ORGANIC CHEMISTRY COURSE

Dr. Nazih El Bizri High School
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Done By: Ms. Hiba Nahhas

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- **Carboxylic Acids:** ... 17
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Chapter: 8 (functional Groups) Page: 195

- Organic Compounds: are insoluble in water, but soluble in organic solvents and the bonds in organic compounds are covalent bonds.

  All organic compounds contain carbon (C), but they may contain other elements such as: Nitrogen (N), Hydrogen (H), and Oxygen (O).

- Quantitative Analysis: Determination of the percent mass composition of each element in a compound and determination of empirical and molecular formula.

% by mass of element = $\frac{m\,(element)}{m\,(compound)} \times 100$

For Carbon (C): $C + O_2 \rightarrow CO_2$

% C = $\frac{m\,(C)}{m\,(compound)} \times 100$

For Hydrogen (H): $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$ and $2H \rightarrow H_2$

% H = $\frac{m\,(H)}{m\,(compound)} \times 100$

For Nitrogen (N): $N_2 + 3H_2 \rightarrow 2NH_3$ and $2N \rightarrow N_2$

% N = $\frac{m\,(N)}{m\,(compound)} \times 100$

%O = 100 – (percentages of the other elements)

Application 1:

0.6g of an organic compound is analyzed to obtain 0.88g of CO_2 and 0.36 of H_2O vapor.
Given: Molar masses in $g.mol^{-1}$ M(C)= 12, M(O)= 16, M(H)= 1.
1- Determine the percent mass composition of each element C and H in the compound.
2- Does the compound contain other elements than C and H? Justify.

Answer:

1- For C: $C\ O_2 \rightarrow CO_2$

M (CO_2) = MC + MO x2= 12+16x2= 44 $g.mol^{-1}$

Acc. to. St. ratio: n (C) = n (CO_2), then $\frac{m\,(C)}{M\,(C)} = \frac{m\,(CO_2)}{M\,(CO_2)}$, $\frac{m\,(C)}{12} = \frac{0.88}{44}$

m (C) = $\frac{0.88\times12}{44}$ = 0.24 g.

% C = $\frac{m\,(C)}{m\,(compound)} \times 100 = \frac{0.24}{0.6} \times 100 = 40$ %

For H: $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$

M(H_2) = 2, M(H_2O) = 18.

Acc. to. St. ratio: n (H_2) = n (H_2O), then $n(H_2) = \frac{m\,(H_2O)}{M\,(H_2O)}$, n($H_2$) = $\frac{0.36}{18}$ = 0.02 moles.

$2H \rightarrow H_2$

Acc. to. St. ratio: $n(H_2) = \frac{n\,(H)}{2} = \frac{m\,(H)}{M(H)\times2}$ then m(H) = n (H_2) x 2 x 1 = 0.02 x 2 = 0.04g.

% H = $\frac{m\,(H)}{m\,(compound)} \times 100 = \frac{0.04}{0.6} \times 100 = 6.67$ %

2- Yes, since % H + % C = 46.67% < 100%

%(O) = 100 -46.7 = 53.33%

- Molecular and Empirical Formula: The empirical formula is the simplest form of the molecular formula.

Example:

Molecular Formula (M.F.)	Empirical Formula (E.F.)
C_4H_{10}	C_2H_5
$C_6H_{12}O_6$	CH_2O
C_6H_6	CH
H_2O	H_2O

Empirical Formula

In empirical formula in 100g of sample % by mass (element) = mass (element)

Since % by mass (element) = $\frac{m\,(element)}{m\,(compound)} \times 100 = \frac{m\,(element)}{\cancel{100}} \times \cancel{100}$ = m (element)

1st step: Calculate number of moles of each element where n = $\frac{m}{M} = \frac{\%\,m}{M}$

2nd step: Divide the number of moles of each element by the smallest n.

3rd step: Write the number in molecule as a whole number

Molecular Formula

1st Method:

If you know the empirical formula and the Molar mass of molecular formula is given, then compare the molar masses of both formulas. $M(C_xH_yO_z)$ and $M\,(C_xH_yO_z)_n$.

If n = 1 then the molecular formula is the same as the empirical formula

If n ≠ 1 then multiply n by (x,y,z) to deduce the molecular formula.

Example 1:

If empirical formula is $C_6H_{12}O_{11}$ and M(molecular formula) = 260 g.mol^{-1}

Given M(C)=12, M(H) =1, M(O) =16.

M(E.F.) = M(M.F.) = 260 g.mol^{-1}

Then n = 1 and M.F. is $C_6H_{12}O_{11}$

Example 2:

If empirical formula is C_5H_{11} and M (Molecular formula) = 142g.mol^{-1}

M(E.F.) = (5x12) + (11x1) = 71 g.mol^{-1}

M(M.F.) = M(E.F.) x 2 then n = 2 and M.F. is $C_{10}H_{22}$

Application 2:

The analysis of an organic substance (S) gives the following mass composition: % (C)= 30.6%, %(H)= 3.8%, %(Cl) = 45.2%

M(C)= 12, M(H)=1, M(O)=16, M(Cl)=45.2%

1- Determine the empirical formula

2- Deduce the molecular formula knowing that its molar mass is 78.5 g.mol^{-1}

2nd Method:

Acc. to law of definite proportion : $\frac{M\,(compound)}{100} = \frac{m\,(H)}{\%\,H} = \frac{m\,(C)}{\%\,C} = \frac{m\,(O)}{\%\,o}$

M(C) = 12, M(H)=1, M(O)=16. $C_xH_yO_z$

$\frac{M\,(compound)}{100} = \frac{y}{\%\,H} = \frac{12x}{\%\,C} = \frac{16z}{\%\,o}$

Note that: $\frac{dA}{A} = \frac{MA}{MB}$ then, $\frac{dA}{air} = \frac{MA}{Mair}$, M(air) = 29 $g.mol^{-1}$

Application 3:

A saturated hydrocarbon C_nH_{2n+2} has a percentage by mass of carbon = 83.7%, prove that the molecular formula of the compound is C_6H_{14} M(C)=12, M(H)=1.

