

Analytical Chemistry

Qualitative and Quantitative Analysis

First Stage / Lecture 1

Presented by

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2023-2024

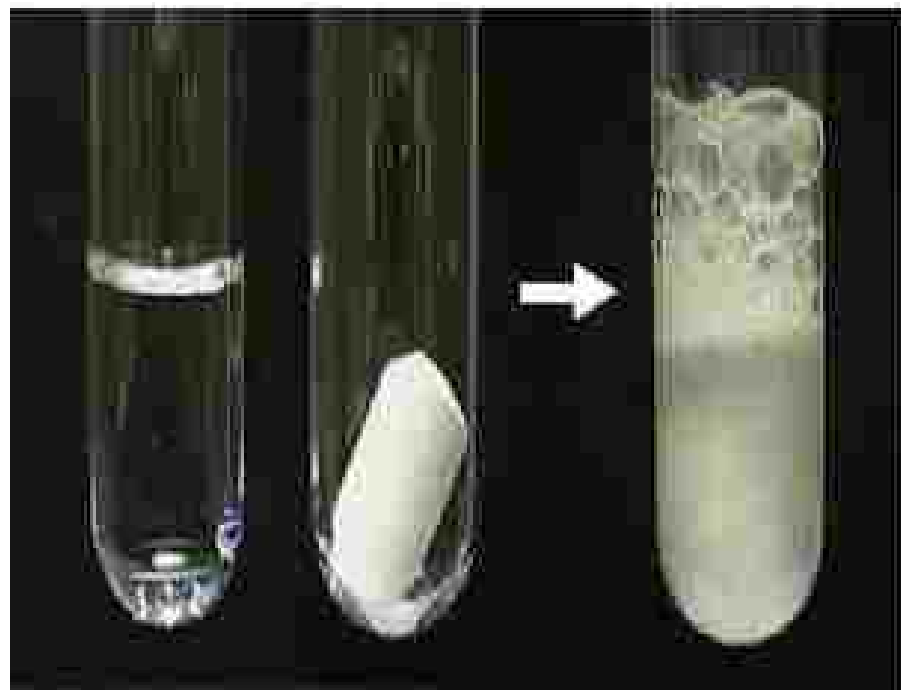
What is Analytical Chemistry ?

A branch of chemistry that deals with the identification of compounds and mixtures (qualitative analysis) or the determination of the proportions of the constituents (quantitative analysis),

Techniques commonly used are titration, precipitation, spectroscopy, chromatography, etc.

Qualitative Analysis

Qualitative Analysis is the determination of non-numerical information about a chemical species, a reaction, etc. Examples would be observing that a reaction is creating gas that is bubbling out of solution or observing that a reaction results in a color change. Qualitative analysis is not as reliable as quantitative analysis but is often far easier, faster and cheaper to perform.



Qualitative analysis

Qualitative analysis is used to

separate an analyte from interferences existing in a sample and to detect the previous one.

It gives negative, positive, or yes/no types of data.

It informs whether or not the analyte (An analyte is the substance in a sample that is being investigated.) is present in a sample.



Flame test

The flame test is used to visually determine the identity of an unknown metal or metalloid ion based on the characteristic color the salt turns the flame of a Bunsen burner. The heat of the flame excites the electrons of the metals ions, causing them to emit visible light. Every element has a signature emission spectrum that can be used to differentiate between one element and another.

Sodium Bright yellow (intense, persistent)

Potassium Pale violet (slight, fleeting)

Calcium Brick red (medium, fleeting)

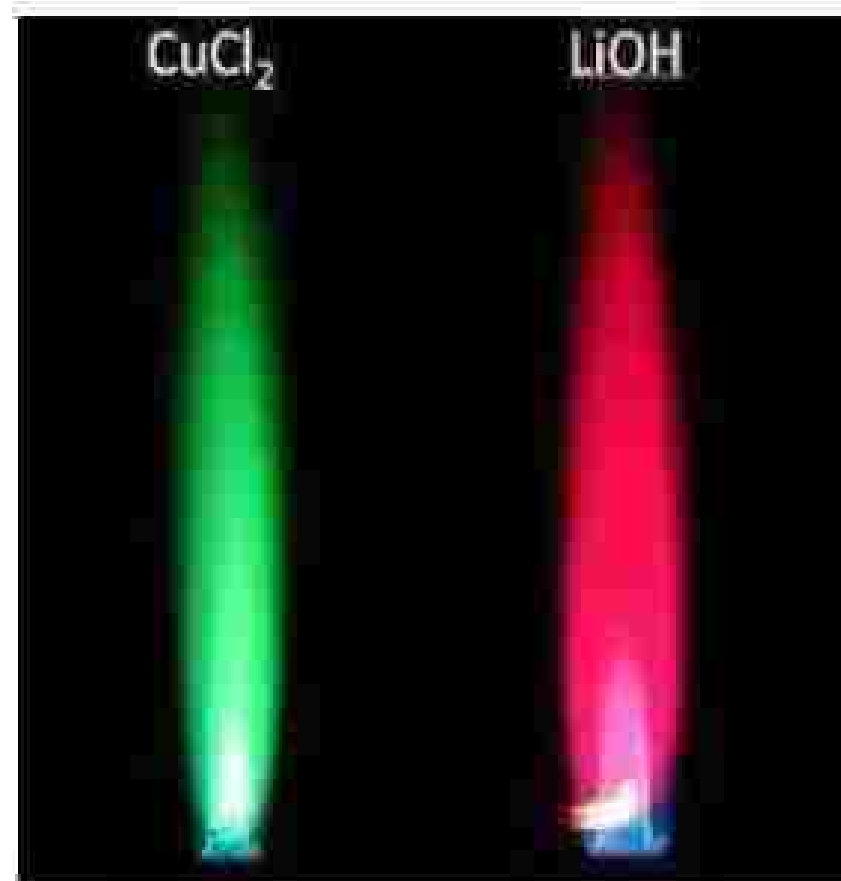
Strontium Crimson (medium)

Barium Light green (slight)

Lead Pale bluish (slight, fleeting)

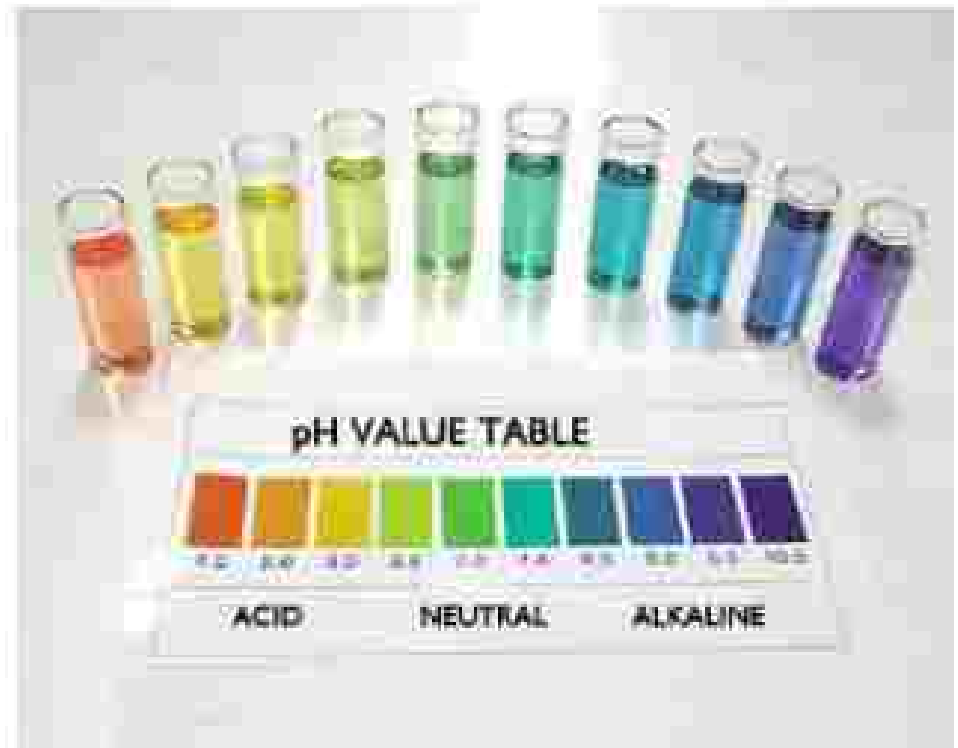
Copper Green or blue (medium, persistent)

Flame test as qualitative analysis of cations



Quantitative analysis

- It determines number of moles or mass of particular substance in a sample.



Methods used in quantitative analysis involve:

- classical methods

 - ✓ gravimetric,

 - ✓ volumetric,

- Instrumental methods

 - Electroanalytical (potentiometry, conductometry)

 - Spectroscopic (UV-VIS, IR, AAS, FES)

 - Mass spectrometry

 - Methods which involve both separation and quantitative analysis (chromatography, electrophoresis)

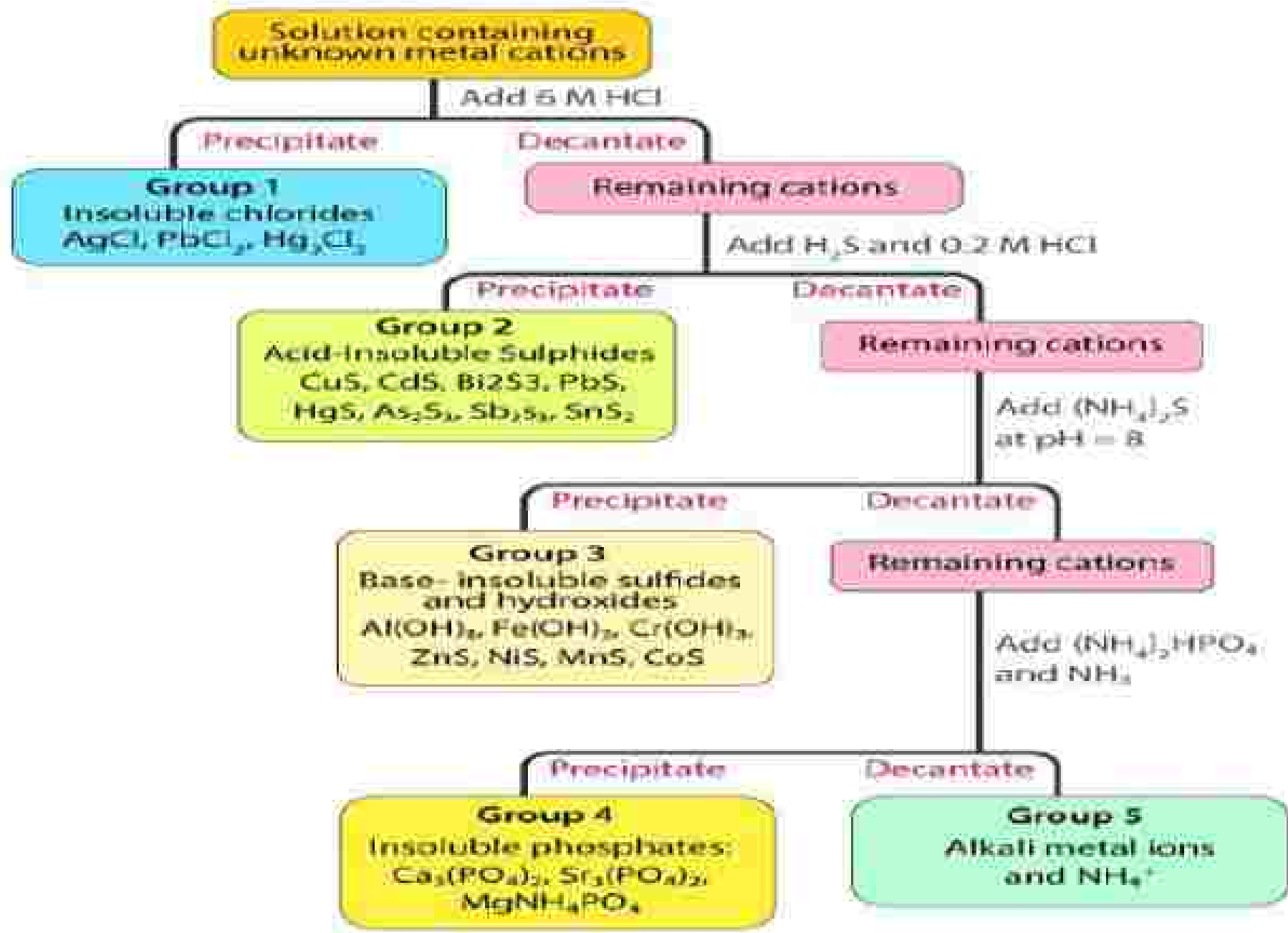
 - Other

Determination of cation or anion (inorganic)

The procedure is based on treating the solution with a succession of reagents which are specified to a certain group of constituents.

The groups are then treated successively with reagents that divide a large group into subgroups or separate the constituents singly.

Portions of the material are dissolved separately, and different procedures are used for each to detect the cationic and anionic constituents



Analysis of organic compounds

The organic nature of a compound is generally indicated by its behaviour on being heated in the air. Solids usually melt, then burn with either a smoky or nonsmoky flame, in some instances leaving a black residue of carbon.

The following elements are usually present in these compounds: carbon, hydrogen, oxygen, nitrogen, sulfur, occasionally, phosphorus, halogens, and some metals. Specific tests are available for each of the individual elements.

Classical methods of quantitative analysis

Gravimetric analysis (gravimetry)

is the quantitative isolation of a substance by precipitation and weighing of the precipitate.

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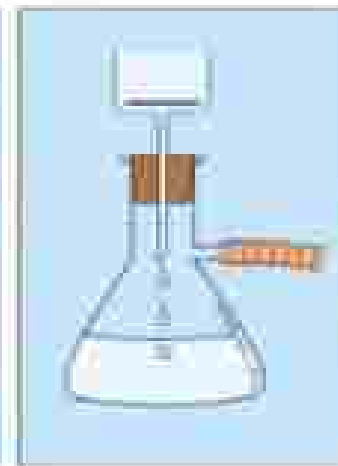
(a) Weighing the sample to be analysed



(b) Dissolving this sample in water



(c) Adding a suitable chemical to form a precipitate



(d) Filtering to collect the precipitate



(e) Repeated drying and weighing until a constant mass of precipitate is obtained

Procedure of gravimetric analysis:

- Weigh the sample to be analyzed
- Dissolve the sample in a suitable solvent, e.g., water
- Add an excess of the precipitating reagent to precipitate the analyte
- Filter the mixture to separate the precipitate from the solution
- Wash the precipitate to remove any impurities
- Dry the precipitate by heating to remove water
- Cool the precipitate in a desiccator to prevent the precipitate absorbing moisture from the air
- Weigh the cooled precipitate
- Repeat the drying and weighing process until a constant mass for the precipitate is achieved

Gravimetric analysis yields more accurate data about the composition of a sample than volumetric analysis does. However, the first one takes more time to perform in the laboratory. Volumetric analysis in the other side doesn't take that much time and the results that we obtain are in the most cases satisfactory.

There are two main areas of application for gravimetric methods:

1. Analysis of standards to be used for the testing and calibration of instrumental techniques.
2. Analysis requiring high accuracy, although the time consuming nature of gravimetry limits this application to small numbers of determinations

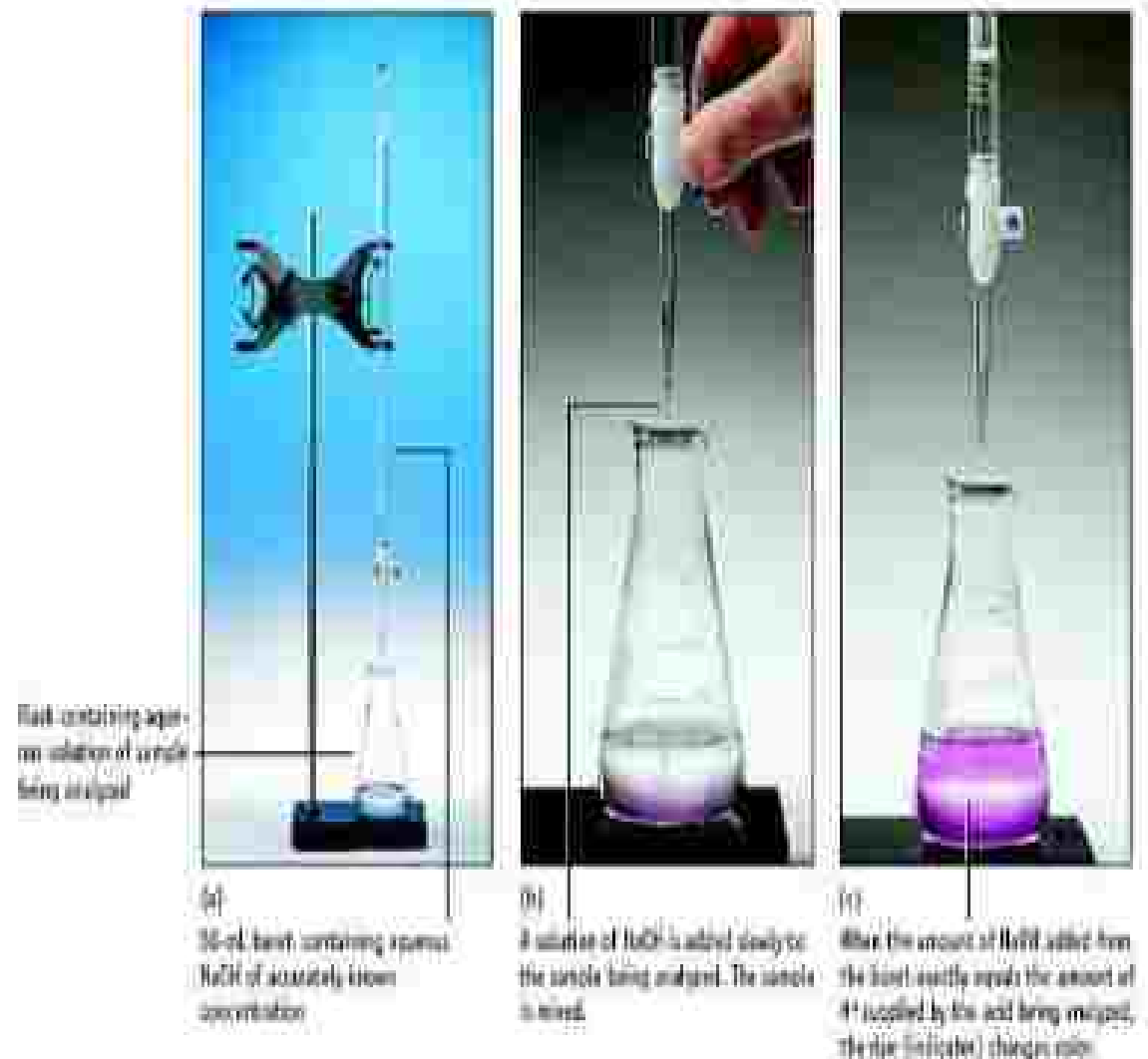
Volumetric analysis

(Simple Titration)

Volumetric analysis is the use of the titration technique to determine the concentration of a solution whose concentration is not known.

