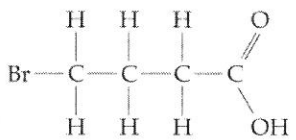
Calculation of the empirical formula

	28.7%	4.2%	19.2%	47.4%
Elements present	C	H	O	Br
Mass ratio (g)	0.04312	0.0630	0.2874	0.7184
Mole ratio	0.03590	0.0625	0.01796	0.008991
Simple ratio	3.993	6.951	1.998	1
Whole No. ratio	4	7	2	1

Therefore, the empirical formula is $\mathbf{C_4H_7O_2Br}$

b) The empirical mass of the compound is = 48.04 + 7.056 + 32.0 + 79.9 = 167.0
Using the relationship, PV = nRT and [n = (PV ÷ RT)], the number of moles of the compound of mass 1.95 g is calculated as follows:
n = {(95.0 × 0.387) ÷ [8.314 × (273 + 105)]} = [36.765 ÷ (8.314 × 378)] = 0.01170 mol
Since 0.01170 mol of the compound has a mass of 1.95 g
1.00 mol of the compound (the molecular mass) is = (1.95 ÷ 0.01170) = 166.7 g mol^{-1}
As the empirical mass (167.0 g) and the molar mass (166.7 g) are equal within the limits of the experimental error, the molecular formula is the same as the empirical formula.
The molecular formula of the compound is = $\mathbf{C_4H_7O_2Br}$.

c) A possible structure for the formula is given below.

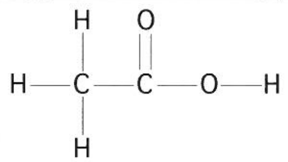
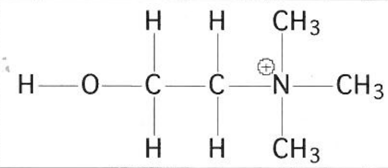


4-bromobutanoic acid

This compound could be 4-bromobutanoic acid. Other position isomers involving the -Br functional groups are also possible.

7.(2016:38) a) Enzymes are proteins which act as biological catalysts. They are more efficient than inorganic catalysts.

b)

Ethanoic acid	Choline
	

c)

CHNO	+	O_2	→	CO_2	+	H_2O	+	NO_2
4.270 g				9.020 g		5.169 g		1.886 g
				n = 9.020/44.01 = 0.2050 mol m = 0.2050 × 12.01 = 2.461 g		n = 5.169/18.016 = 0.2869 mol of H But there are 2 × H m = 0.2869 × 2 × 1.008 = 0.5784 g		n = 1.886/46.01 = 0.0410 mol m = 0.0410 × 14.01 = 0.5743 g

Mass of oxygen = total mass – mass of C – mass of H – mass of N
= 4.270 – 2.4614 – 0.5784 – 0.5743 = 0.6559 g

Ratio of mol =

	C	H	O	N
n	0.20495	0.57382	0.04099	0.04099
÷ n(O)	5	14	1	1

Therefore the empirical formula is $C_5H_{14}ON$

d) The acetylcholine produced 4.270 g of a compound with the molecular formula $C_5H_{14}NO$. This compound matches the structure of choline, so it is evident that the enzyme is active as it has produced the product of the equation rather than the reactant.