Answer:

Acc. to law of definite proportion $\frac{M\,(compound)}{100} = \frac{m\,(H)}{\%\,H} = \frac{m\,(C)}{\%\,C}$

%H= 100 – 83.7 = 16.3%

M(compound) = 12n + 2n+ 2 = 14n+2

mH = n x M = 2n+2 x 1 = 2n +2, mC = n x M = n x 12 = 12n

$\frac{14n+2}{100} = \frac{2n+2}{16.3} = \frac{12n}{83.7}$, then $\frac{14n+2}{100} = \frac{12n}{83.7}$ → 83.7 (14n +2) = 1200n , 1171.8n +167.4 = 1200n

1200n – 1171.8n = 167.4 then n =5.93 ~ 6 then C_nH_{2n+2} is C_6H_{14}

Application 4:

The combustion of 225mg of a nitrogenous organic substance (S) produces 220mg of CO_2, 135mg of H_2O and 60mL of N_2.

Given: V_m = 24L.mol^{-1}, M in g.mol^{-1} : MC =12, MN =14, MH=1, MO=16.

1- Calculate the percentage composition by mass of S

2- Knowing that the molar mass of (S) = 45 g.mol^{-1}, determine its molecular formula.

Application 5:

An organic compound contains the elements C, H and O with a mass 0.814g. Quantitative analysis gives 1.936g of CO_2 and 0.99g of H_2O

Given: M(C)=12, M(H)=1, M(O)= 16

1- Determine the percent composition by mass of each constituent element in this compound

2- Determine its empirical formula

3- Deduce its molecular formula knowing that its molar mass is 74 g.mol^{-1}

Solve Ex 3 and 6 page 204 (book)

Chapter: 9 (Alcohols) Page: 207

Hydrocarbons: are organic compounds formed of only Carbon and Hydrogen.

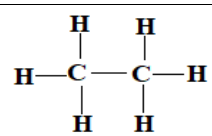
Notes:

Hydrogen: **H•** make only 1 connection → 1 single covalent bond

Carbon: **•C•** make 4 connections → 4 singles, or 2 double, or 1 double and 2 singles, or 1 triple and 1 single.

Oxygen: **•Ö:** make 2 connections → 2 singles, or 1 double.

Nitrogen: **•N̈•** make 3 connections → 3 singles, or 1 double and 1 single, or 1 triple

Molecular Formula (M.F.)	**Structural Formula (S.F.)**	**Condensed Structural Formula (C.S.F.)**
Number of atoms that makes a molecule	Shows the bonds between all atoms	Shows the bonds only between carbon atoms
C_2H_6		$CH_3 — CH_3$

Naming

Nb. of Carbon	Prefix
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hex
7	Hept
8	Oct
9	Non
10	Dec

Linear Chain

Continuous chain of Carbon atoms, no C is bonded to more than 2 other C atoms.

Branched Chain

At least one carbon atom is bonded to more than 2 C atoms.

Branches Names				**Alkyl Branches Names (C_nH_{2n+1})**		
Bromo	Chloro	Iodo	Fluoro	methyl	ethyl	propyl
Br	Cl	I	F	-(CH_3)	-(C_2H_5)	-(C_3H_7)

<u>Nomenclature Steps:</u>

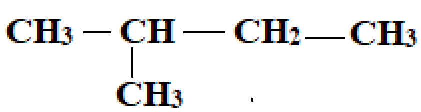
1- Select the longest chain of carbon atoms

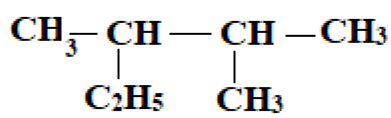
2- Choose numbering closer to the branch where the branches takes the lowest possible number

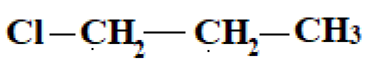
3- Follow alphabetical order

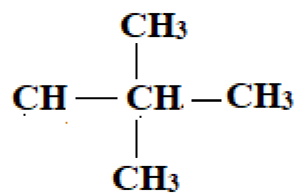
Note: Use di, tri and tetra for having 2,3, and 4 same identical branches.

Application: Name the following Alk**ane**







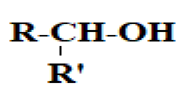


Family	Functional Group	Molecular Formula	General Formula	Name	Example
Alcohol	Hydroxyl (OH)	C_nH_{2n+2}	R-OH	Alkan-ol	CH-OH Methan**ol**

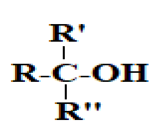
- **<u>Alcohols:</u>** are organic compounds containing one or more hydroxyl (OH) groups. Alcohols having 1 hydroxyl group are known as mono-alcohols.
- **<u>General Formula:</u>** $C_nH_{2n+2}O$ or $C_nH_{2n+1}OH$
- **<u>Classes of Alcohols:</u>**

Primary Alcohol 

when the carbon holding the hydroxyl group is connected to 1 alkyl group (and 2 Hydrogen atoms).

Secondary Alcohol 

when the carbon holding the hydroxyl group is connected to 2 alkyl group (and 1 Hydrogen atoms).

Tertiary Alcohol 

when the carbon holding the hydroxyl group is connected to 3 alkyl group (and 0 Hydrogen atoms).