In a titration, a measured volume of a solution of known concentration is added (from a burette) to a known volume of another solution (measured from a pipette) whose concentration we don't know until the reaction is complete.

The point at which the reaction is complete,



(Volumetric analysis)

Titrant :is the substance whose solution is used to estimate the concentration of the unknown solution.

Titrate: is the substance whose concentration is to be estimated.

classification of Simple Titration

Simple titration can be classified into four different types:

- Acid-base titrations
- Redox titrations
- Precipitation titrations
- Complexometric titrations

Rules for successful volumetric analysis

- The titrant should either be a standard or be standardized.
- The reaction should proceed to a stable and well defined equivalence point.
- The equivalence point must be able to be detected.
- The titrant's and sample's volume or mass must be accurately known.
- The reaction must proceed by a definite chemistry.
- The reaction should be nearly complete at the equivalence point.
- The reaction rate should be fast enough to be practical

Application of volumetric analysis

Volumetry analyses:

1. wastewater e.g. measure ammonia levels in combination with other reactants to quantify other chemicals present.
2. food products - help determine their nutritional implications.e.g. acidity of the orange juice
3. pharmaceutical industry to ensure quality control or to make the process more efficient.

primary standard

In chemistry, a **primary standard** is a [reagent](#) that is very pure, stable, not hygroscopic, and has a high molecular weight. Ideally, it's also non-toxic, inexpensive, and readily available. A primary standard provides a reference to find unknown concentrations in titrations and is used to prepare secondary standards and working solutions.

Primary Standard in Chemistry

A primary standard is a chemical reagent used to make standard solutions for titration and preparing secondary standards.

- High purity
- High stability
- High equivalent weight
- Not hygroscopic
- Low toxicity
- Inexpensive
- Readily available



secondary standard

A **secondary standard** is a reagent that has been standardized against a primary standard. In other words, a secondary standard's concentration is known by titrating it against a measured volume of a primary standard instead of by weighing it out and dissolving it in a solvent. A secondary standard may be less pure and more reactive than a primary standard, but it still upholds some of the properties of a standard. It's stable enough that its concentration remains known for a long time. Sodium hydroxide (NaOH) is a common secondary standard.

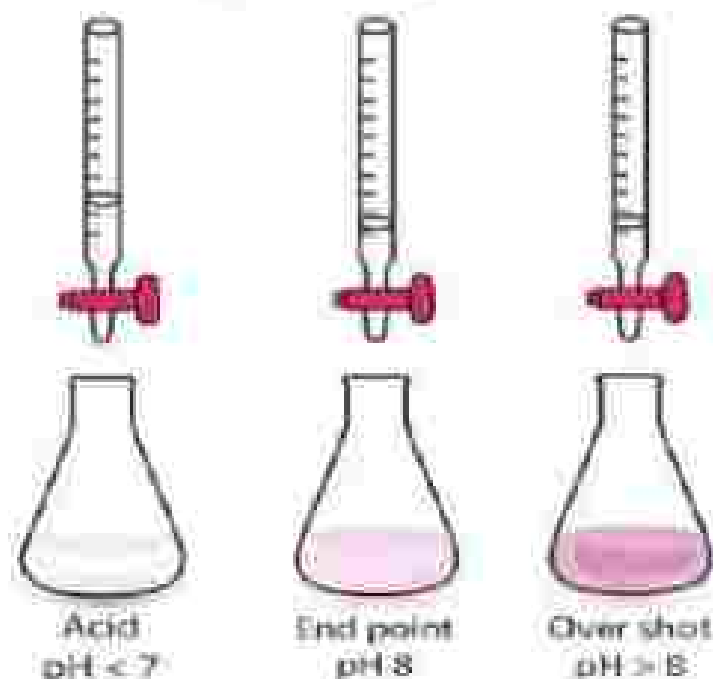


Indicators

Chemical indicators are organic substances that are used to determine the endpoint. Indicators are generally weak acids or weak bases. Indicators change their colors at a certain pH range due to ionization. Unionized forms essentially have a different color than ionized forms. Most of the pH indicators work at a pH range from 3 to 11. Commonly used indicators are phenolphthalein, litmus, methyl oranges, etc



Acid-base titration
Phenolphthalein pH indicator



Acid-base indicators

Acid-base indicators are weak acids or bases commonly used to find out the endpoint in acid/base neutralization titration. Indicators change their color with the change of pH.

Characteristics of Acid-Base Indicators

While choosing an indicator, it should have some characteristics for appropriate use. Some of them are as follows:

1. It should be chemically pure and must not react with other substances in the solution that has to be tested.
2. An indicator should remain chemically inert and must not degrade in the whole reaction.
3. When the reaction reaches the equilibrium point or end-point during titration, the indicator must have noticeable colouration.

Thank you for your
Listening



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جامعة الفرات الأوسط التقنية
المعهد التقني نجف - قسم الأدلة الجنائية

Analytical Chemistry solutions

Lecture 2 / First Stage

Presented by
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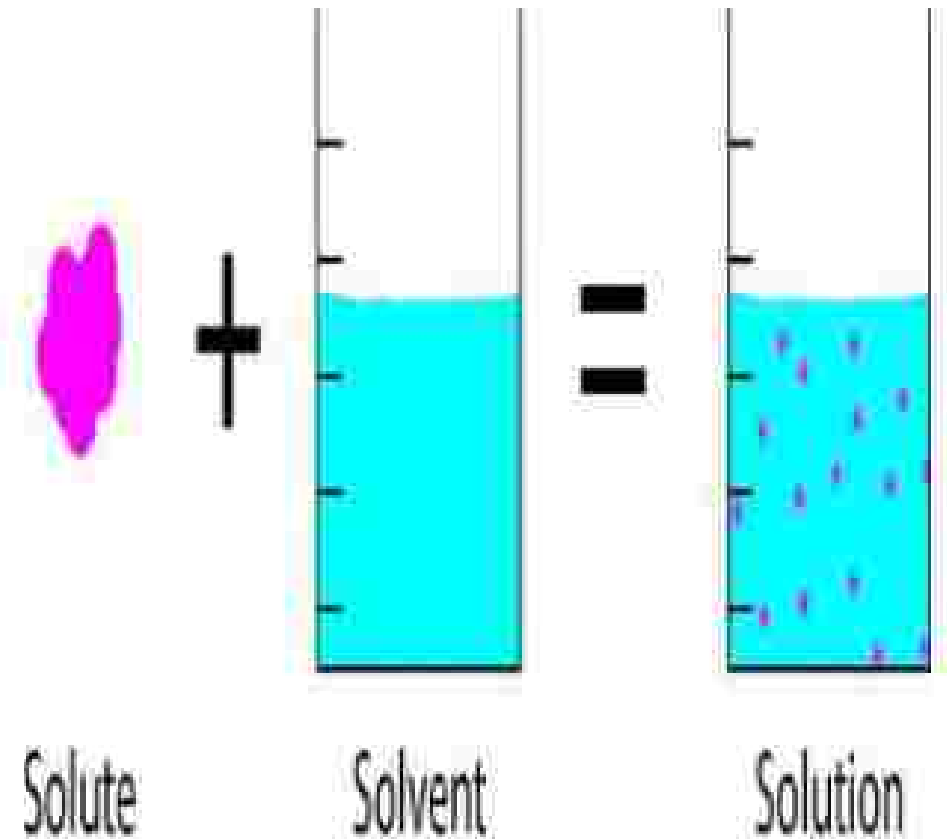
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What is a Solution in Chemistry?

Solution: Homogeneous mixture of two or more substances produced from dissolved (disappeared) solute particles (ions, atoms, molecules) (lesser amount) between solvent particles (larger amount).

Concentrated Solution has a large amount of solute.

Dilute Solution has a small amount of solute.



Classification of solutions according to amount of solute:

(1) **Unsaturated solutions:** if the amount of solute dissolved is less than the solubility limit, or if the amount of solute is less than capacity of solvent.

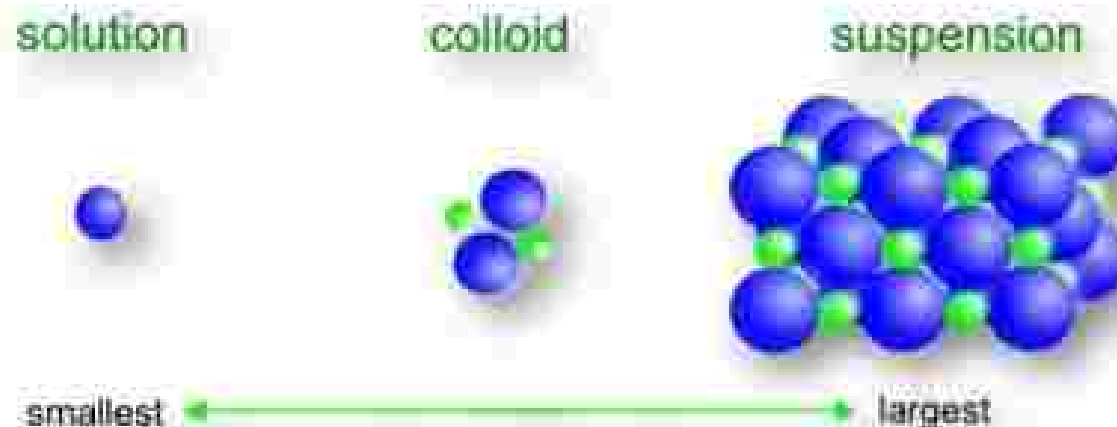
(2) **Saturated solutions:** is one in which no more solute can dissolve in a given amount of solvent at a given temperature, or if the amount of solute equal to capacity of solvent.

(3) **Super saturated solutions:** solution that contains a dissolved amount of solute that exceeds the normal solubility limit (saturated solution). Or a solution contains a larger amount of solute than capacity of solvent at high temperature.



Classification of solution based on solute particle size:

- (1) True solution: A homogeneous mixture of two or more substance in which substance (solute) has a particle size less than 1 nm dissolved in solvent. Particles of true solution cannot be filtered through filter paper and are not visible to naked eye (NaCl in water).
- (2) Suspension solution: heterogeneous mixtures which settles on standing and its components can be separated by filtrating (Amoxycycline Antibiotics), particle of solute visible to naked eye.
- (3) Colloidal solution: homogeneous mixture which does not settle nor are their components filterable, solute particle visible with electron microscope (milk).



How do we express concentrations
of solutions

Important Terms

Mole Concept:-

Mole: which is Avogadro's number (6.022×10^{23}) of atoms, molecules, ions or other species. Numerically: it is the atomic, molecular, or formula weight of a substance expressed in grams.

$$\text{The number of moles (n)} = \frac{\text{weight of substance (w)}}{\text{molar mass of substance (M)}}$$

$$n = \frac{w}{M}$$

Molecular Mass

Molecular Mass: The sum of the atomic masses of all atoms in a molecule.

For example, the molecular mass of water, which has two atoms of hydrogen and one atom of oxygen, is 18 (i.e., $2 + 16$). Also called *molecular weight*.

Example:

What is the mass molar of Calcium sulfate, Heptahydrate, $\text{CaSO}_4 \cdot 7\text{H}_2\text{O}$?

(Ca = 40.08 , S = 32.06 , O = 16 , H = 1.01)

$$\begin{aligned}\text{CaSO}_4 \cdot 7\text{H}_2\text{O} &= 40.08 + 32.06 + (16.0 \times 4) + 7[(2 \times 1.01) + 16.00] \\ &= 262.25 \text{ g/mol}\end{aligned}$$

Periodic Table of the Elements

Number
Symbol
Name
Mass

1 H Hydrogen 1.008																	2 He Helium 4.003
3 Li Lithium 6.941	4 Be Beryllium 9.012											5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305											13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.065	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.96	35 Br Bromine 79.904	36 Kr Krypton 83.798
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.94	43 Tc Technetium 98.906	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.36	47 Ag Silver 107.868	48 Cd Cadmium 112.415	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.757	52 Te Tellurium 127.6	53 I Iodine 126.905	54 Xe Xenon 131.29
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71 Lanthanide Series	72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.222	78 Pt Platinum 195.084	79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium 209	85 At Astatine 210	86 Rn Radon 222
87 Fr Francium 223	88 Ra Radium 226	89-103 Actinide Series	104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 266	107 Bh Bohrium 264	108 Hs Hassium 277	109 Mt Meitnerium 268	110 Ds Darmstadtium 285	111 Rg Roentgenium 282	112 Cn Copernicium 285	113 Nh Nihonium 284	114 Fl Flerovium 289	115 Mc Moscovium 288	116 Lv Livermorium 293	117 Ts Tennessine 294	118 Og Oganesson 294

Lanthanide Series	57 La Lanthanum 138.905	58 Ce Cerium 140.12	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.054	71 Lu Lutetium 174.967
Actinide Series	89 Ac Actinium 227	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium 252	100 Fm Fermium 257.105	101 Md Mendelevium 258	102 No Nobelium 259	103 Lr Lawrencium 262

Alkali Metal	Alkaline Earth	Transition Metal	Base Metal	Metalloid	Nonmetal	Halogens	Noble Gas	Lanthanide	Actinide
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1-A :- Molarity concentration for solutions prepared from dissolving solid solute in liquid solvent:-

Molarity:- defined as a number of solute moles dissolved in solution volumes in litre.

$$\text{Molarity (M)} = \frac{\text{No. of mole solute}}{\text{solution volume (L)}} = \frac{\text{mole}}{\text{L}}$$

$$\text{Molarity (M)} = \frac{\text{No. of mmole solute}}{\text{solution volume (mL)}} = \frac{\text{mmole}}{\text{mL}}$$

$$M = \frac{\text{No of mole solute}}{\text{Volume solution (L)}} = \frac{\frac{\text{wt (g)}}{\text{M.wt } (\frac{\text{g}}{\text{mole}})}}{\frac{V (\text{mL})}{1000 (\frac{\text{mL}}{\text{L}})}} = \frac{\text{wt (g)}}{\text{M.wt } (\frac{\text{g}}{\text{mole}})} \times \frac{1000}{V (\text{mL})}$$

Example (1):- A solution is prepared by dissolving 1.26 gm AgNO₃ in a 250 mL volumetric flask and diluting to volume. Calculate the molarity of the silver nitrate solution. How many millimoles AgNO₃ were dissolved.

Solution:

$$M = \frac{\text{wt (g)}}{\text{M. wt } \left(\frac{\text{g}}{\text{mol}}\right)} \times \frac{1000}{V \text{ (mL)}}$$
$$= \frac{1.26 \text{ (g)}}{169.9 \left(\frac{\text{g}}{\text{mol}}\right)} \times \frac{1000}{250 \text{ (mL)}} = 0.0297 \text{ mol/L}$$

$$\text{Millimoles} = M \left(\frac{\text{mmol}}{\text{mL}}\right) \times V \text{ (mL)}$$
$$= 0.0297 \left(\frac{\text{mmol}}{\text{mL}}\right) \times 250 \text{ mL} = 7.42 \text{ mmole}$$

Example (2):-How many grams per millilitre of NaCl are contained in a 0.250 M solution?

$$M = \frac{\text{wt (g)}}{\text{M. wt } \left(\frac{\text{g}}{\text{mol}}\right)} \times \frac{1000}{V \text{ (mL)}}$$

$$0.250 \text{ M} = \frac{\text{wt (g)}}{58.4 \left(\frac{\text{g}}{\text{mol}}\right)} \times \frac{1000}{1 \text{ (mL)}} , \quad \text{wt (g)} = 0.0146 \frac{\text{g}}{\text{mL}}$$

Homework

How many grams Na₂SO₄ should be weight out to prepare 500 mL of a 0.100 M solution?

1-B:-Molarity concentration for solution prepared from dissolved liquid solute in liquid solvent.

$$\mathbf{M = \frac{\% \times \text{density} \times 1000}{\text{M. wt}} = \frac{\% \times \text{sp. gr.} \times 1000}{\text{M. wt}} =}$$

$$\% = \left(\frac{\text{wt}}{\text{wt}} \% \right) = \frac{\text{wt solute (g)}}{\text{wt solution (g)}} \times 100$$

Density: is the weight per unit volume at the specified temperature, usually (gm/mL) or (gm/cm³) or (gm.cm⁻³) in 20 C (is the ratio of the mass in (gm) and volume (mL)).

Specific gravity (sp. gr.): defined as the ratio of the mass of a body (e.g. a solution) usually at 20 C to the mass of an equal volume of water at 4 C (or sometimes 20 C) or (is the ratio of the densities of the two substances).

Example (1):-Calculate the molarity of 28.0% NH₃, specific gravity 0.898.

