Exercise: 14 **Synthesis of Some Organic Compounds**

The percentage by mole of carbon in an alcohol (A) is 26.66%

A) Molecular formula of an organic compound (A)

1) Determine the molecular formula of compound (A).
2) Write all the possible isomers of (A).

B) Dehydrogenation reactions and different tests

The catalytic dehydrogenation of two straight isomers of (A) gives two compounds (C) and (D). A series of tests are carried out on (C) and (D) and the results are tabulated below:

Compounds	Sodium bisulfite	Fehling solution
(C)	Positive	Positive
(D)	Positive	Negative

1) Based on the results obtained in the above table, identify the chemical family of (C) and (D).
2) Identify the two isomers of compound (A)
3) Write the equations of dehydrogenation reactions of both isomers. Name the products obtained.

C) Oxidation of compound (C) with potassium dichromate

The oxidation of compound (C) with potassium dichromate gives a compound (G) that turns litmus red.

1) Write the condensed structural formula of (G) and circle its functional group.
2) Write the equation of the oxidation reaction of compound (C) with potassium dichromate.

D) Esterification reaction

28.75 mL of an alcohol (E) is mixed with an equimolar amount of (G) in presence of few drops of sulfuric acid. The molecular formula of the ester formed is $C_6H_{12}O_2$. The yield of the reaction is 65%.

1) Deduce the molecular formula of alcohol (E).
2) Write the equation of the esterification reaction. Name the ester formed.
3) Show that the initial number of moles of both reactants is 0.5 mol.
4) Determine the equilibrium constant K_c of the esterification reaction.

Given: $\int_E$: 0.8 g/mL C = 12 H = 1 O = 16 g/mol

Exercise: 14

A)

1) (A): $C_nH_{2n+2}O$ % by mole C = 26.66 %

% by mole (C) = $\frac{n}{3n+3} \times 100 = 26.66 \longrightarrow 100\ n = 26.66\ (3n + 3)$

$100\ n = 79.98\ n + 79.98 \longrightarrow 20.02\ n = 79.98$

$n = 4 \longrightarrow C_4H_{10}O$

2) **Isomers of $C_4H_{10}O$**

1-butanol

$CH_3CH_2CH_2CH_2OH$

2-butanol

$CH_3 - CH_2 - CH(OH) - CH_3$

2-methyl-1-propanol

$CH_3 - CH(CH_3) - CH_2 - OH$

2-methyl-2-propanol

$CH_3 - C(CH_3)(OH) - CH_3$

B)

1) (C) and (D) react with sodium bisulfite thus they are carbonyl compounds. (C) reacts with fehling solution while (D) doesn't.
(C) is an aldehyde and (D) is a ketone.

2) The two isomers are 1-butanol: $CH_3CH_2CH_2CH_2OH$ and
2-butanol: $CH_3 - CH(OH) - CH_2 - CH_3$

Since dehydrogenation of a primary alcohol gives an aldehyde. While dehydrogenation of a secondary alcohol gives a ketone.

3) $CH_3CH_2CH_2CH_2OH \xrightarrow[300^0C]{Cu} \underset{\text{butanal}}{CH_3CH_2CH_2-\overset{\overset{O}{\|}}{C}-H} + H_2$

$$CH_3-\underset{\underset{OH}{|}}{CH}-CH_2-CH_3 \xrightarrow[300^0C]{Cu} \underset{\text{2- butanone}}{CH_3-\overset{\overset{O}{\|}}{C}-CH_2-CH_3} + H_2$$

C)

1) (C): butanal: $CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-H$

$(C) + Cr_2O_7^{2-} \rightarrow (G)$

(G) turns litmus red $\Rightarrow$ (G) is a carboxylic acid.

(G) is butanoic acid: $CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-OH$

The functional group of (G) is COOH (carboxyl group).

2) $CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-H + Cr_2O_7^{2-} \rightarrow CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-OH + Cr^{3+}$

$$3 \times \left(CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-H + H_2O \rightarrow CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-OH + 2H^+ + 2e^-\right)$$

$$Cr_2O_7^{2-} + 14H^+ + 6e^- \rightarrow 2Cr^{3+} + 7H_2O$$

$$3\,CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-H + Cr_2O_7^{2-} + 8H^+ \rightarrow 3\,CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-OH + 2Cr^{3+} + 4H_2O$$

D)

1) Let (E) be $C_xH_yO_z$

$$C_xH_yO_z + CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-OH \rightleftarrows C_6H_{12}O_2 + H_2O$$

According to the law of conservation of atoms the total number of atoms in the reactants is equal to the total number of atoms in the products.

w.r.to carbon: $x + 4 = 6 \rightarrow x = 2$

w.r.to hydrogen: $y + 8 = 14 \rightarrow y = 6$

w.r.to oxygen: $z + 2 = 3 \rightarrow z = 1 \rightarrow$ (E): C_2H_6O: CH_3CH_2OH

2) $CH_3 - CH_2OH + CH_3 - (CH_2)_2 - \overset{\overset{O}{\|}}{C} - OH \rightleftarrows CH_3(CH_2)_2 - \overset{\overset{O}{\|}}{C} - O - CH_2CH_3 + H_2O$

The ester formed is ethyl butanoate

3) m alcohol (E) = $\rho \times V = 0.8\ g/mL \times 28.75\ mL = 23\ g$

$n\ (Alcohol) = \frac{m}{M} = \frac{23}{46} = 0.5$ mol, since (E) and (G) are equimolar

$\Rightarrow n(E) = n(G) = 0.5$ mol

4)

	Alcohol	+ Acid	$\rightleftarrows$ Ester	+ H_2O
$t = 0$	0.5 mol	0.5 mol	0	0
$t = t_{eq}$	$0.5 - x$	$0.5 - x$	x	x

$$\%\ yield = \frac{act\ quantity}{theo\ quantity} \times 100 \quad 65 = \frac{x}{0.5} \times 100 \rightarrow x = \frac{65 \times 0.5}{100} = 0.325\ mol$$

At equilibrium: n(alcohol) = n(acid) = 0.5 – 0.325 = 0.175 mol

$$n\ (Ester) = n\ (H_2O) = 0.325\ mol \rightarrow Kc = \frac{[Ester][H_2O]}{[Alcohol][Acid]} = \frac{\frac{0.325}{V}\ \frac{0.325}{V}}{\frac{0.175}{V}\ \frac{0.175}{V}} = 3$$