<u>Note:</u> The carbon atom holding the OH is included in the main chain and the position of OH is given the lowest number.

Application: Name the following alcohols

$CH_3-CH_2-CH_2-OH$		$CH_3-CH-CH-CH_2OH$ | | CH_3 CH_3	
$CH_3-CH-CH_3$ | OH		$CH_3-CH-CH_2-CH_2OH$ | OH	
CH_3 | $CH_3-CH_2-C-CH-CH_3$ | | CH_3 OH		OH | $CH_3-CH_2-C-CH_2-CH-CH_3$ | | CH_3 CH_3	
$CH_3-CH-CH-CH_2-CH-CH_3$ | | | CH_3 C_2H_5 OH		$CH_3-CH-CH-CH-CH-CH_3$ | | | | CH_3 CH_3 C_2H_5 OH	

Solve Ex: 2 (book) page: 225

- **Isomers**

Skeletal Isomers: same position of OH but different carbon skeleton (different structure)
Positional Isomers: the position of OH group is different in the carbon chain.

Application 1:

$C_4H_{10}O$ alcohol

1- Write the condensed structural formula of all the possible isomers of the alcohol.
2- Give the systematic name of each.
3- Indicate the class of alcohol of each. Justify.
4- Give 2 positional isomers and 2 skeletal isomers. Justify.

- **Chemical Reactions of Alcohols:**

1-Catalytic oxidation (Cu or Pt) in the presence of oxygen or air.

Primary Alcohol	Aldehyde → Carboxylic Acid
Secondary Alcohol	Ketone
Tertiary Alcohol	No rxn

Note: Primary Alcohol in continuous oxidation (presence of excess oxygen) gives directly carboxylic acid.

Primary Alcohol:

$$R-CH_2-OH + 1/2\ O_2 \xrightarrow[300^0C]{Cu\ or\ Pt} R-CH{=}O + H_2O$$

Aldehyde

$$\mathbf{R\text{-}CH{=}O + 1/2\ O_2 \xrightarrow[300^0C]{Cu\ or\ Pt} R\text{-}\underset{\substack{|\\ OH}}{C}{=}O}$$

Carboxylic acid

However, in presence of excess oxygen (continuous oxidation) primary alcohol gives directly carboxylic acid as follows:

$$\mathbf{R\text{-}CH_2\text{-}OH + O_2 \xrightarrow[300^0C]{Cu\ or\ Pt} R\text{-}\underset{\substack{|\\ OH}}{C}{=}O + H_2O}$$

Carboxylic acid

<u>Example:</u>

$CH_3\text{-}CH_2\text{-}CH_2OH + ½\ O_2 \rightarrow CH_3\text{-}CH_2\text{-}CH{=}O + H_2O$

$$CH_3\text{-}CH_2\text{-}CH{=}O + ½\ O_2 \xrightarrow[300^0C]{Cu\ or\ Pt} CH_3\text{-}CH_2\text{-}\underset{\substack{|\\ OH}}{C}{=}O$$

$$\text{Continuous Oxidation: } CH_3\text{-}CH_2\text{-}CH_2OH + O_2 \xrightarrow[300^0C]{Cu\ or\ Pt} CH_3\text{-}CH_2\text{-}\underset{\substack{|\\ OH}}{C}{=}O + H_2O$$

<u>Secondary Alcohol:</u>

$$R\text{-}\underset{\substack{|\\ R'}}{CH}\text{-}OH + 1/2\ O_2 \xrightarrow[300^0C]{Cu\ or\ Pt} R\text{-}\underset{\substack{||\\ O}}{C}\text{-}R' + H_2O$$

Ketone

<u>Example:</u>

$$CH_3\text{-}CH_2\text{-}\underset{\substack{|\\ CH_3}}{CH}\text{-}OH + 1/2\ O_2 \xrightarrow[300^0C]{Cu\ or\ Pt} CH_3\text{-}CH_2\ \text{-}\ \underset{\substack{||\\ O}}{C}\text{-}\ CH_3 + H_2O$$

2-Catalytic dehydrogenation in the absence of oxygen.

Primary Alcohol	Aldehyde
Secondary Alcohol	Ketone
Tertiary Alcohol	No rxn

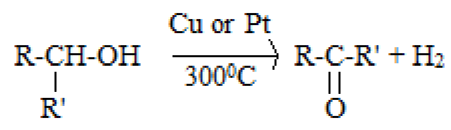
<u>Primary Alcohol:</u>

$$\mathbf{R\text{-}CH_2\text{-}OH \xrightarrow[300^0C]{Cu\ or\ Pt} R\text{-}CH{=}O + H_2}$$

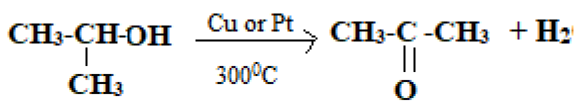
<u>Example:</u>

$$\mathbf{CH_3\text{-}CH_2OH \xrightarrow[300^0C]{Cu\ or\ Pt} CH_3\text{-}\underset{\substack{||\\ O}}{C}\ \text{-}H + H_2}$$

Secondary Alcohol:



Example:



3-Oxidation in the presence of an oxidant.

Primary Alcohol	Aldehyde → Carboxylic Acid
Secondary Alcohol	Ketone
Tertiary Alcohol	No rxn

Note: Primary Alcohol in (presence of excess oxidant) gives directly carboxylic acid.