Solution:

$$\text{M. wt NH}_3 = 14 + (3 \times 1) = 17$$

$$M = \frac{\% \times \text{sp. gr. or (density)} \times 1000}{\text{M. wt}}$$

$$M = \frac{\frac{28}{100} \times 0.898 \times 1000}{17} = 16.470 \frac{\text{mol}}{\text{L}} = 16.470 \frac{\text{mmol}}{\text{mL}} = 16.470 \text{ M}$$

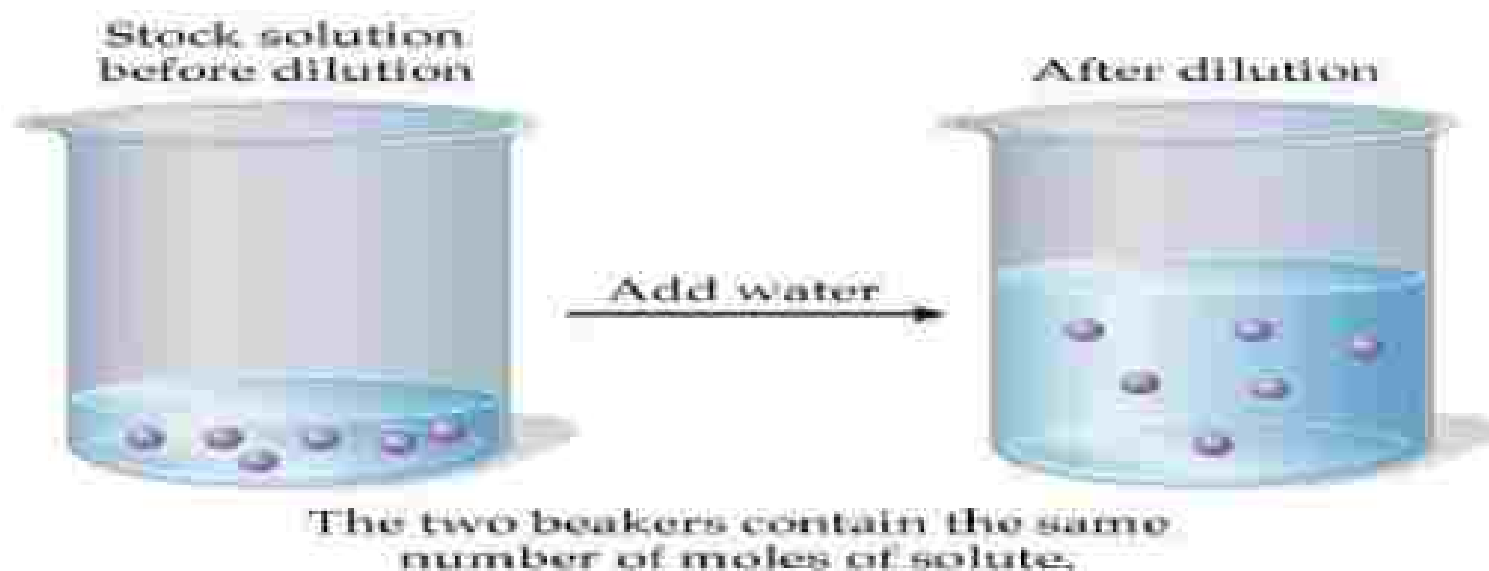
Diluting Solutions:-

We often must prepare dilute solutions from more concentrated stock solutions. For example, we may prepare a dilute HCl solution from concentrated HCl to be used for titration. Or, we may have a stock standard solution from which we wish to prepare a series of more dilute standards. The millimoles of stock solution taken for dilution will be identical to the millimoles in the final diluted solution.



What happens to the volume and concentration in a dilution?

When additional water is added to an aqueous solution, the **concentration** of that solution ***decreases***. This is because the **number of moles** of the solute ***does not change***, while the **volume** of the solution ***increases***



Example (2) :-How many millilitres of concentrated sulphuric acid, 94.0% (g/100g solution), density 1.831 g/cm³, are required to prepare 1 liter of a 0.100 M solution.

$$M = \frac{\frac{94}{100} \times 1.831 \times 1000}{98.1} = 17.5 \left(\frac{\text{mmol}}{\text{mL}} \right)$$

$$\text{no. of mmol (conc.)} = \text{no. mmol (dilu.)}$$

$$(M_1 \times V_1)_{\text{conc.}} = (M_2 \times V_2)_{\text{dilu.}}$$

$$17.5 \times V_1 = 0.1 \times 1000$$

$$V_1 = 5.71 \text{ mL}$$

Example ():-You wish to prepare 500 mL of 0.1 M $K_2Cr_2O_7$ solution from a 0.250 M solution. What volume of the 0.250 M solution must be diluted to 500 mL.

$$(\text{no. of mmol})_{\text{conc.}} = (\text{no. of mmol})_{\text{dilu.}}$$

$$(M_1 \times V_1)_{\text{conc.}} = (M_2 \times V_2)_{\text{dilu.}}$$

$$0.250 \left(\frac{\text{mmol}}{\text{mL}} \right) \times V_1(\text{mL}) = 0.1 \left(\frac{\text{mmol}}{\text{mL}} \right) \times 500 \text{ mL}$$

$$V_1 = 200 \text{ mL}$$

Example ():-You wish to prepare a calibration curve for the spectrophotometric determination of permanganate. You have a stock 0.100 M solution of KMnO_4 and a series of 100 mL volumetric flasks. What volumes of the stock solution will you have to pipet into the flasks to prepare standards of 1.00, 2.00, 5.00, and 10.0×10^{-3} M KMnO_4 solutions.

Solution-1: 1.0×10^{-3} M

$$(M_1 \times V_1)_{\text{conc.}} = (M_2 \times V_2)_{\text{dilu.}}$$

$$0.1 \left(\frac{\text{mmol}}{\text{mL}} \right) \times V_1 = 1.0 \times 10^{-3} \left(\frac{\text{mmol}}{\text{mL}} \right) \times 100 \text{ (mL)}$$

$V_1 = 1.0$ mL stock solution (conc.), Also to prepare 2.0, 5.0, 10.0×10^{-3} M

Percentage Concentration

Mass Percent: The mass percent is used to express the concentration of a solution when the mass of a solute and the mass of a solution is given:.

$$\left(\frac{\text{wt}}{\text{wt}}\right)\% = \frac{\text{wt solute (g)}}{\text{wt solution or sample (g)}} \times 100$$
$$= \frac{\text{wt solute (mg)}}{\text{wt solution or sample (mg)}} \times 100$$



Mass/Volume Percent : Another version of a percentage concentration is mass/volume percent, which measures the mass or weight of solute vs. the volume of solution. An example would be a 0.9% (w/v) NaCl solution in medical saline solutions that contains 0.9 g of NaCl for every 100 mL of solution

$$\left(\frac{\text{wt}}{\text{V}}\right)\% = \frac{\text{wt solute (g)}}{\text{V solution or sample (mL)}} \times 100$$
$$= \frac{\text{wt solute (mg)}}{\text{V solution or sample (\mu\text{L})}} \times 100$$



Volume Percent: The volume percent is used to express the concentration of a solution when the volume of a solute and the volume of a solution is given:

$$\left(\frac{V}{V}\right)\% = \frac{V \text{ solute (mL)}}{V \text{ solution or sample (mL)}} \times 100$$
$$= \frac{V \text{ solute } (\mu\text{L})}{V \text{ solution or sample } (\mu\text{L})} \times 100$$



Example():-Calculate the weight percentage of solution prepared by mixing 5.0g AgNO₃ with 100mL water (density 1g/cm³).

Solution:

$$\left(\frac{\text{wt}}{\text{wt}}\%\right) = \frac{\text{wt solute (g)}}{\text{wt solution (g)}} \times 100$$

$$\left(\frac{\text{wt}}{\text{wt}}\%\right) = \frac{\text{wt solute (AgNO}_3\text{)(g)}}{\text{wt solute + wt solvent (H}_2\text{O) (g)}} \times 100$$

$$\left(\frac{\text{wt}}{\text{wt}}\%\right) = \frac{5 \text{ g}}{5 \text{ g} + (100 \text{ mL} \times 1 \frac{\text{g}}{\text{mL}})} \times 100 = \frac{5 \text{ g}}{105 \text{ g}} \times 100 = 4.76\%$$

Example ():- Calculate the weight of glucose in liter solution (wt/v % = 5 %).

Solution:

$$\left(\frac{\text{wt}}{\text{V}}\%\right) = \frac{\text{wt solute (g)}}{\text{V solution (mL)}} \times 100 = \frac{\text{wt glucose (g)}}{\text{V solution (mL)}} \times 100$$

$$5\% = \frac{\text{wt glucose (g)}}{1000 \text{ (mL)}} \times 100, \quad \text{wt glucose} = \frac{5 \times 1000}{100} = 50 \text{ g}$$

Example():-Calculate the volume percentage of solution preparing by mixing 50mL methyl alcohol with 200mL water

Solution:

$$\left(\frac{V}{V}\right)\% = \frac{V \text{ solute (mL)}}{V \text{ solution or sample (mL)}} \times 100$$
$$= \frac{V \text{ methyl alcohol (mL)}}{V \text{ methyl alcohol} + V \text{ water (mL)}} \times 100 = \frac{50 \text{ mL}}{(50 + 200)\text{mL}} \times 100 = 20\%$$

Concentration in parts per million

$$\text{part per million (ppm)} \left(\frac{\text{wt}}{\text{wt}} \right) = \frac{\text{wt solute (g)}}{\text{wt solution (sample)(g)}} \times 10^6 = \frac{\text{wt } (\mu\text{g})}{\text{wt (g)}} = \frac{\text{wt (mg)}}{\text{wt (kg)}}$$

$$\text{part per million (ppm)} \left(\frac{\text{wt}}{\text{V}} \right) = \frac{\text{wt solute (g)}}{\text{V solution (sample)(mL)}} \times 10^6 = \frac{\text{wt } (\mu\text{g})}{\text{V (mL)}} = \frac{\text{wt (mg)}}{\text{V (L)}}$$

Example : 2.6 g sample of plant tissue was analyzed and found to contain 3.6 μg zinc, what is the concentration of zinc in the plant in ppm?

$$\text{ppm} = \frac{\text{wt } (\mu\text{g})}{\text{wt } (\text{g})} = \frac{3.6 \mu\text{g}}{2.6 \text{ g}} = 1.4 \frac{\mu\text{g}}{\text{g}} = 1.4 \text{ ppm}$$

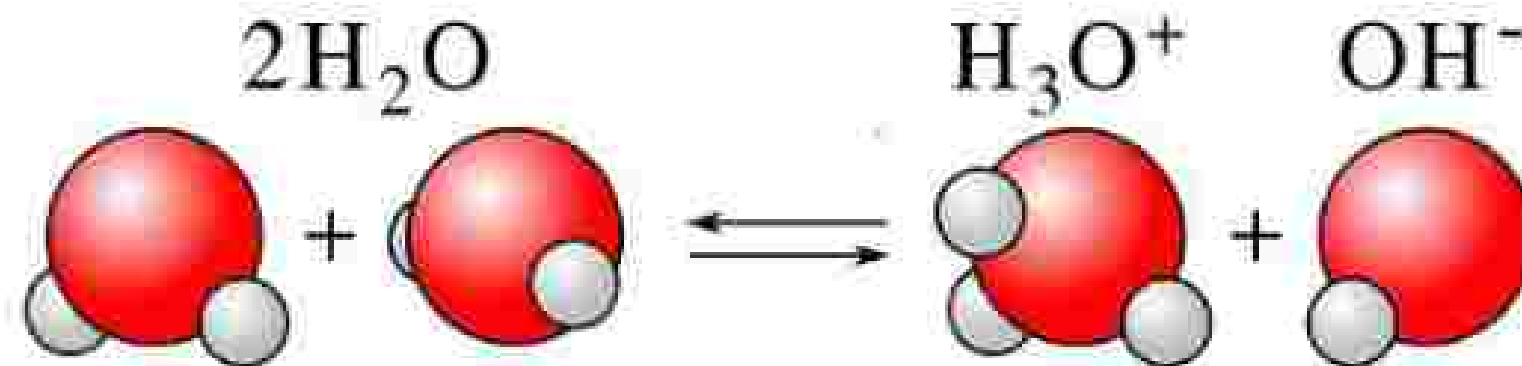
Example :- 25.0 μL serum sample was analyzed for glucose content and found to contain 26.7 μg . Calculate the concentration of glucose in ppm.

$$\begin{aligned}\text{ppm} &= \frac{\text{wt } (\mu\text{g})}{\text{V (mL)}} = \frac{26.7 (\mu\text{g})}{\frac{25.0 (\mu\text{L})}{1000 \left(\frac{\mu\text{L}}{\text{mL}}\right)}} = \frac{26.7 (\mu\text{g})}{0.025 (\text{mL})} \\ &= 1.07 \times 10^3 \left(\frac{\mu\text{g}}{\text{mL}}\right) = 1.07 \times 10^3 \text{ ppm}\end{aligned}$$

Thank you for your
Listening

Water Ionization

Pure water or distilled water is amphoteric in nature. This means that in its pure state, water goes through the self-ionization process. **Self-ionization** in this case, means that water molecules donate and accept protons to form H_3O^+ and OH^- ions. The former hydronium ion acts as a strong acid, the latter hydroxide ion is a strong base.



When they come together, they form a water molecule ion. Water maintains a state of equilibrium where both hydronium and hydroxide ions are present, but the state of equilibrium leans to the left side of the water molecule equation. Hence, the concentration of these ions is comparatively less in the water.

The **equilibrium constant** for this autoionisation of water is known as K_w .

Thus

$$K_w = [\text{H}_3\text{O}^+] [\text{OH}^-]$$

Or simply

$$K_w = [\text{H}^+] [\text{OH}^-]$$

Acids and bases can be defined via three different theories.

- The *Arrhenius theory* of acids and bases states that “an acid generates H^+ ions in a solution whereas a base produces an OH^- ion in its solution”.
- The *Bronsted-Lowry theory* defines “an acid as a proton donor and a base as a proton acceptor”.
- Finally, the *Lewis definition* of acids and bases describes “acids as electron-pair acceptors and bases as electron-pair donors”.

pH of pure water

For pure water the concentration of $[H^+]$ and $[OH^-]$ ions are same.
That means, $[H^+] = [OH^-]$

So, from equation ($K_w = [H^+] [OH^-]$) we can write,

$$K_w = [H^+]^2 \quad \text{As} \quad K_w = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$$

$$[H^+]^2 = 1.00 \times 10^{-14} \text{ mol}^2 \text{ dm}^{-6}$$

$$\text{Thus} \quad [H^+] = 1.00 \times 10^{-7} \text{ mol dm}^{-3}$$

$$\text{And} \quad \text{pH} = -\log [H^+] = -\log (1.00 \times 10^{-7}) \quad \text{So} \quad \text{pH} = 7$$

So, we can say that the pH of the pure water is 7. And the concentration of $[H^+] = [OH^-] = 10^{-7} \text{ mol dm}^{-3}$.

Acidic, basic and neutral solution

In pure water the concentration of hydronium ion and hydroxide ion are same and equal to 10^{-7} M at 25° C . This types of solution is known as neutral solution. But depending on the difference between their concentration, the solution is named as acidic or basic. Such as

- If $[H^+] = [OH^-]$, it is a neutral solution.
- If $[H^+] > [OH^-]$, it is an acidic solution.
- If $[H^+] < [OH^-]$, it is a basic solution.

Relation between pH and pOH from K_w

We can derive a relation between pH and pOH from the equation below:

$K_w = [H^+][OH^-]$ Taking logarithm on both side, we get

$$\log K_w = \log [H^+] + \log [OH^-]$$

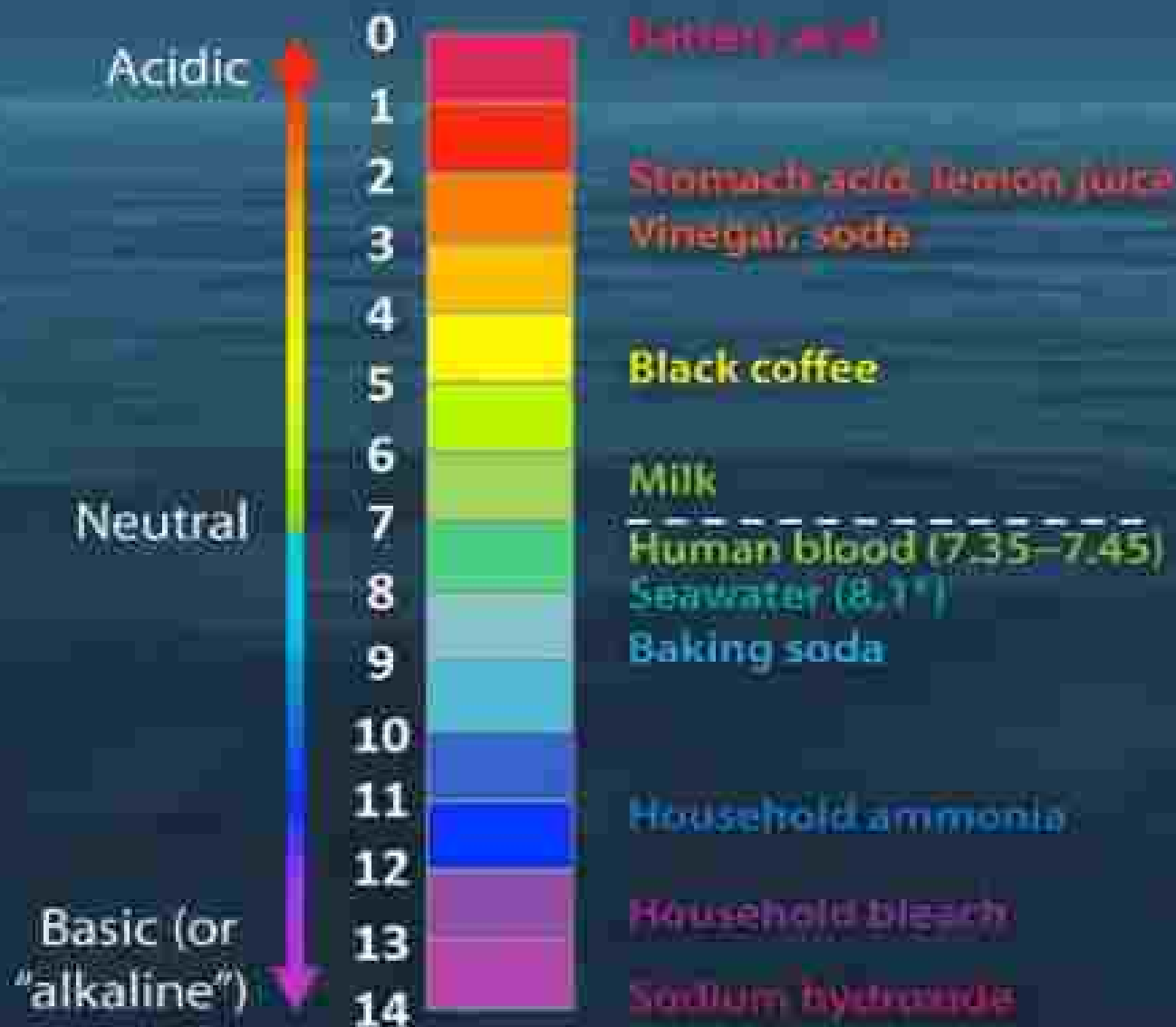
Or $-\log K_w = -\log [H^+] - \log [OH^-]$

So $pK_w = pH + pOH$

As $pK_w = 14$

Thus **$pH + pOH = 14$** .

