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B.SC. II SEM

BIOORGANIC AND MEDICINAL CHEMISTRY

- 400+ MCQs
- Brief and Intensive Notes

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BSc SEM II

Code B020201T Bioorganic and Medicinal Chemistry

SYLLABUS

UNIT I	**Chemistry of Carbohydrates** : Classification of carbohydrates, reducing and non-reducing sugars, General Properties of Glucose and Fructose, their open chain structure. Epimers, mutarotation and anomers. Mechanism of mutarotation Determination of configuration of Glucose (Fischer's proof). Cyclic structure of glucose. Haworth projections. Cyclic structure of fructose. Inter conversions of sugars (ascending and descending of sugar series, conversion of aldoses to ketoses). Lobry de Bruyn-van Ekenstein rearrangement; stepping–up (Kiliani Fischer method) and stepping–down (Ruff's &Wohl's methods) of aldoses; end-group interchange of aldoses Linkage between monosaccharides, structure of disaccharides (sucrose, maltose, lactose)
UNIT II	**Chemistry of Proteins**: Classification of amino acids, zwitter ion structure and Isoelectric point. Overview of primary, secondary, tertiary and quaternary structure of proteins. Determination of primary structure of peptides, determination of N-terminal amino acid (by DNFB and Edman method) and C–terminal amino acid (by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection & C-activating groups and Merrifield solid phase synthesis. Protein denaturation/ renaturation Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and
UNIT III	**Chemistry of Nucleic Acids**: Constituents of Nucleic acids: Adenine, guanine, thymine and Cytosine (Structure only), Nucleosides and nucleotides (nomenclature), Synthesis of nucleic 05 17 acids, Structure of polynucleotides; Structure of DNA (Watson-Crick model) and RNA (types of RNA), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation.
UNIT IV	**Introductory Medicinal Chemistry** : Drug discovery, design and development; Basic Retrosynthetic approach. Drug action-receptor theory. Structure –activity relationships of drug molecules, binding role of –OH group, -NH2 group, double bond and aromatic ring. Mechanism of action of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide); antiviral agents (Acyclovir),

	Central Nervous System agents (Phenobarbital, diazepam), Cardiovascular (Glyceryl trinitrate), HIV-AIDS related drugs (AZT- Zidovudine)
UNIT V	**Solid State** Definition of space lattice, unit cell. Laws of crystallography – (i) Law of constancy of interfacial angles, (ii) Law of rationality of indices and iii) Symmetry elements in crystals and law of symmetry .X-ray diffraction by crystals. Derivation of Bragg equation. Determination of crystal structure of NaCl, KCl and CsCl (powder method) their role in biological reactions)
UNIT VI	**Introduction to Polymer**: Monomers, Oligomers, Polymers and their characteristics, Classification of polymers : Natural synthetic, linear, cross linked and network; plastics, elastomers, fibres, Homopolymers and Co-polymers, Bonding in polymers : Primary and secondary bond forces in polymers ; cohesive energy, and decomposition of polymers. Determination of Molecular mass of polymers: Number Average molecular mass (Mn) and Weight average molecular mass (Mw) of polymers and determination by (i) Viscosity (ii) Light scattering method (iii) Gel permeation chromatography (iv) Osmometry and Ultracentrifuging. Silicones and Phosphazenes –Silicones and phosphazenes as examples of inorganic polymers, nature of bonding in triphosphazenes.
UNIT VII	**Kinetics and Mechanism of Polymerization** Polymerization techniques, Mechanism and kinetics of copolymerization,Addition or chaingrowth polymerization, Free radical vinyl polymerization, ionic vinyl polymerization, ZieglerNatta polymerization and vinyl polymers, Condensation or step growth-polymerization, Polyesters, polyamides, phenol formaldehyde resins, urea formaldehyde resins, epoxy resins and polyurethanes.
UNIT VIII	**Synthetic Dyes**: Colour and constitution (electronic Concept), Classification of dyes, Chemistry and synthesis of Methyl orange, Congo red, Malachite green, crystal violet, phenolphthalein, fluorescein, Alizarin and Indigo.