Primary Alcohol:

Example 1:

In presence of limited amount of oxidant. **Alcohol→ Aldehyde**

$Cr_2O_7^{2-}$ / Cr^{3+} with CH_3-CH_2-OH

(CH_3-CH_2-OH → CH_3-CH=O +2 H^+ + 2e-) x 3

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

Then: 3 CH_3-CH_2-OH → 3 CH_3-CH=O +6 H^+ + 6e-

Overall: $Cr_2O_7^{2-}$ + 8H^+ + 3CH_3-CH_2-OH → 3 CH_3-CH=O + 2 Cr^{3+} + 7H_2O

Example 2:

In presence of excess amount of oxidant. **Alcohol→ Carboxylic acid**

Note

Before the reaction the solution color is purple (MnO_4^-).

After the reaction the solution color is colorless (Mn^{2+}).

Oxidation occur when color changes from purple to colorless.

MnO_4^- / Mn^{2+} with CH_3-CH_2-OH

(CH_3-CH_2-OH + H_2O → CH_3-COOH +4 H^+ + 4e-) x 5

(MnO_4^- + 8H^+ + 5e- → Mn^{2+} + 4H_2O) x 4

Then: 5 CH_3-CH_2-OH + 5 H_2O → 5 CH_3-COOH + 20 H^+ + 20e-

4 MnO_4^- + 32 H^+ + 20 e- → 4 Mn^{2+} + 16 H_2O

Overall: 5 CH_3-CH_2-OH + 4 MnO_4^- + 12 H^+ → 5 CH_3-COOH 4 Mn^{2+} + 11 H_2O

<u>Secondary Alcohol:</u>

<u>Example:</u>

$Cr_2O_7^{2-}$ / Cr^{3+} and $\underset{\displaystyle OH}{CH_3\text{-}\overset{|}{C}H\text{-}CH_3}$

Note

Before the reaction the solution color is yellow ($Cr_2O_7^{2-}$).

After the reaction the solution color is green (Cr^{3+}).

Oxidation occur when color changes from yellow to green.

Alcohol→ Ketone

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

$$CH_3\text{-}\underset{\displaystyle OH}{\underset{|}{C}H}\text{-}CH_3 \longrightarrow CH_3\text{-}\underset{\displaystyle O}{\underset{||}{C}}\text{-}CH_3 + 2H^+ + 2e^- \quad \times 3$$

Then:

$$3CH_3\text{-}\underset{\displaystyle OH}{\underset{|}{C}H}\text{-}CH_3 \longrightarrow 3\,CH_3\text{-}\underset{\displaystyle O}{\underset{||}{C}}\text{-}CH_3 + 6H^+ + 6e^-$$

Overall:

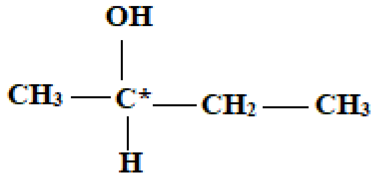
$$3CH_3\text{-}\underset{\displaystyle OH}{\underset{|}{C}H}\text{-}CH_3 + Cr_2O_7^{2-} + 8H^+ \longrightarrow 3\,CH_3\text{-}\underset{\displaystyle O}{\underset{||}{C}}\text{-}CH_3 + 2Cr^{3+} + 7H_2O$$

- **<u>Summary:</u>**

Family	**Functional Group**	**Molecular Formula**	**General Formula**	**Name**	**Example**
Alcohol	Hydroxyl (OH)	C_nH_{2n+2}	R-OH	Alkan-ol	CH-OH Methan**ol**
Aldehyde	Carbonyl (CO) / C=O	$C_nH_{2n}O$	R-CHO	Alkan-al	CH_3-CHO Or CH_3-CH=O Ethanal
Ketone	Carbonyl (CO)/C=O	$C_nH_{2n}O$	R-CO-R’	Alkan-one	CH_3-CO-CH_3 Or $CH_3\text{-}\underset{\displaystyle O}{\underset{\Vert}{C}}\text{-}CH_3$ Propanone
Carboxylic acid	Carboxyl COOH/ $\underset{\displaystyle OH}{\underset{|}{C}}=O$	$C_nH_{2n}O_2$	R-COOH	Alkan-oic acid	CH_3-CH_2-COOH Or $CH_3\text{-}CH_2\text{-}\underset{\displaystyle OH}{\underset{|}{C}}=O$ Propanoic acid

➢ Asymmetric Carbon

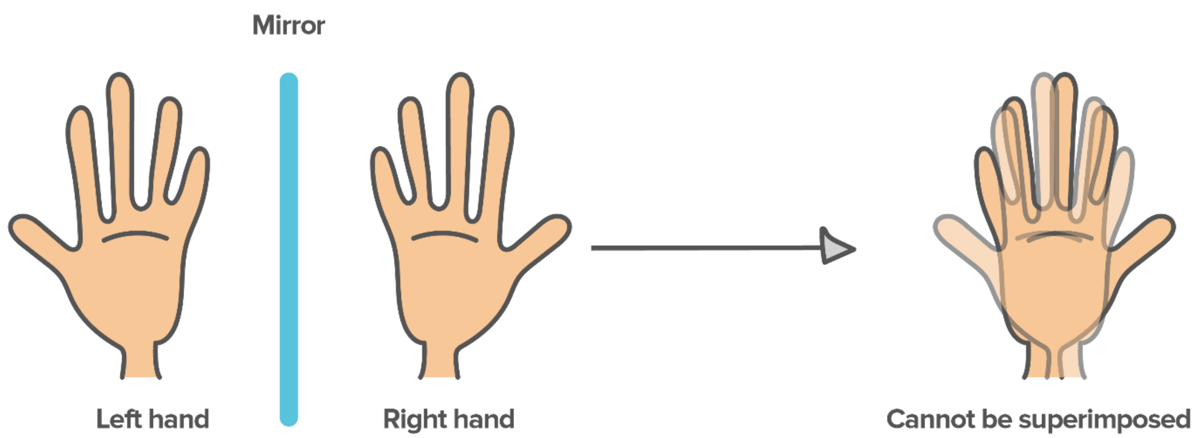
An asymmetric carbon represented by C* is attached to 4 different atoms or group of atoms.
This asymmetric center will lead to a chiral molecule.
2-butanol CH_3-CHOH-CH_2-CH_3 has an asymmetric center