Using this relation we can solve many problems of pH and pOH.



* Average global surface ocean pH

The pH scale, with examples of common solutions and their pH values

Example:- Calculate the pOH and pH of a 5×10^{-2} M NaOH ?

$$[\text{OH}^-] = 5 \times 10^{-2} \text{ M} \quad \text{pOH} = -\log[\text{OH}^-]$$

$$= -\log(5 \times 10^{-2}) = 2 - \log 5 = 2 - 0.70 = 1.30$$

$$\text{pH} + \text{pOH} = 14 \quad \text{pH} = 14 - \text{pOH} = 14 - 1.30 = 12.70$$

Example:- Calculate the pH of a 2×10^{-3} M HCl ?

$$[\text{H}^+] = 2 \times 10^{-3} \quad \text{pH} = -\log[\text{H}^+]$$

$$= -\log(2.0 \times 10^{-3}) = 3 - \log 2.0 = 2.70$$

Buffer solution

Buffers:- solutions that resist change in pH on dilution or on the addition of small amounts of acids or alkali.

A lot of biological and chemical reactions need a constant pH for the reaction to proceed. Buffers are extremely useful in these systems to maintain the pH at a constant value. This does not mean that the pH of buffers does not change. It only means that the change in pH is not as much as it would be with a solution that is not a buffer.



Properties and Types of buffer solutions

Properties of buffer solution are:

1. Its pH doesn't change even when kept for a long time.
2. On diluting the solution, its pH value doesn't change.
3. The solution doesn't shift by adding a little proportion of acid or base.

There are two types of buffer solutions:

- **Acidic buffer solution** : A solution of a weak acid and its salts containing strong bases.

E.g., A solution with CH_3COOH , which is weak acid and CH_3COONa , which is its salt is an acidic buffer solution.

- **Basic buffer solution** : A solution of a weak base and its salt-containing strong acids.

E.g., A solution with NH_4OH as a weak base and NH_4Cl , which is its salt, is an essential buffer solution.

What do you think will happen if the pH of our blood changes from its normal pH of 7.35?

The cells of our body will not function properly and our body systems will fail! Human blood contains a 'buffer' that allows it to maintain its pH at 7.35 to ensure normal functioning of cells. Buffer solutions are also important in chemical and biochemical processes where the control of pH is very important.

Thank you for your
Listening

Colorimetric Analysis

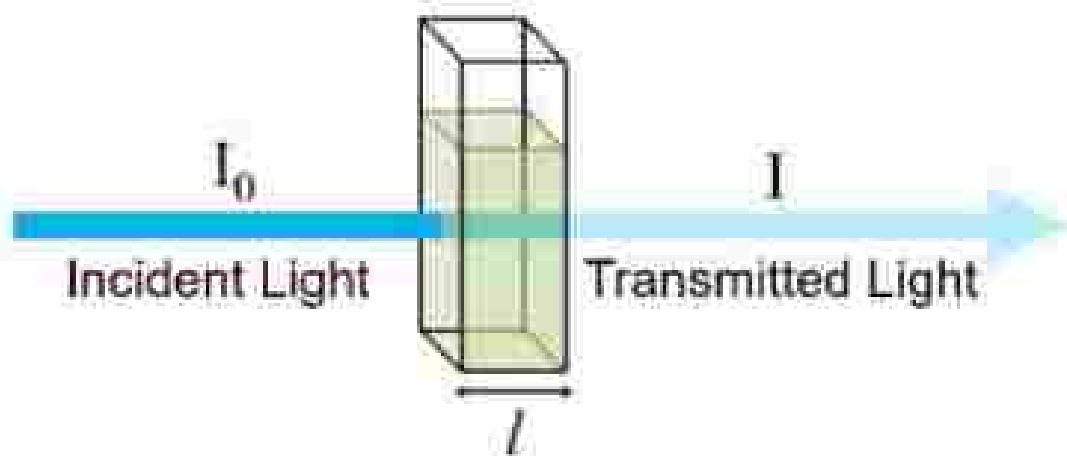
Colorimetric analysis is the **technique normally used to determine the concentration of analyte through comparing the color changes of the solution.**

What are the principles of colorimetry?

Principle of Colorimeter is that **coloured compounds can absorb a certain wavelength of light when monochromatic light is passed through them.** The working of a colorimeter is based on the concept of Beer-Lambert's law

What are Transmittance and absorbance?

Consider monochromatic light transmitted through a solution; with an incident intensity of I_0 and a transmitted intensity of I (Figure 1).



What is the Beer-Lambert Law?

The Beer-Lambert law is a linear relationship between the absorbance and the concentration, molar absorption coefficient and optical path length of a solution:

$$A = \epsilon cl$$

A	Absorbance	
ϵ	Molar absorption coefficient	$M^{-1}cm^{-1}$
C	Molar concentration	M
l	optical path length	cm

The molar absorption coefficient is a sample dependent property and is a measure of how strong an absorber the sample is at a particular wavelength of light. **a measurement of how strongly a chemical species absorbs light at a given wavelength**

The concentration is simply the moles L^{-1} (M) of the sample dissolved in the solution.

the optical path length is the width of the cuvette used for the absorbance measurement and is typically 1 cm.

The Beer-Lambert law states that there is a linear relationship between the concentration and the absorbance of the solution, which enables the concentration of a solution to be calculated by measuring its absorbance.

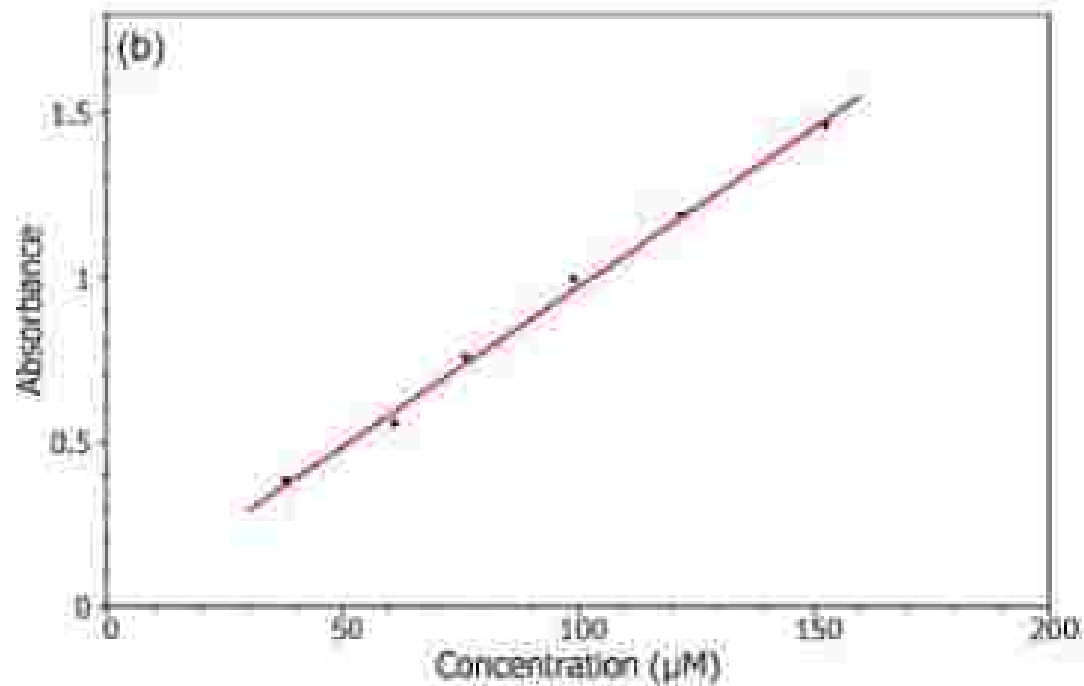
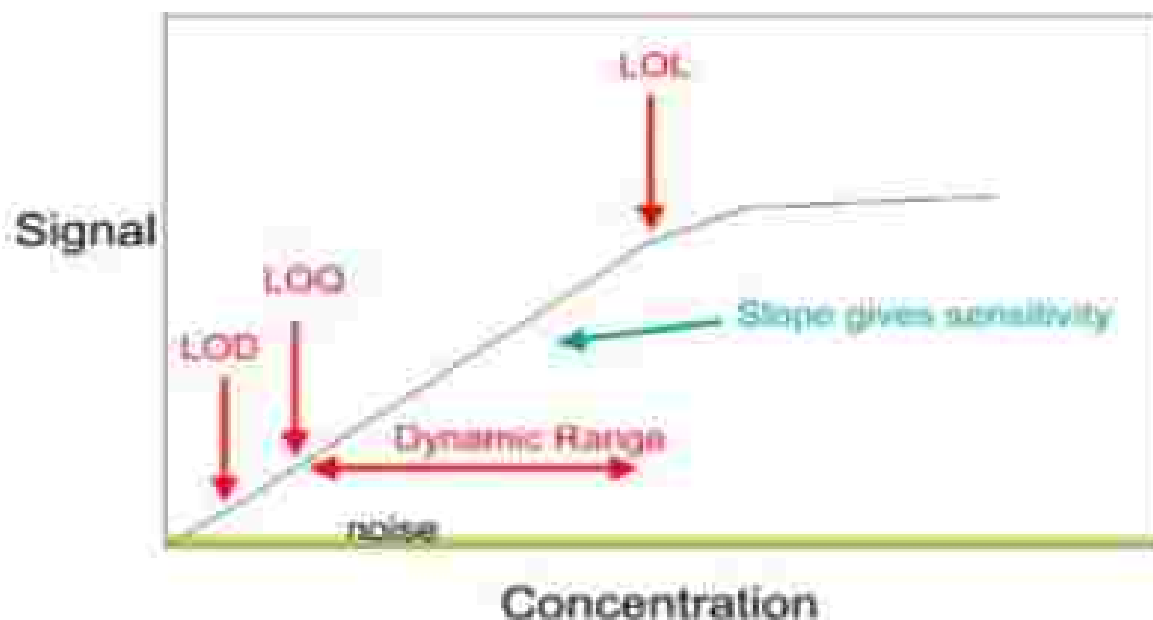


Figure2 : Calibration Curve

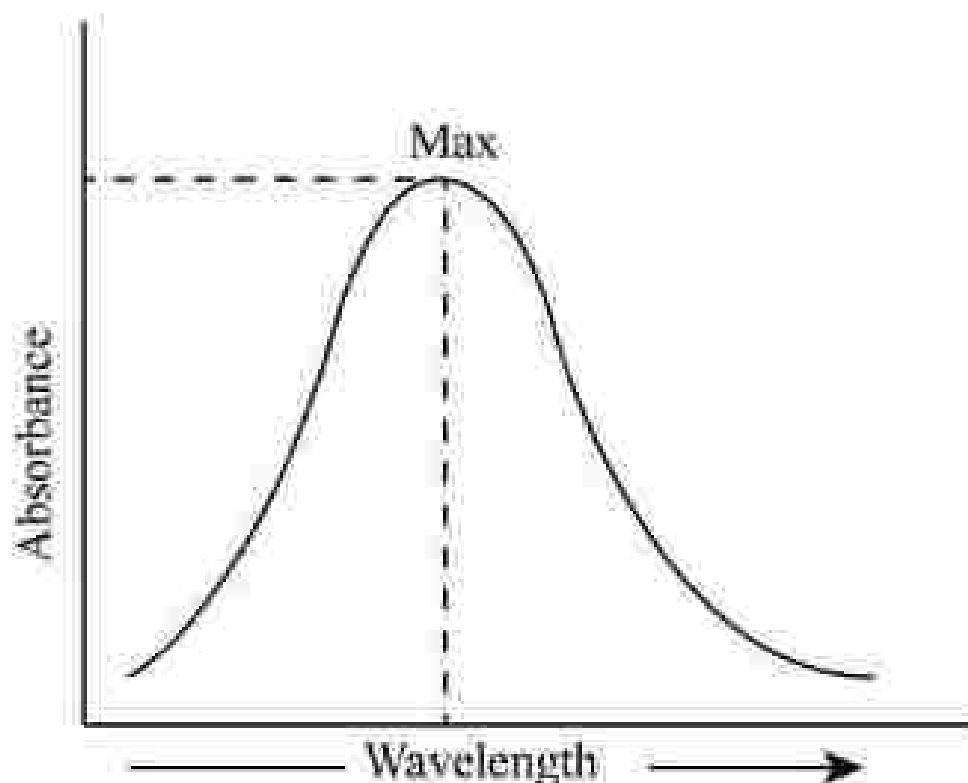
What is a standard calibration curve?

In analytical chemistry, a calibration curve, also known as a standard curve, is a general method for determining the concentration of a substance in an unknown sample by comparing the unknown to a set of standard samples of known concentration.



The Wavelength of Maximum Absorption (Lambda max: λ_{Max})

The absorption of light by the sample in the UV-visible Spectroscopy depends upon the wavelength of the light. That particular wavelength, at which the absorption by the substance is highest, is known as the wavelength of maximum absorption.



What is Colorimeter?

A colorimeter is a device that is used in Colorimetry. It refers to a device which helps specific solutions to absorb a particular wavelength of light. The colorimeter is usually used to measure the concentration of a known solute in a given solution with the help of the Beer-Lambert law.

Principle of Colorimeter

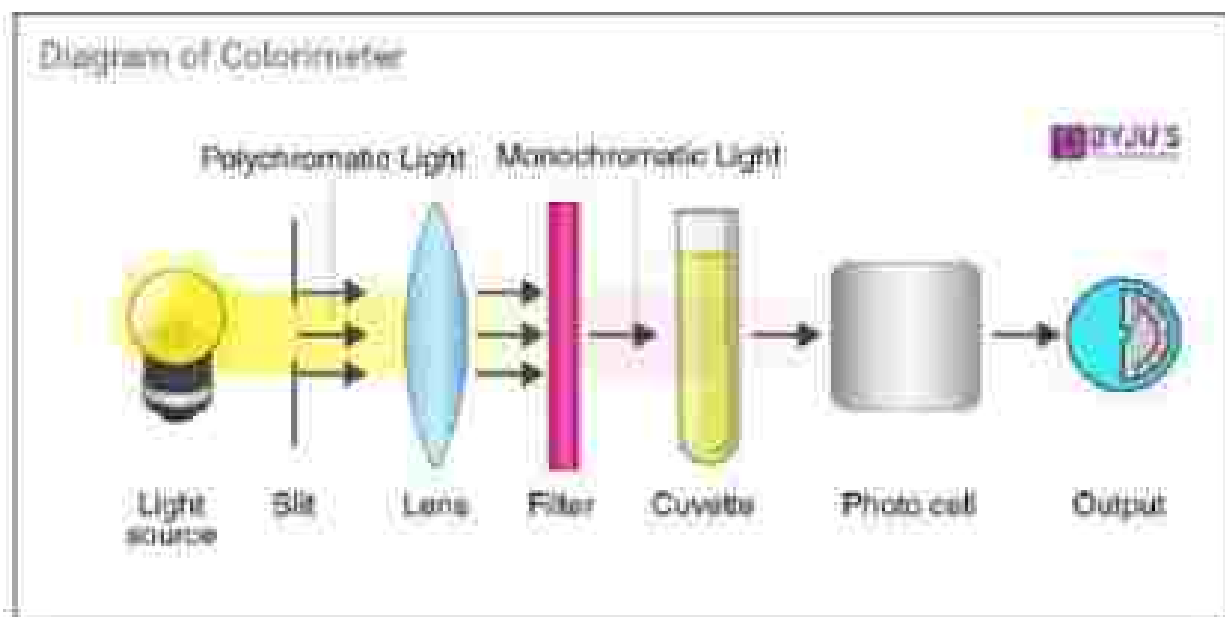
It is a photometric technique which states that when a beam of incident light of intensity I_0 passes through a solution, the following occur:

- A part of it is reflected which is denoted as I_r
- A part of it is absorbed which is denoted as I_a
- Rest of the light is transmitted and is denoted as I_t

Therefore, $I_0 = I_r + I_a + I_t$

To determine I_a the measurement of I_0 and I_t is sufficient therefore, I_r is eliminated. The amount of light reflected is kept constant to measure I_a and I_t .

Diagram of Colorimeter



Uses of Colorimeter

- It is used in laboratories and hospitals to estimate biochemical samples such as urine, plasma, serum, etc.
- It is used in the manufacturing of paints.

- It is used in textile and food industry.
- It is used in the quantitative analysis of proteins, glucose, and other biochemical compounds.
- It is used to test water quality.
- It is used to determine the concentration of haemoglobin in the blood.

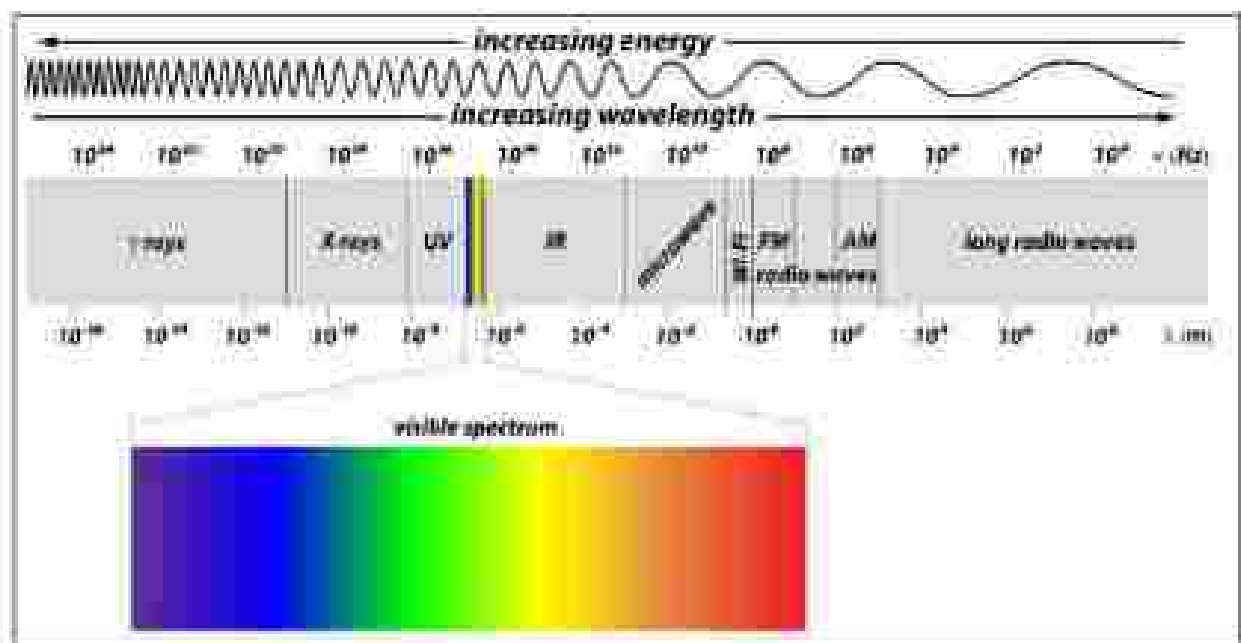
Advantages and disadvantages of colorimetry

Some benefits are as follows:

It is an inexpensive method, widely used in the quantitative analysis of coloured samples, easy to carry, and transport.

Some disadvantages are as follows:

Analysis of colourless compounds is not possible, does not work in IR and UV regions.



Electromagnetic Spectrum

Organic Chemistry

The Origins of Organic Chemistry

The modern definition of organic chemistry is *the chemistry of carbon compounds*. The term organic literally means "derived from living organisms." Originally, the science of organic chemistry was the study of compounds extracted from living organisms and their natural products. Compounds such as sugar, urea, starch, waxes, and plant oils were considered "organic," and people accepted **Vitalism**, the belief that natural products needed a "vital force" to create them. Organic chemistry, then, was the study of compounds having the vital force. Inorganic chemistry was the study of gases, rocks, and minerals, and the compounds that could be made from them.

Importance of organic chemistry

1-Medicine: Most of drugs and medical substances are organic compound

2-Foods : Food materials are solely made of carbon compounds viz carbohydrates (CHO), proteins (NH₂-CH-COOH), and fats (CH₂-COO-CH₂). Even vitamins are organic in nature.

3- Sterilizing agents: Most of the sterilizing agents and disinfectants like phenol, formaldehyde etc. are carbon compounds.

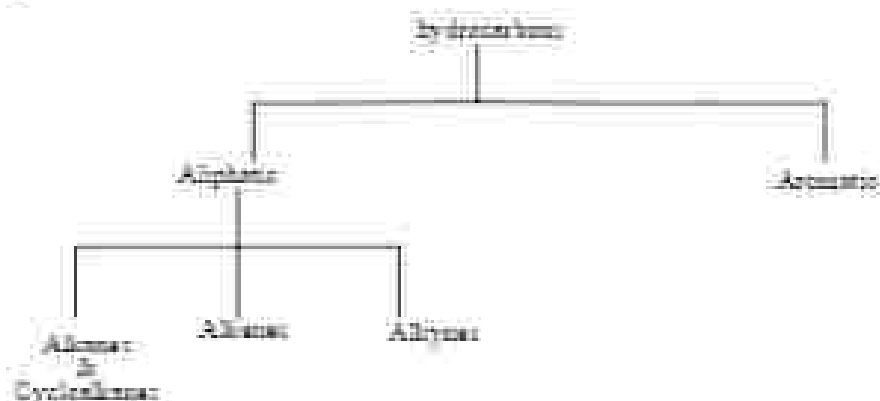
4- Valuables: Diamonds, graphite, petroleum. Interestingly the carbon compounds are found to be highly valuable, durable and hardest in the world.

5-Industry : most of clothes, tools, containers, etc are made of carbon.

6-Cleaning agents : nearly all cleaning agents are organic compounds.

Hydrocarbons

Hydrocarbons are compounds that only contain carbon and hydrogen atoms, and they can be classified as follows depending on the bond types that are present within the molecules.



Methane:



Structure of methane

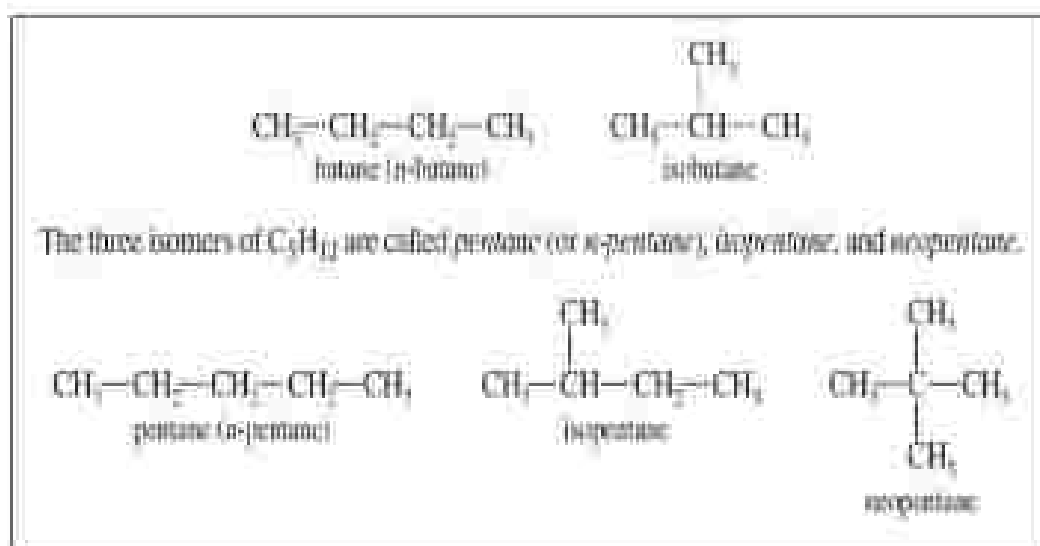
Sources of methane:

Methane is an end product of the anaerobic (without air) decay of plants. It is the major constituent (up to 97%) of natural gas and can be seen as marsh gas bubbling to the surface of swamps.

Nomenclature of Alkanes

1-Common Names

If all alkanes had unbranched (straight-chain) structures, their nomenclature would be simple. Most alkanes have structural isomers, however, and we need a way of naming all the different isomers. For example, there are two isomers of formula C₄H₁₀. The unbranched isomer is simply called *butane* (or *n-butane*, meaning “normal” butane), and the branched isomer is called *isobutane*, meaning an “isomer of butane.”



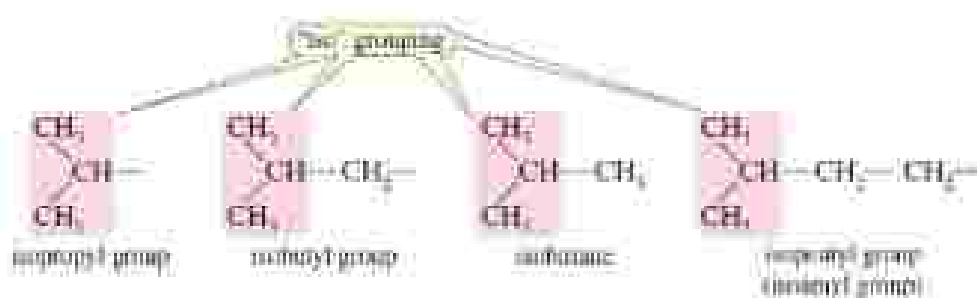
2-IUPAC Nomenclature of Alkanes

The names of alkanes and cycloalkanes are the root names of organic compounds. Beginning with the five-carbon alkane, the number of carbons in the chain is indicated by the Greek or Latin prefix. Rings are designated by the prefix "cyclo". (In the geometrical symbols for rings, each apex represents a carbon with the number of hydrogens required to fill its valence.)

NUMBER OF CARBON ATOMS	PREFIX	NAME OF ALKANE	NUMBER OF CARBON ATOMS	PREFIX	NAME OF ALKANE
1	meth	methane	11	undec	undecane
2	eth	ethane	12	dodec	dodecane
3	prop	propane	13	tridec	tridecane
4	but	butane	14	tetradec	tetradecane
5	pent	pentane	15	pentadec	pentadecane
6	hex	hexane	20	eicos	eicosane
7	hept	heptane	30	triacont	triacontane
8	oct	octane	40	tetracont	tetracontane
9	non	nonane	50	pentacont	pentacontane
10	dec	decane	100	hect	hectane

Notes

- Find the longest continuous chain of carbon atoms, and use the name of this chain as the base name of the compound.
- Number the longest chain, beginning with the end of the chain nearest a substituent.
- Name the substituent groups attached to the longest chain as alkyl groups.
- Give the location of each alkyl group by the number of the main-chain carbon atom to which it is attached.
- The simple branched alkyl groups are usually known by common names. The isopropyl and isobutyl groups have a characteristic "iso" ($(\text{CH}_3)_2\text{CH}$) grouping, just as in isobutane.



When two or more substituents are present, list them in alphabetical order. When two or more of the same alkyl substituent are present, use the prefixes di-, tri-, tetra-, etc. to avoid having to name the alkyl group twice. Include a position number for each substituent, even if it means repeating a number more than once.

di- means 2

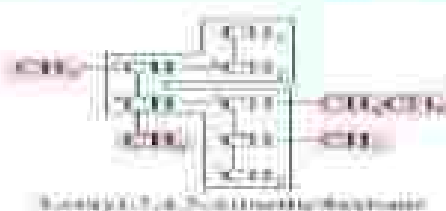
tetra- means 4

hexa- means 6

tri- means 3

penta- means 5

hepta- means 7





Methods of Preparation

Alkanes are saturated hydrocarbons. They are very less reactive towards various reagents; hence, they are also referred to as paraffins (parum means little, affinis means affinity).

- C₁-C₄ are gases
- C₅-C₁₇ liquids
- > C₁₇ solids

1-From Haloalkanes (Alkyl Halides): Monohaloalkanes can be converted to alkanes by following three methods:

a) By reduction of haloalkanes: The replacement of halogen atom of Haloalkanes with hydrogen is called the reduction and can be carried out by the following reagents:

(i) Zinc and dilute HCl



(ii) HI in the presence of red phosphorus



(iii) Catalytic reduction



b) **By using Grignard's Reagent** : A Grignard reagent is a compound of the type RMgX which is prepared by reacting a haloalkane with magnesium metal in the presence of dry ether.



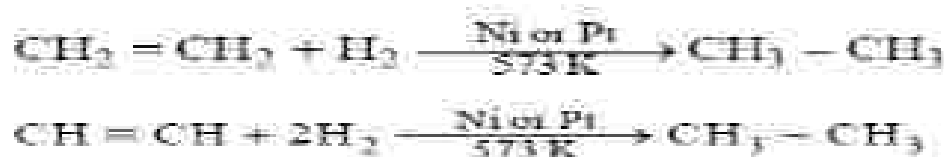
The Grignard's reagents are used to prepare various compounds like hydrocarbons, ethers, alcohols and carboxylic acids. It reacts with the compounds containing active hydrogen and forms alkanes. An easily replaceable hydrogen atom present in the compounds is called active hydrogen. An active hydrogen is present in (i) alcohols and (ii) water and (iii) acids.



d) **By Wurtz Reaction** : In this reaction, an alkyl halide reacts with sodium metal in the presence of dry ether and forms the higher alkanes.



2. **From Unsaturated Hydrocarbons** : The unsaturated hydrocarbons (i.e. alkenes and alkynes) can be converted to alkanes by the addition of hydrogen in the presence of a catalyst like nickel, platinum or palladium.



This reaction is also called hydrogenation and is used to prepare vegetable ghee from edible oils (by converting unsaturated fats to saturated ones.)

Wittig Method : In this method 1, 3 to 1,6-dihalo alkanes react with Na metal 'or' Zn metal to form corresponding cycloalkanes.



Combustion:

When there is sufficient oxygen, alkanes will burn and form water and carbon dioxide as products. Example:



Carboxylic acids

- The carboxylic acid functional group consist of a carbonyl group that has a hydroxyl group attached to the carbonyl carbon.
- Carboxylic acid groups are generally written as $R-COOH$ or $R-CO_2H$.
- Carboxylic acids are generally weak acids that are only partially ionized.



Properties of carboxylic acids

Boiling Points

Higher boiling points than similar alcohols, due to dimer formation.



Hydrogen-bonded acid dimer

Acetic acid, b.p. $118^\circ C$

Melting Points

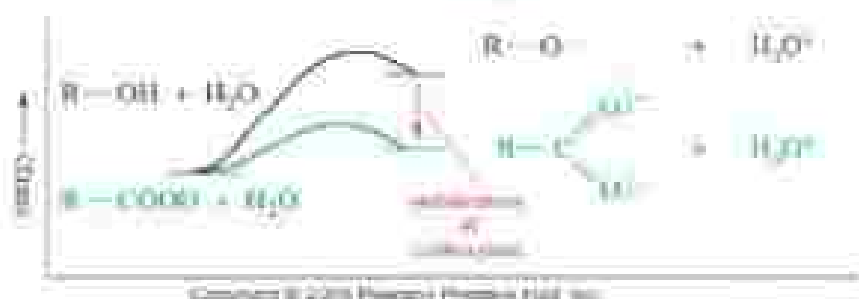
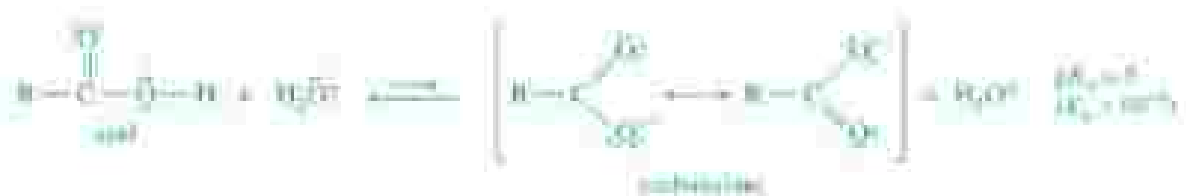
- Aliphatic acids with more than 8 carbons are solids at room temperature.
- Double bonds (especially *cis*) lower the melting point. Note these 18-C acids:
 - Stearic acid (saturated): $72^\circ C$
 - Oleic acid (one *cis* double bond): $16^\circ C$
 - Linoleic acid (two *cis* double bonds): $-5^\circ C$ (*cis,cis*-9,12-octadecadienoic acid)

Properties of carboxylic acids

Solubility

- Water solubility decreases with the length of the carbon chain.
- Up to 4 carbons, acid is miscible in water.
- More soluble in alcohol.
- Also soluble in relatively nonpolar solvents like chloroform because it dissolves as a dimer.

Acidity

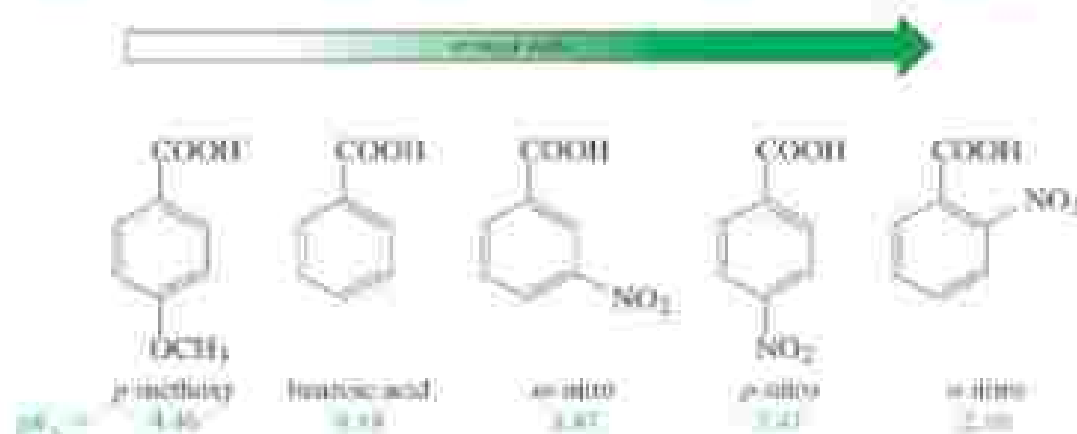


Structure of Carboxyl

- Carbon is sp^2 hybridized.
- Bond angles are close to 120° .
- O-H eclipsed with C=O, to get overlap of π orbital with orbital of lone pair on oxygen.



Substituent Effects on Acidity



Naming Carboxylic acids

- Historical names are **commonly** used for many carboxylic acids.
- Positions of substituents on the chain are labeled with Greek letters.



acetic acid



α -chloropropionic acid



γ -aminobutyric acid

Common Carboxylic acid Names



formic acid



acetic acid



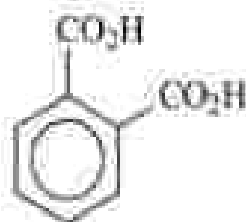
propionic acid



butyric acid



Benzoic acid



phthalic acid



oxalic acid



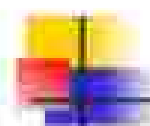
malonic acid



succinic acid



adipic acid IUPAC: hexanedioic acid



Naming Carboxylic acids

IUPAC Names

- Remove *-e* from alkane (or alkene) name, add *-oic acid*. The carboxylic acid group has priority over all other groups.
- The carbon of the carboxyl group is #1.



2-chlorobutanoic acid



trans-3-phenyl-2-propenoic acid (cinnamic acid)

- When the $-CO_2H$ is bonded to a cycloalkane ring the compound is named as a cycloalkancarboxylic acids.
- Aromatic acids are named based on benzoic acids.



2-isopropylcyclopentanecarboxylic acid



o-hydroxybenzoic acid (salicylic acid)

Dicarboxylic Acids

- Aliphatic diacids are usually called by their common names (to be memorized).
- For IUPAC name, number the chain from the end closest to a substituent.
- Two carboxyl groups on a benzene ring indicate a phthalic acid.