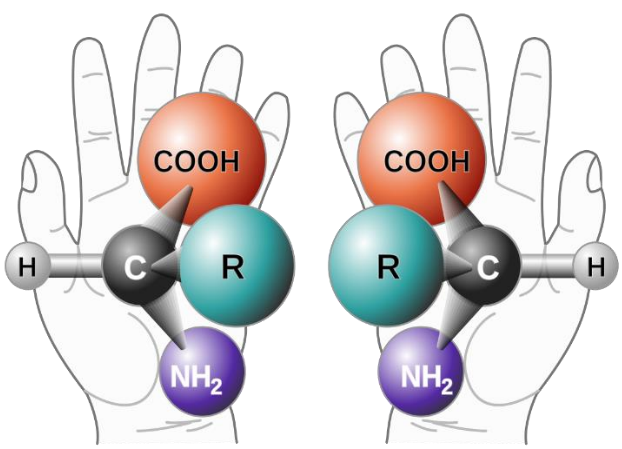


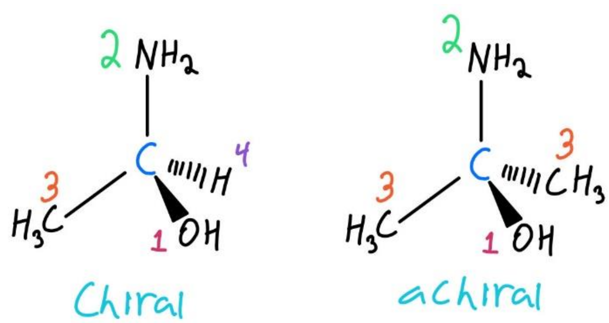
4 different groups (CH_3, H , OH, CH_2-CH_3)

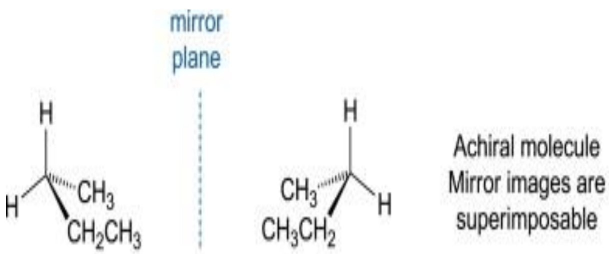
➢ Chiral Molecule

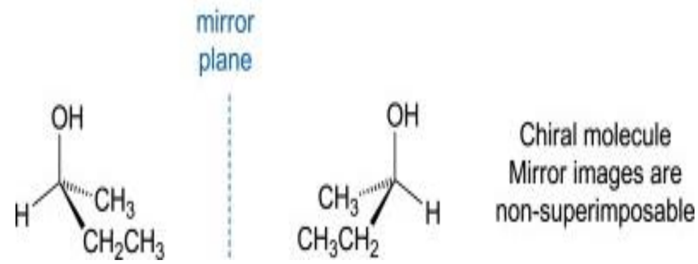
Chiral Molecule is a molecule with a non-superimposable mirror image.
Chiral ≠ Achiral (has a superimposable mirror image)











- **Enantiomers**

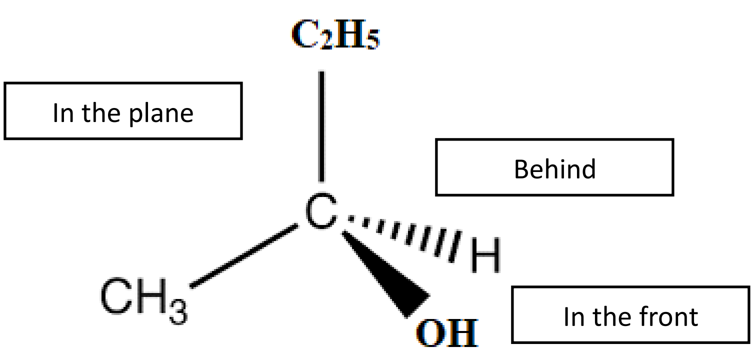
The construction of the two non-superimposable images using cram representation is called enantiomers.

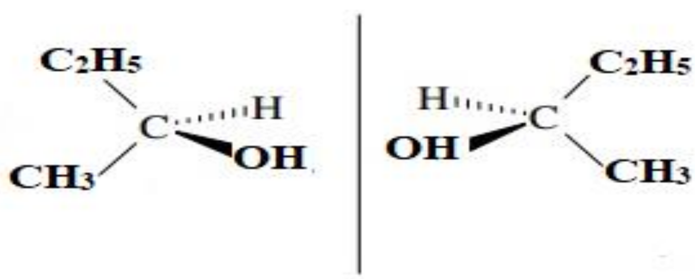
- **Cram Representation**

The molecules in the plane are represented by a continuous line ——

The bonds in the front of the plane are represented by 

The bonds behind the plane are represented by 





mirror
nonsuperimposable—chiral

Solve Ex: 4-5 page 225 and Ex: 8-9 page:226 and Ex: 12-15 page: 227

Chapter:10 (Aldehyde and Ketone) Page: 231

- **Aldehyde:**

Molecular Formula	$C_nH_{2n}O$
Functional Group	Carbonyl (CO) C=O
General Formula	R-CO-H or R-CH=O
Naming	Alkan-al

- **Naming:**

Structure	**Name**
O ‖ H-C-H	Methanal
O ‖ CH_3-C-H	Ethanal
CH_3-CH_2-CHO	Propanal
CH_3-CH_2-CH_2-CHO	Butanal
CH_3 | CH_3-C-CHO | CH_3	2,2-dimethyl propanal
CH_3-CH_2-CH-CH-CHO | | CH_3 C_2H_5	2-ethyl-3-methyl-pentanal

Note: The functional group (CHO) is always numbered 1.