3-bromoterephthalic acid

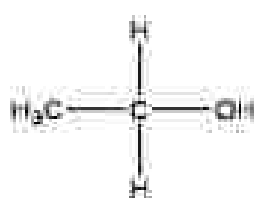
β -bromodipic acid



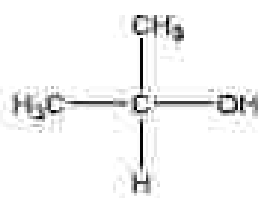
1,3-benzenedicarboxylic acid
m-phthalic acid

Alcohols: ROH

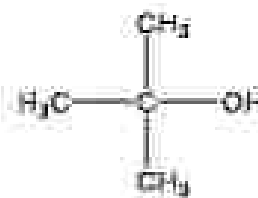
Alcohols are compounds in which (one , two , or more hydrogen atoms) in an alkane compound have been replaced by an (-OH) group. For example:



Primary



Secondary



Tertiary

Nomenclature:

Common names: Name of alkyl group, followed by word alcohol, eg ethyl alcohol, isopropyl alcohol

2.IUPAC :

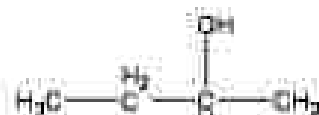
(a) Parent structure - longest chain containing -OH group: name by replacing -e of alkane by -ol examples:



butane



1-butanol

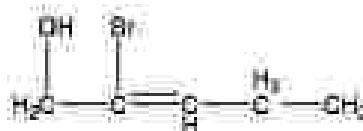


2-butanol

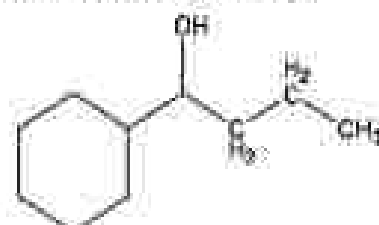
(b) Position of -OH is indicated by a number, usually the lowest one possible (-OH takes precedence over double and triple bonds if any are present, i.e. number from the end that gives the -OH a lower number).



3-ethyl-3-butene-2-ol



2-bromo-2-pentene-1-ol



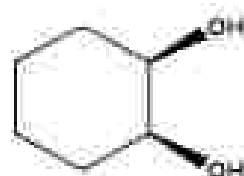
1-cyclohexylbutane-1-ol

(c) Substituents on parent chain indicated by name and position number.



3-chloro-4-phenyl-2-butanol

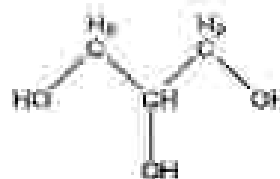
(d) More than one -OH group: -diol, -triol, etc eg



cis-cyclohexane-1,2-diol



ethane-1,2-diol



propane-1,2,3-triol

Physical Properties

Hydrogen bonds can form between a lone pair on an oxygen on one molecule and the hydrogen on the (-OH) group

Up to ~6 carbons: soluble in water owing to hydrogen bonding and dipole-dipole interactions with water. The larger the alkyl group, the more alkane-like the alcohol, and the less soluble it is in water. Owing to H-bonding and dipole-dipole interactions, the solubility of alcohols are high compared to alkanes of same MW.



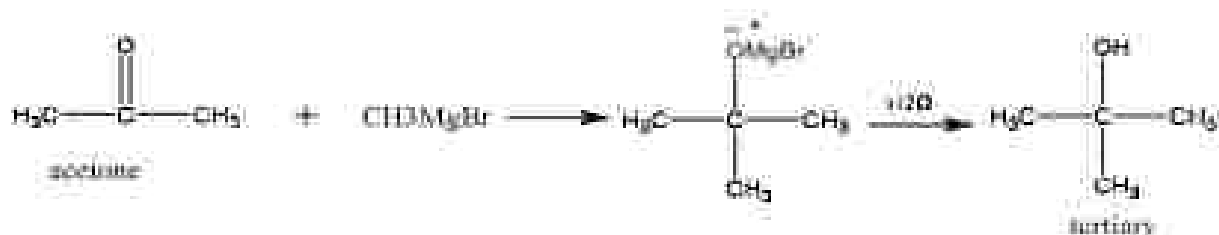
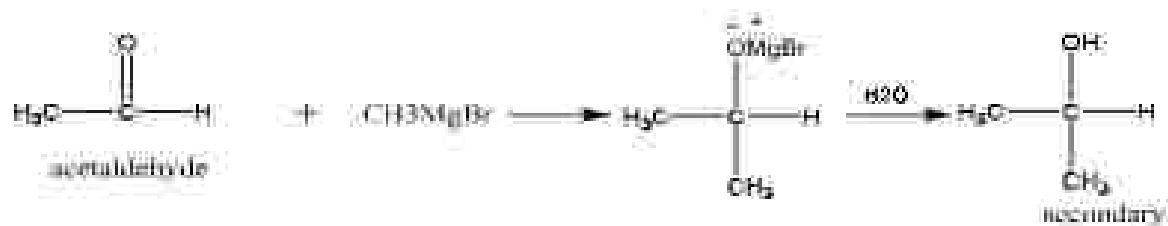
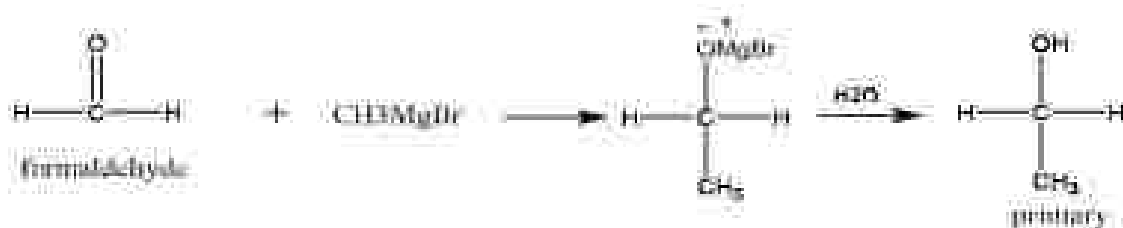
Hydrogen bonded

Preparation of Alcohols :

1-Addition of H₂O to alkene with acid :



2- Reaction of Carbonyl compounds with Grignard reagent:

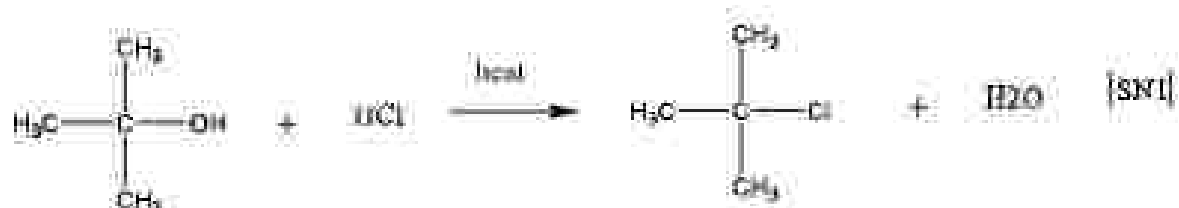


Reactions of Alcohols:

Alcohols are capable of being converted to metal salts, alkyl halides, esters, aldehydes, ketones, and carboxylic acids.

1-Alkyl halide formation:

Alcohols are converted to alkyl halides by SN1 and SN2 reactions with halogen acids.



Primary alcohols favor S_N2 substitutions ,while S_N1 substitutions occur mainly with tertiary alcohols. A more efficient method of preparing alkyl halides from alcohols involves reactions with thionyl chloride (SOCl₂) or with the sulfur dioxide.

2-Oxidation of Alcohols

Oxidizing agents such as those listed below are often used. Cr(VI) reagents (Chromic acid)(most common) ,KMnO₄ ,HNO₃

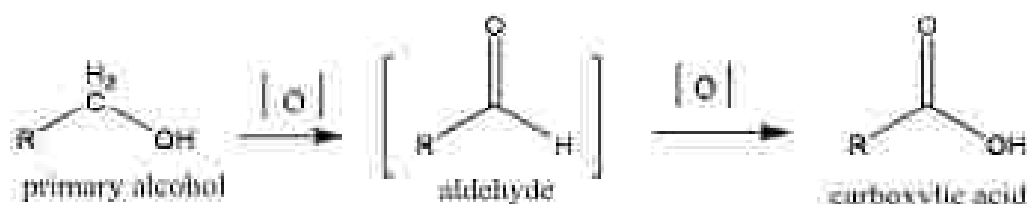
A-Secondary alcohols will always produce ketones. Chromic acid is a common reagent used to carry out oxidation of alcohols.



Example:



B-Primary alcohols will also be oxidized by chromic acid. An aldehyde is first produced and react further to give the corresponding carboxylic acid.



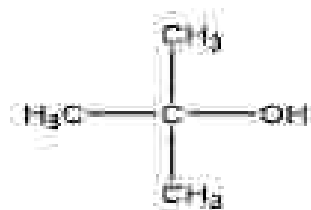
Example:



cyclohexylmethanol

cyclohexanecarboxylic acid

C-Tertiary alcohols cannot be oxidized to a carbonyl compound, as it would involve the breaking of one C-C bond in the process.

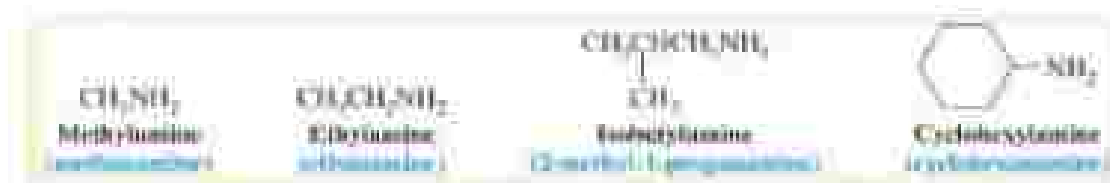


tertiary alcohol

Organic Chemistry.....

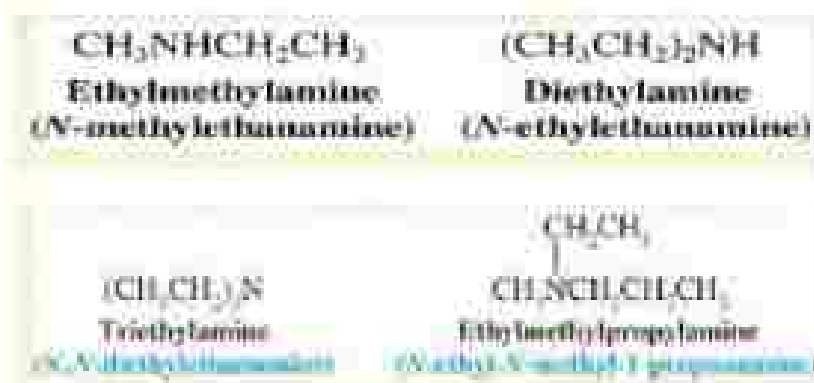
• Nomenclature of Amines

Primary amines are named in systematic (IUPAC) nomenclature by replacing the -e of the corresponding parent alkane with -amine. • In common nomenclature they are named as alkyl amines



• Simple secondary and tertiary amines are named in common nomenclature by designating the organic groups separately in front of the word amine

• In systematic nomenclature, the smaller groups on the amine nitrogen are designated as substituents and given the locant N



• In IUPAC nomenclature the substituent -NH₂ is called the amino group



– Aryl Amines

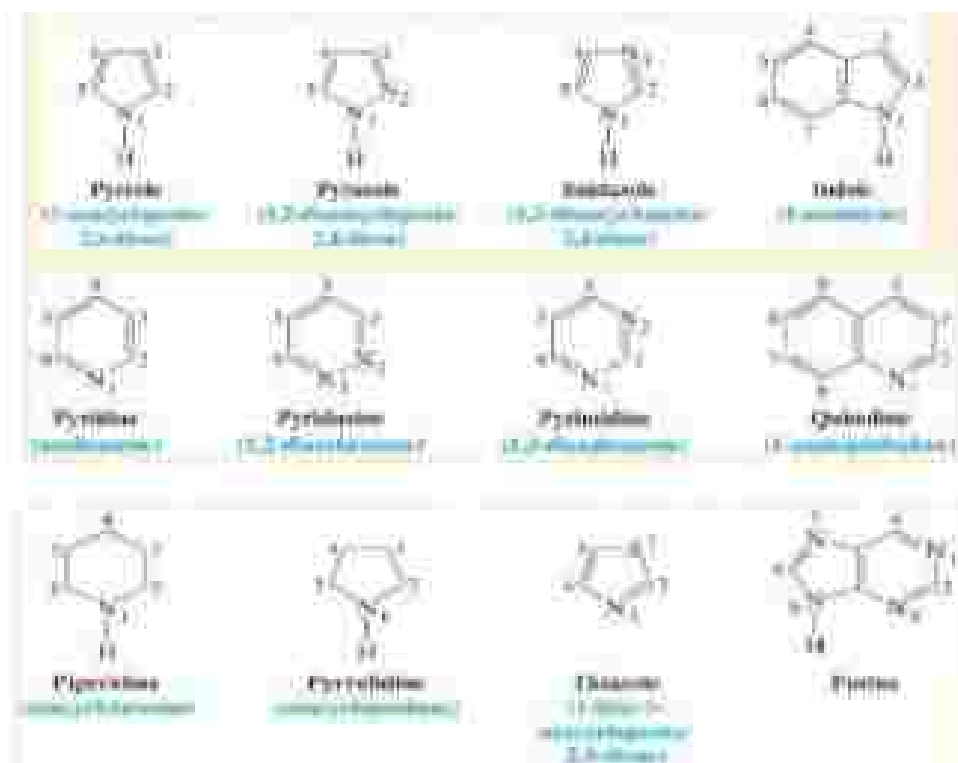
• The common aryl amines have the following names:



Organic Chemistry.....

– Heterocyclic Amines

- The important heterocyclic amines have common names
- In IUPAC nomenclature the prefixes aza-, diaza- and triaza- are used to indicate that nitrogen has replaced carbon in the corresponding hydrocarbon – The nitrogen is assigned position 1 and the ring is numbered to give the lowest overall set of locants to the



Physical Properties:

Physical Properties and Structure of Amines

- Primary and secondary amines can form hydrogen bonds to each other and water
- Tertiary amines cannot form hydrogen bonds to each other but can form hydrogen bonds to hydrogen bond donors such as water
- Tertiary amines have lower boiling points than primary or secondary amines of comparable molecular weights
- Low molecular weight amines tend to be water soluble whether they are primary, secondary or tertiary

Structure

Structure of Amines

- The nitrogen atom in an amine is sp^3 hybridized - tetrahedral geometry
- only the groups - trigonal pyramidal



- It is usually impossible to resolve amine enantiomers that are chiral at nitrogen because they interconvert rapidly – The interconversion occurs through a pyramidal or nitrogen inversion involving the unshared electron pair



Basicity

- Amines are weak bases
- Relative basicity of amines can be compared in terms of pK_a values for their respective conjugate acids – The more basic the amine, the higher the pK_a of its conjugate acid will be



- Primary alkyl amines are more basic than ammonia – An alkyl group helps to stabilize the alkylammonium ion

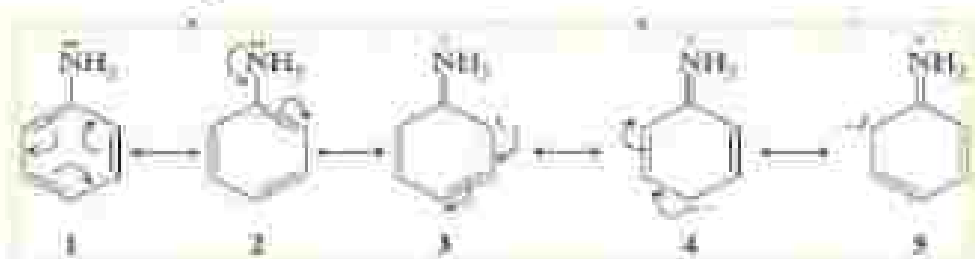
Conjugate acid pK_a	NH_3	CH_3NH_2	$\text{CH}_3\text{CH}_2\text{NH}_2$	$\text{CH}_3\text{CH}_2\text{CH}_2\text{NH}_2$
	9.26	10.64	10.75	10.67



- Arylamines are weaker bases than nonaromatic cyclohexylamines

	Cyclo- $C_6H_{11}NH_2$	$C_6H_5NH_2$	<i>p</i> -Cl- $C_6H_4NH_2$
Conjugate acid pK_a	10.64	4.55	5.08

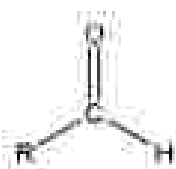
- The unshared electron pair is delocalized to the ring – The lone pair is less available for protonation, i.e., it is less basic



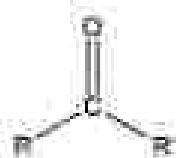
Ketones and Aldehydes

The carbonyl group is of central importance in organic chemistry because of its ubiquity.

The simplest carbonyl compounds are aldehydes and ketones. A ketone has two alkyl (or aryl) groups bonded to the carbonyl carbon



Aldehyde

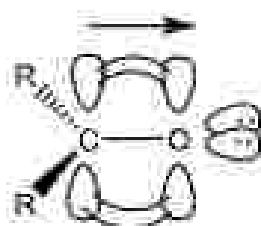


Ketone

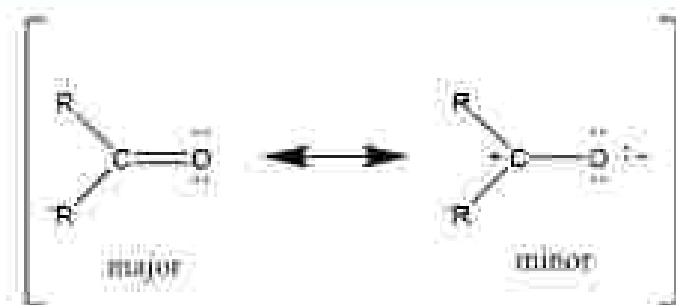
An aldehyde has one alkyl (or aryl) group and one hydrogen bonded to the carbonyl carbon.

Structure of the carbonyl group

The carbonyl carbon is sp^2 hybridized, and has a partially filled unhybridized p orbital perpendicular to the σ framework



The oxygen is also sp^2 hybridized, with the 2 lone pairs occupying sp^2 orbitals. This leaves one electron in a p orbital. These p orbitals form the carbon oxygen π bond. The C=O double bond is like a C=C double bond except the carbonyl double bond is shorter and stronger. The carbonyl group has a large dipole moment due to the polarity of the double bond. Oxygen is more electronegative than carbon, and so the bond is polarized toward the oxygen. The attraction of the weakly held π electrons toward oxygen can be represented by the two following resonance structures.



The first resonance structure is the major contributor, but the other contributes in a small amount, which helps explain the dipole moment.

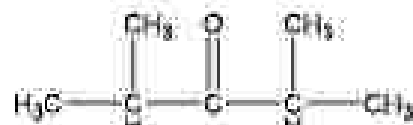
It is this polarization that creates the reactivity of the carbonyl groups (carbon is electrophilic, and the oxygen is nucleophilic).

Nomenclature

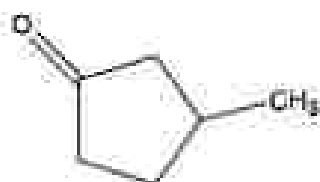
IUPAC nomenclature: requires ketones to be named by replacing the -e ending of the alkyl name with -one. Alkane → alkanone.



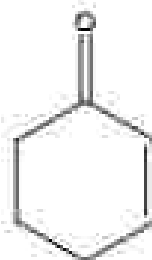
2-butanone
or butane-2-one



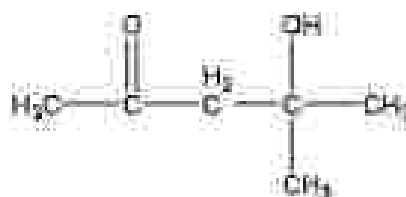
2,4-dimethyl-3-pentanone
or 2,4-dimethylpentane-3-one



3-methylcyclopentanone



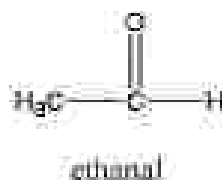
2-cyclohexanone



4-hydroxy-4-methyl-2-pentanone

Organic Chemistry

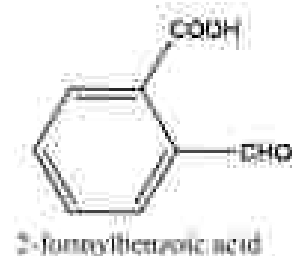
Systematic names for aldehydes are obtained by replacing *-e* with *-al*. An aldehyde has to be at the end of a chain, and therefore it is carbon number 1.



If the aldehyde is attached to a large unit, the suffix *-carbaldehyde* is used.

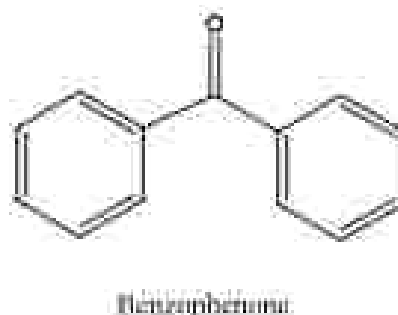
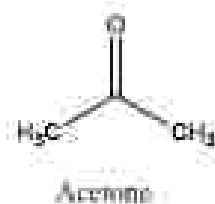


A ketone or aldehyde group can also be named as a substituent on a molecule with another functional group as its root. The ketone carbonyl is given the prefix *oxo-*, and the aldehyde group is named as a *formyl-* group. (This is especially common for carboxylic acids).

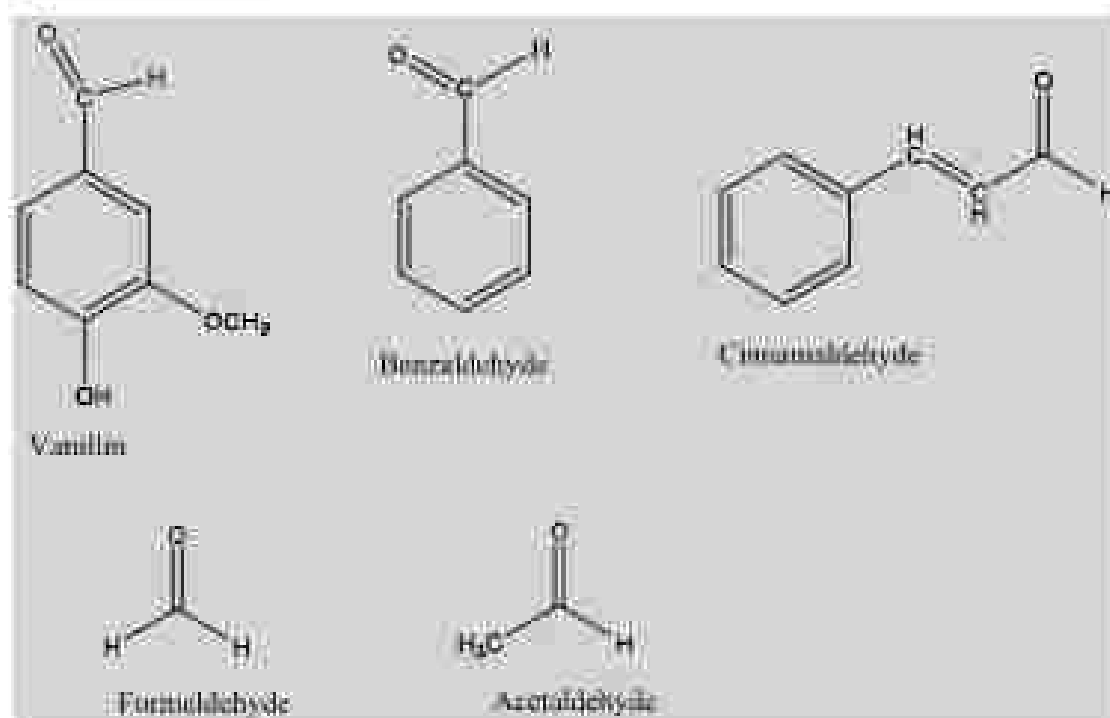


Common Names

The wide spread use of carbonyl compounds means many common names are entrenched in their everyday use



Common name:



Physical Properties of Aldehydes and Ketones :

Aldehydes and ketones are the class of organic compounds that have a carbonyl group i.e. carbon-oxygen double bond ($-C=O$). As they do not have any other reactive groups like $-OH$ or $-Cl$ attached to the carbon atom in the carbonyl group they are very simple compounds. The chemistry of aldehydes and ketones is greatly influenced by the presence of carbonyl group.

1. Boiling Points of Aldehydes and Ketones:

The boiling point of aldehydes and ketones is higher than that of non-polar compounds (hydrocarbons) but lower than those of corresponding alcohols and carboxylic acids as aldehydes and ketones do not form (H-bonds) with themselves.

Because of the presence of carbon-oxygen double bond both aldehydes as well as ketones are polar in nature. There will be attraction between permanent dipoles as well as the molecules which are near to it. This is the reason for aldehydes and ketones having boiling point higher than the similar sized hydrocarbons.

2. Solubility of Aldehydes and Ketones:

The lower members (up to 4 carbons) of aldehydes and ketones are soluble in water due to H-bonding. The higher members do not dissolve

Organic chemistry

in water because the hydrocarbon part is larger and resists the formation of hydrogen bonds with water molecules.

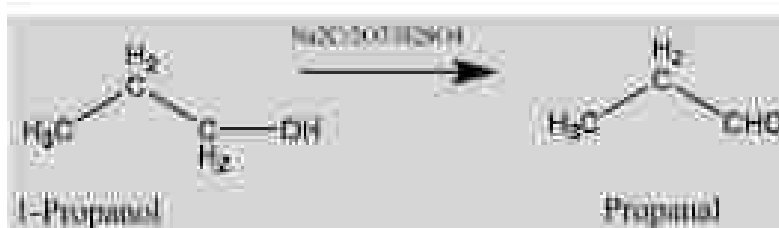
Method of Preparation of Aldehydes and Ketones :

Aldehydes and Ketones can be prepared by a number of methods. Let's discuss the method one by one.

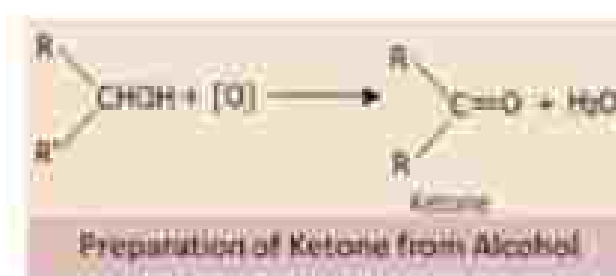
1. Formation by Oxidation of Alcohols

Oxidation of primary and secondary alcohols leads to the formation of aldehydes and ketones. The oxidation is possible with the help of common oxidizing agents are KMnO_4 , $\text{K}_2\text{Cr}_2\text{O}_7$, and CrO_3 . Strong oxidizing agents helps in the oxidation of the primary alcohol to aldehyde then to a carboxylic acid.

Example:



Ketones can be prepared by using similar oxidizing agents from secondary alcohols.



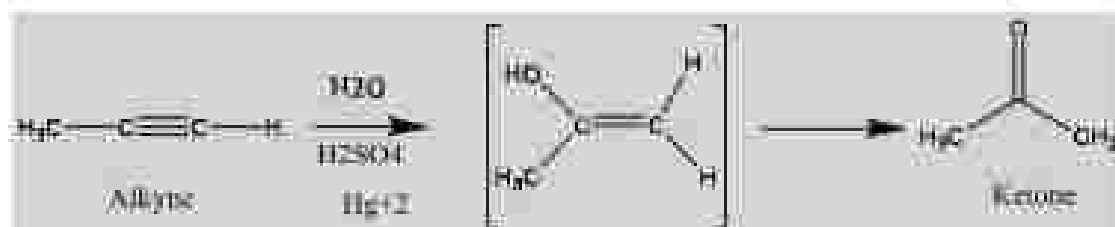
Example:



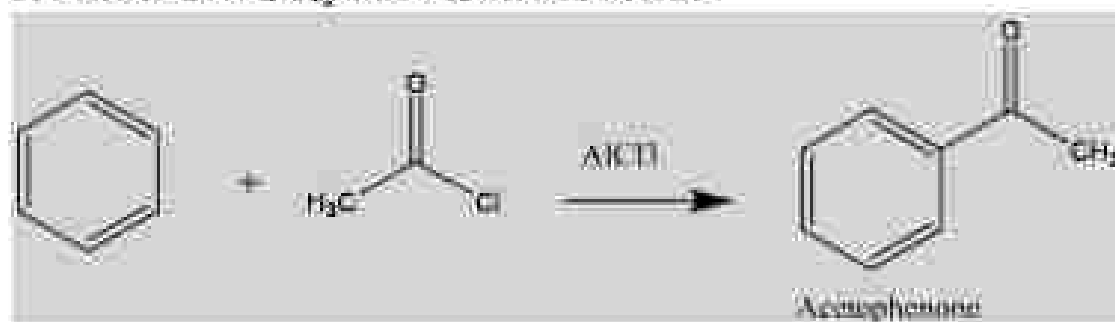
Organic chemistry

2. Hydration of an alkyne to form ketones

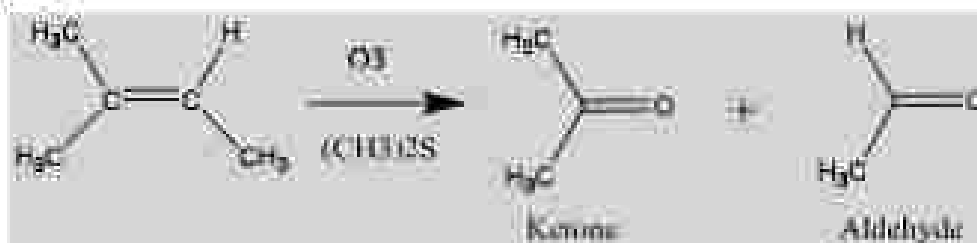
The addition of a hydroxyl group to an alkyne causes tautomerization which subsequently forms a carbonyl. Markovnikov addition of a hydroxyl group to an alkyne forms a ketone.



3. Friedel-Crafts acylation to form a ketone



4. Alkenes can be cleaved using ozone (O_3) to form aldehydes and/or ketones



Biochemistry

Introduction to biochemistry

Biochemistry or biological chemistry is the branch of life science which deals with the study of chemical reactions that occur inside the body. Life is chemical process involving thousands of different reactions occurring in an organized manner. These are called metabolic reaction.

Biochemistry consists of four main classes of molecules (often called biomolecules), where the biomolecules is composed of major elements such as carbon, hydrogen, oxygen and nitrogen that combine together to form a great variety of molecules. The four major biomolecules are carbohydrate, proteins, lipids, and nucleic acids, it is very important to know the nature and functions of these biomolecules.

Large organic molecules

Small organic molecules

- | | | |
|-------------------------|--------|---------------|
| 1- <u>Carbohydrates</u> | —————> | Simple sugars |
| 2- <u>Proteins</u> | —————> | Amino acids |
| 3- <u>Lipids</u> | —————> | Fatty acids |
| 4- <u>Nucleic acids</u> | —————> | Nucleotides |

Many newer disciplines have been emerged from Biochemistry such of Clinical Biochemistry (study of diseases), Enzymology (study of enzymes) and Endocrinology (study of hormones).

Carbohydrate

Carbohydrates are defined as polyhydroxy aldehydes or ketones which are widely distributed in plants where they are formed from carbon dioxide of the atmosphere and water by **photosynthesis**. Animals obtain their carbohydrates from plants.



The importance of carbohydrates includes:

- 1) Provide energy through oxidation.
- 2) Provide carbon for synthesis of cell components.
- 3) Serve as a stored form of chemical energy.
- 4) Form part of the structural elements of some cells and tissues.

There are more carbohydrates on Earth than any other known type of biomolecule.

Types of Metabolism

Metabolism include all of the chemical reactions that take place in a living system, a cell, a tissue, an organ, or an organism. Metabolic reactions are almost all enzyme-catalyzed and **include** transformations of energy and nutrients, **syntheses** and **degradations**, and **excretions** of waste products.

Metabolism is the whole range of biochemical processes that occur within a living organism. Metabolism consists of *anabolism* (the buildup of substances) and *catabolism* (the breakdown of substances). The term metabolism is commonly used to refer specifically to the breakdown of food and its transformation into energy.

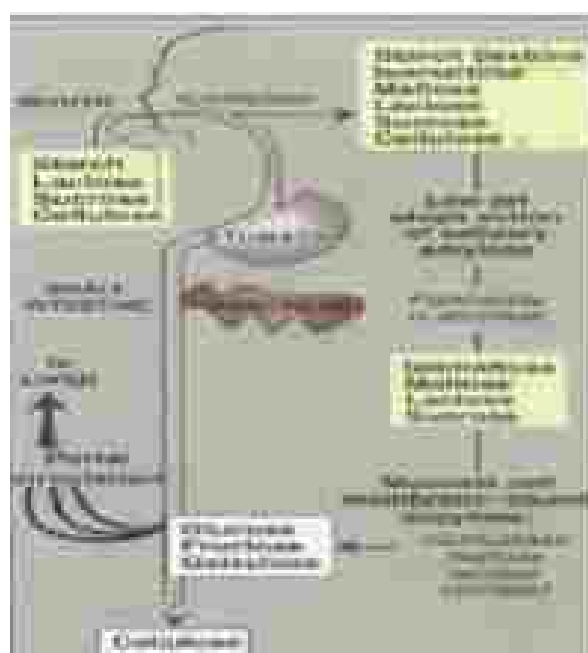
1- Catabolism

Catabolism is the set of metabolic pathways that **breaks down** **molecules into smaller units** that are either oxidized to release energy (ATP), or used in other anabolic reactions. Catabolism breaks down large molecules (such as polysaccharides, lipids, nucleic acids and proteins)

into smaller units (such as monosaccharides, fatty acids, nucleotides, and amino acids, respectively). The pathways for catabolism and anabolism use different enzymes but are regulated by the same molecules, so they take place in different locations and organelles (eukaryotes) in cells to avoid interfering with one another.

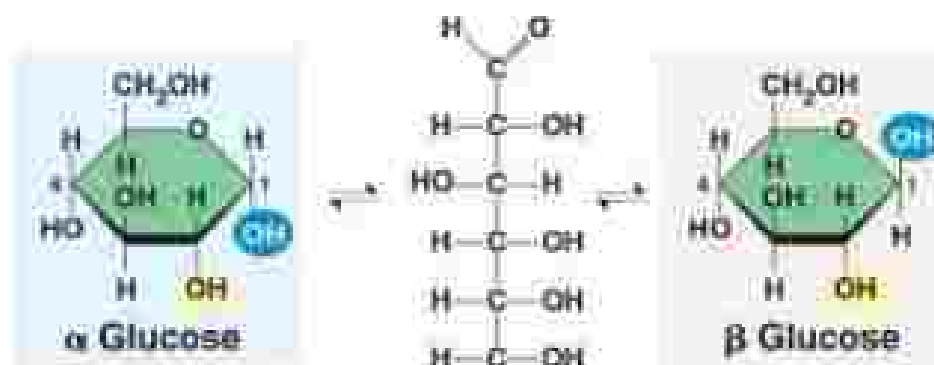
2- Anabolism

Anabolism is the set of **constructive metabolic processes** where the energy released by **catabolism is used to synthesize complex molecules**.



Glucose and its normal value.

Glucose ($C_6H_{12}O_6$) is one of the most important carbohydrates where the glucose is in important sugar of blood. Human blood containing 60-100 gm of glucose in 100 ml of blood in fasting. It serves as the major metabolic fuel in cells and tissues. Oxidation of glucose quickly provides energy for the cell. Hence, **glucose** is described as the chief source of energy. In human nutrition, **Galactose** can be found most readily in milk and dairy products, while **fructose** is found mostly in vegetables and fruits.



- **Random blood sugar test.** A blood sample will be taken at a random time. No matter when you last ate, a blood sugar level of **200 milligrams per deciliter (mg/dL)** or higher suggests diabetes.
- **Fasting blood sugar test.** A blood sample will be taken after you haven't eaten anything the night before (fast). A fasting blood sugar level less than **100 mg/dL** is normal. A fasting blood sugar level from **100 to 125 mg/dL** is considered prediabetes. If it's **126 mg/dL (7 mmol/L)** or higher on two separate tests, you have diabetes.