- **Ketone:**

Molecular Formula	$C_nH_{2n}O$
Functional Group	Carbonyl (CO) C=O
General Formula	R-CO-R' or O ‖ R-C-R'
Naming	Alkan-one

- **Naming:**

Structure	**Naming**
CH_3-CO-CH_2-CH_3	2-butanone
O ‖ CH_3-CH-C-CH_3 | CH_3	3-methyl-2-butanone
CH_3-CH-CH-CO-CH-CH_3 | | | CH_3 C_2H_5 CH_3	4-ethyl-3,5-dimethyl-3-hexanone

<u>Note:</u> Since Aldehyde and Ketone have same molecular formula ($C_nH_{2n}O$) but different families then they are known as functional isomers.

Application:

1- Write all the isomers of $C_5H_{10}O$ then name each isomer.

2- Give skeletal isomers, positional isomers, and functional isomers.

Answer:

1-

	Structure	**Name**
1	CH_3-CH_2-CH_2-CH_2-CH=O	pentanal
2	CH_3-CH_2-CH_2-CO-CH_3	2-pentanone
3	CH_3-CH_2-CO-CH_2-CH_3	3-pentanone
4	CH_3-CH_2-CH-C-H | || CH_3 O	2-methyl-butanal
5	CH_3-CH-CH_2-C-H | || CH_3 O	3-methyl-butanal
6	CH_3-CH-C-CH_3 | || CH_3 O	3-methyl-2-butanone
7	CH_3 | CH_3-C-C-H | || CH_3 O	2,2-dimethyl-propanal

2- 1,4,5,7 are skeletal isomers since they have same molecular formula ($C_5H_{10}O$) but different structure.

2, and 6 are skeletal isomers since they have same molecular formula, same position of functional group but different structure.

2 and 3 are positional isomers since they have same molecular formula, same structure, but different position of the functional group.

1 and 2 are functional isomers since they have same molecular formula, different functions (different families)

<u>Note:</u>

Aldehyde and Ketone are functional isomers (same molecular formula $C_nH_{2n}O$) however Carboxylic acid and ester are also functional isomers (same molecular formula $C_nH_{2n}O_2$)

➢ <u>Identification Tests</u>

To identify the presence of carbonyl group (C=O) one test is available:

Test: DNPH (2,4-dinitro phenyl hydrazine) gives yellow-orange color if there is a carbonyl group (positive), while there is no change in color if there is no carbonyl group (negative).

To differentiate between aldehyde and ketones 4 tests are available:

Reagent	**Aldehyde**	**Ketone**
$NaHSO_3$	+ (White precipitate)	-
Schiff's reagent	+ (Pink color)	-
Fehling's Test	+ (Brick red color)	-
Tollen's reagent	+ (Silver mirror color)	-

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Chapter:11 (Carboxylic acid and ester) Page: 249

➢ Carboxylic Acids:

Molecular Formula	$C_nH_{2n}O_2$
Functional Group	C-OH || Carbonyl (COOH) O
General Formula	R-CO-OH
Naming	Alkan-oic acid

➢ Naming:

Structure	**Name**
H-COOH	Methanoic acid
CH_3-COOH	Ethanoic acid
CH_3-CH_2-CH_2-COOH	Butanoic acid
CH_3-CH-COOH | CH_3	2-methyl propanoic acid
CH_3 | CH_3-C-COOH | CH_3	2,2-dimethyl propanoic acid
CH_3-CH-CH_2-COOH | CH_3	3-methyl butanoic acid

Note: The functional group (COOH) is always numbered 1.

➢ Ester:

Molecular Formula	$C_nH_{2n}O_2$
Functional Group	-C-O || ester (COO) O
General Formula	O || R-COO-R' or R-C-OR'
Naming	Alkyl Alkanoate

➢ Naming:

Structure	**Naming**
H-COO-CH_3	Methyl methanoate
CH_3-COO-CH_2-CH_3	Ethyl ethanoate

Note: Esters are derivatives and functional isomers of Carboxylic acids.

Application 1:

1- Write all the isomers of $C_5H_{10}O_2$ then name each isomer.

2- Name the type of isomers.

Answer:

1-

	Structure	**Name**
	Carboxylic Acid Isomers	
1	$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}COOH$	Pentanoic acid
2	$CH_3\text{-}CH\text{-}CH_2\text{-}COOH$ | CH_3	3-methyl butanoic acid
3	CH_3 | $CH_3\text{-}C\text{-}COOH$ | CH_3	2,2-dimethyl propanoic acid
4	$CH_3\text{-}CH_2\text{-}CH\text{-}COOH$ | CH_3	2-methyl butanoic acid

2-

1,2,3,and 4 are structural or skeletal isomers since they have same molecular formula, same functional group but different structure.

Note:

Carboxylic acid and aldehyde don't have positional isomers because the functional group is always on number 1.

Note:

In naming of ester alkyl is the name of the chain next to oxygen (O) and alkanoate is the chain next to Carbon (C) where the C takes number 1.