Glucose regulation factors in blood

Or **Blood sugar regulation is the process by which the levels of blood sugar, the common name for glucose dissolved in blood plasma, are maintained by the body within a narrow range.**

This tight regulation is referred to as **glucose homeostasis** (**The process of maintaining blood glucose at a steady-state level is called glucose homeostasis**). **Insulin**, which lowers blood sugar, and **glucagon**, which raises it, are the most well known of the hormones involved, but more recent discoveries of other glucoregulatory hormones have expanded the understanding of this process. The gland called pancreas secrete two hormones and they are primarily responsible to regulate glucose levels in blood.

Glucagon is secreted in hypoglycemia or in carbohydrate deficiency. It acts as inhibitors for glycolytic key enzymes (glucokinase, PFK-1, pyruvate kinase)

Insulin is secreted in hyperglycemia and after carbohydrate feeding. It acts as stimulation of glycolytic key enzymes.

Metabolism in diabetes mellitus

Diabetes mellitus is one of the most common metabolic disorders. It is not a single disorder but is classified into two major types, insulin-dependent and non-insulin dependent; recently identified is a pre-diabetic condition called metabolic syndrome. The insulin-dependent disease, also called type I or juvenile-onset diabetes (because it often appears in childhood) is caused failure of the pancreatic cells to produce enough insulin. **The symptoms by which diabetes (Type I)** is usually detected are **excessive thirst accompanied by frequent urination, abnormally high glucose concentrations in urine and blood, and wasting of the body despite a good diet.** These symptoms result when available glucose does not enter cells where it is needed.

By contrast, in **non-insulin-dependent diabetes, also called Type II** or adult-onset diabetes (because it usually occurs in individuals over about 40 years of age), insulin is in good supply but fails to promote the passage of glucose across cell membranes. **Type II diabetes is thought to result when cell membrane receptors fail to recognize insulin.** This state is sometimes referred to as **insulin resistance.**

- **Lipids** are organic compounds, found in living organisms that are soluble in nonpolar organic solvents.
- Unlike the polysaccharides, proteins, and nucleic acids, lipids are not polymers. They are mostly small molecules.
- **General properties of lipids:**
 - 1- Lipids are relatively soluble in organic solvents such as chloroform and methanol.
 - 2- Lipids are insoluble in water.
 - 3- The hydrophobic (water-hating) nature of lipids is due to the predominance of hydro-carbon chains ($-CH_2-$)_n in their structure.

Function of lipids

1-Lipids are a source of high energy value:

Fat: 1 gram = 9 calories

Protein: 1 gram = 4 calories

Carbohydrate: 1 gram = 4 calories

2- Lipids are the constituents of **membrane structure** and regulate the membrane permeability

3- Lipids serve as a source of fat soluble vitamins (**A, D, K** and **E**)

4- Lipids are important as **cellular metabolic regulators** (steroid hormones and prostaglandins).

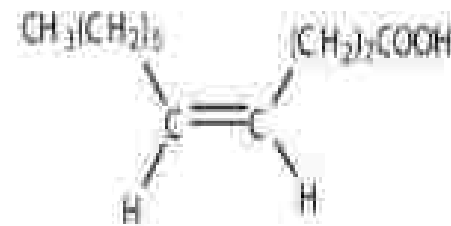
5- Lipids protect the internal organs, serve as insulating materials and give shape and smooth appearance to the body .

6- As compounds of the inner mitochondrial membranes, lipids (phospholipids) participate in **electron transport chain**.

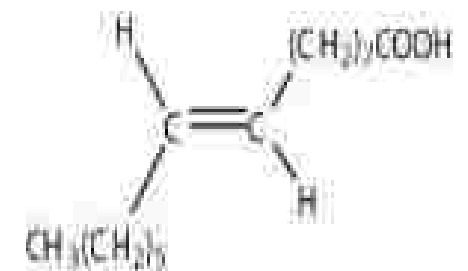
Fatty acids

- **Fatty acids** are long-chain hydrocarbon molecules that terminate with **carboxylic acid groups**. The numbering of carbons in fatty acids begins with the **carbon of the carboxylate group (COOH)**.
- The fatty acid chains in membranes usually contain between **14 and 24** carbon atoms; they may be **saturated** or **unsaturated**. Short chain length and unsaturation enhance the fluidity of fatty acids and their derivatives by lowering the melting temperature.
- The **16- and 18-**carbon fatty acids are most common. The hydrocarbon chain is almost **unbranched** in animal fatty acids.
- The alkyl chain may be saturated or it may contain **one or more double bonds**. The configuration of the double bonds in most unsaturated fatty acids is *cis*.
- The double bonds in polyunsaturated fatty acids are separated by at least one methylene group.
- Fatty acids that contain **no carbon-carbon double bonds** are termed **saturated fatty acids**; those that contain **double bonds are unsaturated fatty acids** and fatty acids with **multiple** sites of unsaturation are termed **polyunsaturated fatty acids (PUFAs)**.

Saturated	Unsaturated
$ \begin{array}{c} \text{H} \text{ H} \\ \quad \\ -\text{C}-\text{C}- \\ \quad \\ \text{H} \text{ H} \end{array} $	$ \begin{array}{c} \text{H} \text{ H} \\ \quad \\ -\text{C}=\text{C}- \\ \quad \\ \text{H} \text{ H} \end{array} $
Carbon-Carbon Single Bond	Carbon-Carbon Double Bond



cis-fatty acid



trans-fatty acid

TYPES OF FATTY ACIDS

(according to the number of double bonds)



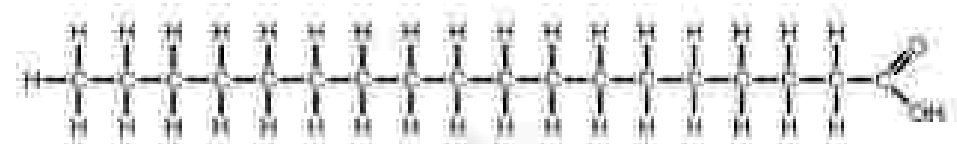
Saturated (No bond)



Monounsaturated (1 bond)



Polyunsaturated (>1 bond)



stearic acid
(saturated fatty acid)



oleic acid
(monounsaturated fatty acid)



linolenic acid
(polyunsaturated fatty acid)

- The physical properties of a fatty acid depend on the length of the **hydrocarbon chain and the degree of unsaturation**.
- The **melting points** of saturated fatty acids **increase with increasing molecular weight** because of increased van der Waals interactions between the molecules.
- The presence of **double bonds** in fatty acids significantly **lowers the melting point** relative to a saturated fatty acid.
- The melting points of the unsaturated fatty acids **decrease as the number of double bonds increases**. For example, an 18-carbon fatty acid melts at 69 °C if it is saturated, at 13 °C if it has one double bond, at -5 °C if it has two double bonds, and at -11 °C if it has three double bonds.
- **Monounsaturated fatty acids** contain **one double bond**, and **polyunsaturated** fatty acids contain **two or more double bonds**

Essential fatty acids

The fatty acids can not be synthesized by the body and, therefore, should be supplied in the diet are known as **essential fatty acids (EFA)**. Chemically, they are **unsaturated** fatty acids, namely linoleic acid (18:2;9,12) and linolenic acid (18:3;9,12,15). Arachidonic acid (20:4;5,8,11,14).

Functions of EFA

- 1- Membrane structure and functions.
- 2- Transport of cholesterol .
- 3- Formation of lipoproteins .
- 4- Prevention of fatty liver .
- 5-They are also needed for synthesis of eicosanoids (prostaglandins, prostacyclins). It derived from arachidonic acid (20) carbon .

□ Length of hydrocarbon chain of fatty acids

Depending on the length of carbon chains, fatty acids are categorized into 3 groups:

1-Short chain with less than 6 carbons.

2- Medium chain with 8 to 14 carbons.

3- Long chain with 16 to 24 carbons.

□ Shorthand representation of fatty acids

Instead of writing the full structures, biochemists employ shorthand notations (by numbers) to represent fatty acids. The general rule is that total number of carbon atoms are written first, followed by the number of double bonds and finally the position of double bonds, starting from the carboxyl end. Thus, saturated fatty acids, palmitic acids is written as 16:0 , oleic acid as 18:1:9 , arachidonic acid as 20:4:5,8,11,14 .

○ **Numbering of carbon atoms and position of double bond:**

- The position of a double bond is designated by the number of the carbon in the double bond that is closest to the carboxyl group. For example, **oleic acid**, which contains 18 carbons and a double bond between position 9 and 10, is designated **18:1, 9**. The number **18** denotes the **number of carbon** atoms, **1** denotes the number of **double bonds**, and **9** denotes the **position of the double bond** between the **9th** and **10th** carbon atoms.
- Oleic acid can also be designated 18:1, without the denotes the position of the double bond between the 9th and 10th carbon atoms.
- Numbering of carbon atoms starts from the carboxyl carbon which taken as number 1. The carbon adjacent to this (carboxyl) are 2,3,4, and so on or alternatively **alpha, beta, gamma**, and so on.

Triacylglycerols

Triacylglycerols (triglycerides) are the esters of glycerol with fatty acids. They are insoluble in water and non-polar solvents and known as neutral fats. TG are the most abundant group of lipids that primarily functions as fuel reserves of animals. The fat reserve of normal humans (men 20%, women 25% by weight) is sufficient to meet the body caloric requirements for 2-3 months.



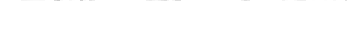
Glycerol



1-Monoacylglycerol



1,2-Diacylglycerol



Triacylglycerol

Properties of triacylglycerols

- Hydrolysis: Triacylglycerols $\xrightarrow{\text{lipase}}$ Free fatty acids + glycerol .
- Antioxidants: prevent the occurrence of oxidative rancidity.
- Lipid peroxidation in vivo: In the living cells, lipids undergo oxidation to produce peroxides and free radicals which can damage the tissue. The free radicals are believed to cause inflammatory diseases, ageing , cancer, atherosclerosis etc.

Classification of Lipids:

1- Simple Lipids

2- Compound (complex) Lipids

3- Derived lipids

Simple lipids are Esters of fatty acids with various alcohols.



a. **Fats and Oils** are esters of fatty acids with **glycerol**. Oil is a liquid, while fat is a solid at room temperature .



b. **Waxes**: Esters of fatty acids (usually long chain) with **alcohol** other than glycerol

- **2- Compound Lipids:** Esters of fatty acids with **alcohols** containing additional groups such as **phosphate, nitrogenous base, carbohydrate, protein** etc.

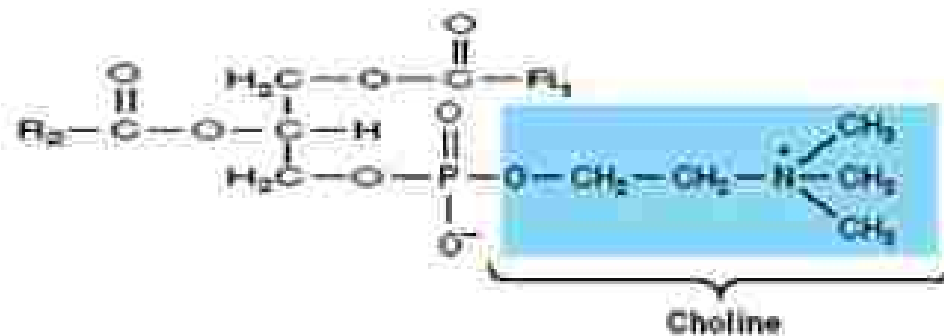
They are divided into :

A- Phospholipids : Lipids containing **phosphoric acid** and frequently a **nitrogenous base**. In addition to **alcohol** and **fatty acids** . Phospholipids enter in the structure of cell membrane .

- **There are two classes of phospholipids:-**

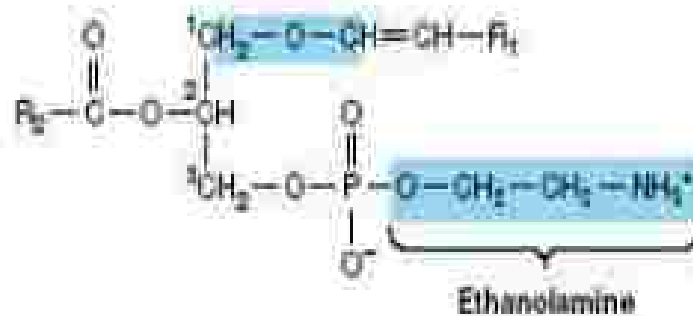
- **1- Glycerophospholipids:** These phospholipids contain **glycerol** as the alcohol e.g.,

➤ **Lecithin** (glycerol +saturated fatty acid + Phosphate+ **choline**).



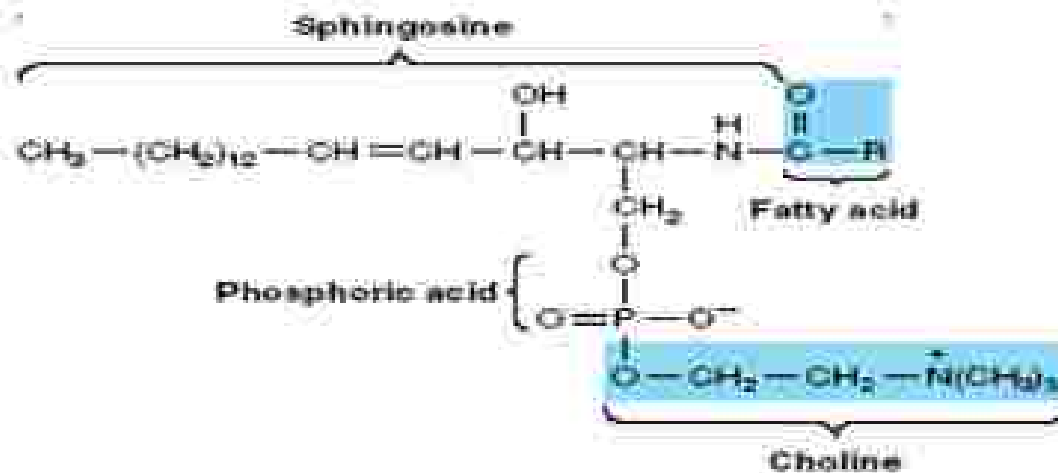
phosphatidylcholine

➤ **Cephalin:** (glycerol + unsaturated fatty acid + Phosphate + ethanol amine)



phosphatidylethanolamine

2- Sphingophospholipids: Sphingosine is the alcohol in this group of phospho-lipids e.g., Sphingomyelin (Sphingosine + fatty acid + Phosphate + choline).

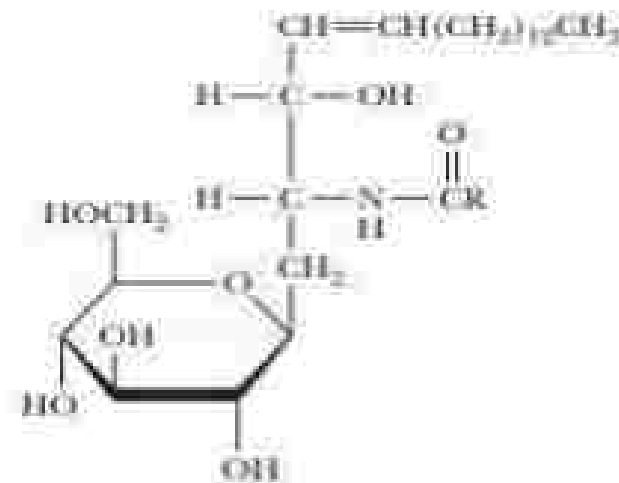


sphingomyelin

- Sphingomyelin is an **insulating material** for **nerve fibres**
- It has a double behaviour where it dissolves in fat and polar solvents.
- It is found in the brain, kidney, liver and blood

b) Glycolipids: These lipids contain a **fatty acid and carbohydrate**. The alcohol is Sphingosine (also called as glycosphingolipids) e.g., Cerebrosides (**Sphingosine + Cerebronic acid + Glucose or Galactose**).

- Cerebrosides is a key component of brain, spinal cord, and nervous cells



β -Gluco-cerebroside

C) Lipoproteins: Macromolecular complex of **lipids and proteins** . They are the transport vehicles for lipids in the circulation.

There are five types of lipoproteins :

1- **Chylomicrons** , transport dietary lipids from intestine to peripheral tissues.

2- **Very low density lipoproteins (VLDL)** , transport the lipids (endogenously synthesized) mainly TG from liver to peripheral tissues).

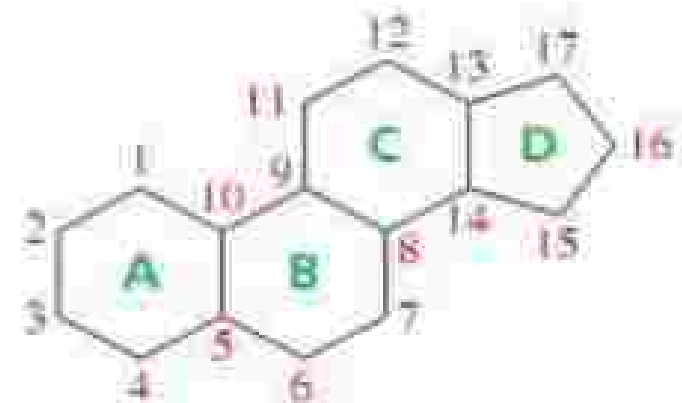
3- **Low density lipoproteins (LDL)** ("bad" cholesterol) , transport cholesterol from liver to peripheral tissues.

4- **High density lipoproteins (HDL)** ("good" cholesterol) , carry cholesterol from peripheral tissues to liver.

5- **Intermediate density lipoproteins (IDL)**.

3- **Derived Lipids**: These are the derivatives obtained by the hydrolysis of simple and compound lipids. These include fatty acids, alcohols, mono-and diacylglycerol, lipid soluble vitamins and Steroids. The most common derived lipids are **steroids**.

- **Steroids** are the compounds containing a cyclic steroid nucleus called cyclopentanoperhydrophenanthrene (CPPP) that contain **17 Carbone atoms**.
- There are several steroids in the biological system. These include **cholesterol, bile acids, vitamin D, sex hormones, adrenocortical hormone**



the steroid ring system

4- **Neutral lipids** : The lipids which are uncharged are referred to as neutral lipids e.g. triacylglycerols