Application 2:

Give the name of each of the following esters.

$H\text{-}COO\text{-}CH_3$

$CH_3\text{-}COO\text{-}CH_3$

$CH_3\text{-}CH_2\text{-}COO\text{-}CH_3$

$H\text{-}COO\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

$CH_3\text{-}CH\text{-}COO\text{-}CH_3$
|
CH_3

$CH_3\text{-}COO\text{-}CH_2\text{-}CH_2\text{-}CH_3$

$CH_3\text{-}CH_2\text{-}COO\text{-}CH_2\text{-}CH_3$

$H\text{-}COO\text{-}CH\text{-}CH_2\text{-}CH_3$
|
CH_3

$H\text{-}COO\text{-}CH_2\text{-}CH\text{-}CH_3$
|
CH_3

- **Esterification Reaction:**

Alcohol reacts with carboxylic acid to give ester and water according to the following reaction:

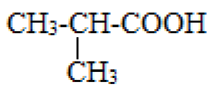
Alcohol + Carboxylic acid ↔ ester + water

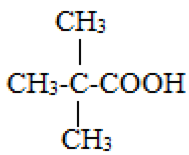
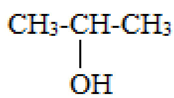
R-COOH + R'-OH ↔ R-COO-R' + H_2O

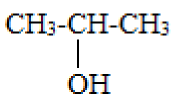
Examples: Complete the following reactions

1- CH_3OH + CH_3-COOH ↔ H_2O +

2- CH_3-CH_2OH + CH_3-CH_2-COOH ↔ H_2O +

3-  + CH_3-CH_2OH ↔ H_2O +

4-  +  ↔ H_2O +

5-  + CH_3-CH_2-COOH ↔ H_2O +

Note: reaction in direction 1 (forward direction) is the esterification reaction however reaction in direction 2 (backward direction) is the hydrolysis reaction.

Starting from an equimolar mixture

Proportion by mole of ester formed depend on the class of alcohol used

Class of alcohol	% by mole of ester
Primary Alcohol	67%
Secondary Alcohol	60%
Tertiary Alcohol	1 to 5%

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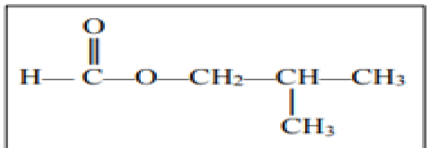
Application **Synthesis of an Organic Compound**

The organic compound (E) of raspberry odor is used in food industry. The condensed structural formula of this compound is represented in **document-1.**



Document-1

1. **Study of the Structure of The Compound (E)**
   - **1.1.** Name the functional group of this compound.
   - **1.2.** Give the systematic name of (E).
2. **Preparation of the compound (E)**

   The compound (E) can be obtained from the reaction of a carboxylic acid (A) and an alcohol (B).
   - **2.1.** Identify the carboxylic acid (A) and the alcohol (B).
   - **2.2.** Indicate the class of the alcohol (B).
   - **2.3.** Write, using condensed structural formulas, the equation of the preparation reaction of the compound (E) starting from the compounds (A) and (B).

Application 2 **Esterification Reaction**

Available is a mono-functional organic compound (A) of saturated non cyclic hydrocarbon chain. The analysis of this compound shows the following results:
- M(A) = 74 $g.mol^{-1}$.
- % by mass of (C) = 48.65; % by mass of (H) = 8.11% and the remaining is oxygen.

Given : M (H) = 1 $g.mol^{-1}$; M (C) = 12 $g.mol^{-1}$; M (O) = 16 $g.mol^{-1}$

1- Molecular formula of (A)

1.1- Show that the molecular formula of (A) is $C_3H_6O_2$

1.2- Write the condensed structural formulas of the possible isomers of (A).

1.3- Identify the compound (A) knowing that the pH of an aqueous solution of (A) is less than 7.0

2- Esterification reaction

A mixture of 0.2 mol of the acid (A) and 0.2 mol of 2-methyl-1-propanol is heated. Heating is stopped after a certain time.
(All the constituents of the reacting mixture form one single liquid phase).
The obtained organic compound (B) is extracted. After the purification of this product, it is weighed and its mass is found to be 13 g.

2.1- Write, using the condensed structural formulas of the organic compounds, the equation of the reaction that takes place.

2.2- Give the systematic name of the organic compound obtained.

2.3- Determine the yield of this reaction.

2.4- Specify whether the equilibrium state is reached at the end of heating , knowing that the equilibrium constant K_c of this reaction is equal to 4.12

Application: 3 <u>Importance and Characteristics of the Ester</u>

Two skiers broke their legs in Faraya during a ski session. The leg of the first skier was treated with a metal screw while the leg of the second skier was treated with a screw formed of the ester-based polymers. Three months later the first skier was subjected to a second surgery to remove the screw while there is no need for further surgery for the second skier. Among the constituents of the ester-based screw we note the presence of an ester (X) to be identified.
Ester (X) is derived from an alcohol (A) C_3H_8O and an acid (B) CH_3-COOH.
Given: − Molar masses: M(C) = 12 $g.mol^{-1}$; M(H) = 1 $g.mol^{-1}$; M(O) = 16 $g.mol^{-1}$

1. Characteristics of the Disappearance Reaction of the Ester (X).

1.1. Knowing that human body is very rich in water, explain the fact of the disappearance of the ester-based screw in the body of the second skier.

1.2. Referring to the text , give one characteristic for the reaction of disappearance of the este

2- Identification of class of (A).

• The catalytic oxidation of (A) gives an organic compound (C).
• The compound (C) is subjected to two successive tests and the results are given in the following table.

Experiment	Result
(C) + 2,4-DNPH	Formation of yellow-orange precipitate .
(C) + Schiff's reagent	The solution remains colorless.

2.1. Identify(C), and deduce the class of alcohol.

2.2. Write the condensed structural formula of ester (X) .Give its systematic name.

3- Study of Hydrolysis Reaction Of (X).

• A mixture of 1 mol of ester (X) and 1 of water, in the presence of few mL of concentrated sulfuric acid, are heated under reflux for about 45 min.
The volume of alcohol (A) obtained is 30 mL
. • The percentage yield of hydrolysis of ester at equilibrium, for an equimolar mixture, is 40 % when the obtained alcohol is secondary and 33% when the obtained alcohol is primary.
• Density of alcohol (A): ρ (A) = 0.8 $g.mL^{-1}$

Document-3-

3.1. Referring to document-3-:

3.1.1. Determine the percentage yield of the hydrolysis reaction at t = 45 min.

3.1.2. Deduce whether t = 45 min represents the equilibrium time.

3.2. Indicate the role of reflux heating.

3.3. Specify whether the following proposition is correct:
The experiment is repeated by introducing 1.5 mol of (X) and 2 mol of water. The yield of reaction remains the same.

Exercise : 1

Isobutyl Propanoate

Esters of general formula RCOOR' are very abundant in nature. Many of them have agreeable characteristic odor and contribute to natural or artificial tastes and flavors of certain fruits, plants, and candies.

The aim of this exercise is to study the preparation reaction of isobutyl propanoate which characterizes the rum odor.

1. Study of the Structure of Propanoic Acid

The molecular formula of propanoic acid is $C_3H_6O_2$

1.1. Write the condensed structural formula of propanoic acid.

1.2. Circle and name the functional group of this acid.

2. Isobutyl Alcohol

The condensed structural formula of isobutyl alcohol is given in **Document-1.**

$$\begin{array}{l} CH_3 - CH - CH_2OH \\ \qquad\;\; | \\ \qquad CH_3 \end{array}$$

Document-1

2.1. Give the systematic name of isobutyl alcohol.

2.2. Identify the class of this alcohol.

3. Synthesis of Isobutyl Propanoate

Isobutyl propanoate can be prepared starting from isobutyl alcohol and propanoic acid.

3.1. Write, using condensed structural formulas, the equation of the preparation reaction of isobutyl propanoate.

3.2. Give the systematic name of the ester formed.

3.3. An equimolar mixture (M) containing 0.1 mol of isobutyl alcohol and 0.1 mol of propanoic acid is heated to reflux for 40 min in the presence of few drops of concentrated sulfuric acid as a catalyst.

- For an initial equimolar mixture of a carboxylic acid and a primary alcohol, the yield of the reaction at equilibrium is 67%.
- Molar mass of isobutyl propanoate is: $M = 130\ g.mol^{-1}$.

Document-2

3.3.1. Indicate the importance of the reflux heating.

3.3.2. Determine the yield of this esterification reaction at t = 40 min.

3.3.3. Verify that the reacting system is at equilibrium at this instant.

3.3.4. Another reacting mixture containing 0.1 mol of isobutyl alcohol and 0.1 mol of propanoyl chloride is prepared.

3.3.4.1. Write, using condensed structural formulas, the equation of the preparation of propanoyl chloride starting from propanoic acid.

3.3.4.2. Choose, with justifying, the correct answer.
The mass m of the ester obtained at the end of the reaction is:

a) $m = 8.71\ g$ **b)** $m < 8.71\ g$ **c)** $m > 8.71\ g$

Exercise: 2 **Study of an Esterification Reaction**

Four flasks are available each contains, one of the following organic compounds:
Propanoic acid, 1-propanol, 3-pentanol and 2-butanol.
The available flasks are numbered and their contents are noted as follows:

Number of flask	1	2	3	4
Organic compound	A	B	C	D

Document-1

The aim of this exercise is to identify the content of each flask in order to carry out an esterification reaction.

1. Identification of The Content of Each Flask

The following tests are carried out:

Chemical test	Experimental result
Mild oxidation of compound (A) by an acidified potassium permanganate solution.	An organic compound (F) is obtained which reacts with DNPH and Fehling solution.
The pH of an aqueous solution of compound (B) is measured.	The pH is clearly less than 7.0

Document-2

1.1. Referring to document-2, identify the organic compounds (A) and (B).

1.2. Knowing that the molecule of compound (C) is chiral:

1.2.1. Write its condensed structural formula. Justify its chirality.

1.2.2. Represent according to Cram its two enantiomers.

2. Esterification Reaction

- For an initial equimolar mixture of a carboxylic acid and a secondary alcohol, the yield of the reaction at equilibrium is 60%.
- Density of the propanoic acid is d = 0.99 $g.mL^{-1}$.
- Molar masses in $g.mol^{-1}$: M (propanoic acid) = 74 ; M (E) = 130.

Document-3

A mixture of 0.25 mol of 2-butanol and a volume V = 30 mL of propanoic acid is heated to reflux. At instant t, heating is stopped. The mass of the ester (E) obtained at instant t is 19.5 g.

2.1. Write, using condensed structural formulas, the equation of the esterification reaction taking place. Name the obtained ester (E).

2.2. Calculate the initial number of moles of propanoic acid.

2.3. Determine the yield of this reaction at instant t.

2.4. Referring to document-3, verify whether the equilibrium is reached at this instant t.

2.5. It is suggested to realize the following modifications during this study:

- Modification 1: Extend the duration of heating.
- Modification 2: Add a catalyst to the initial mixture of the reactants.

Specify the effect of each modification on the yield of this reaction.