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UNIT I

B.Sc. SEM II

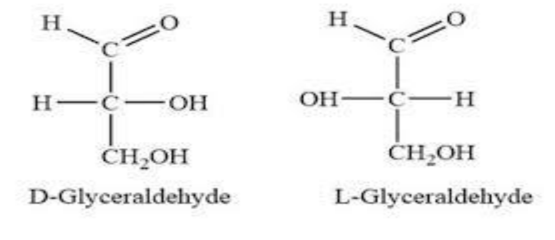
SYLLABUS OF UNIT I

Chemistry of Carbohydrates : Classification of carbohydrates, reducing and non-reducing sugars, General Properties of Glucose and Fructose, their open chain structure. Epimers, mutarotation and anomers. Mechanism of mutarotation Determination of configuration of Glucose (Fischer's proof). Cyclic structure of glucose. Haworth projections. Cyclic structure of fructose. Inter conversions of sugars (ascending and descending of sugar series, conversion of aldoses to ketoses). Lobry de Bruyn-van Ekenstein rearrangement; stepping–up (Kiliani Fischer method) and stepping–down (Ruff's &Wohl's methods) of aldoses; end-group interchange of aldoses Linkage between monosachharides, structure of disacharrides (sucrose, maltose, lactose

Chemistry of Carbohydrates

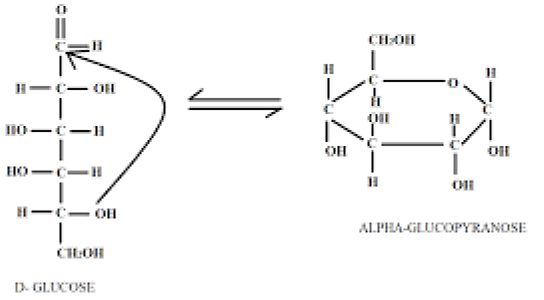
- **Carbohydrates are defined as "optically active polyhydroxy aldehydes or ketones or the compounds which produce units of such type on hydrolysis."**
- Carbohydrates can be classified into three classes: monosaccharides, oligosaccharides, polysaccharides.
- Glucose has four stereocenters (chiral center) in the open-chain form. Open chain structure having several chiral centers are depicted by Fischer projection formulas. The number of stereoisomers of carbohydrates is determined by the formula 2^n, Where n =number of chiral centres.
- **Monosaccharides** are polyhydroxy aldehydes or ketones which cannot be hydrolyzed to simpler molecules. Their general formula is $(CH_2O)_n$ where n = 3-7. Monosaccharides are of two types: aldoses and ketoses depending on the presence of aldehyde or keto functional groups.
- **Disaccharides ($C_{12}H_{22}O_{11}$) These disaccharides on hydrolysis give two units of monosaccharides.**
- **Oligosaccharides** are carbohydrates that upon hydrolysis give 2-10 molecules of the same or different monosaccharides. These are classified as di, tri, tetra saccharides, etc. as they give 2,3,4, etc. molecules of monosaccharides on hydrolysis.
- **Trisaccharides.** ($C_{18}H_{32}O_{16}$)-Raffinose on hydrolysis gives one unit each of glucose, fructose, and galactose.
- **Polysaccharides are complex substances that** on hydrolysis give hundreds to thousands of molecules of monosaccharides.
- **Sugars.** The monosaccharides and disaccharides being sweet in taste are called sugars. Fructose is the sweetest sugar, followed by invert sugar, sucrose.

- **Reducing and non-reducing sugars.** All the monosaccharides (aldoses and ketoses) and disaccharides (except sucrose) reduce Fehling's solution or Tollens' reagent and hence, are called reducing sugars. Other sugars that do not reduce these reagents are called non-reducing sugars.
- **[D&L] Configuration**. All the naturally occurring monosaccharides belong to the D-series, carbohydrates are classified depending upon whether the OH group at the stereocenter next to the primary alcohol at the end of the chain is oriented towards the right-hand side of the viewer [D family] as in D glyceraldehyde or to the left [L family]as in L glyceraldehyde.



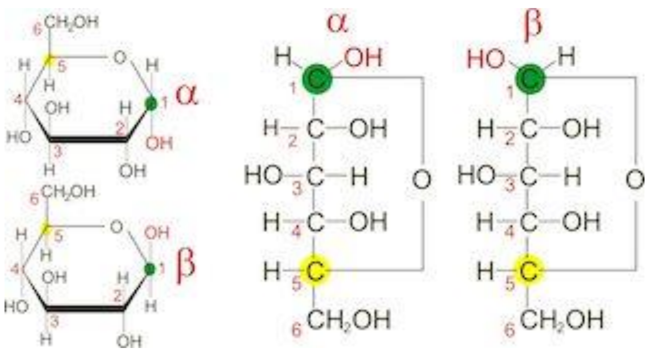
D-Glyceraldehyde L-Glyceraldehyde

- **Ring structure**. Carbohydrates, because they have both hydroxyl and carbonyl groups within the same molecule, react internally and forms ring structure i.e. cyclic hemiacetals or hemi ketals.
- six-membered cyclic structures called pyranose form and five-membered cyclic structure called the furanose form.Ring structures i.e. pyranose and furanose form is shown by Haworth projection formulas.

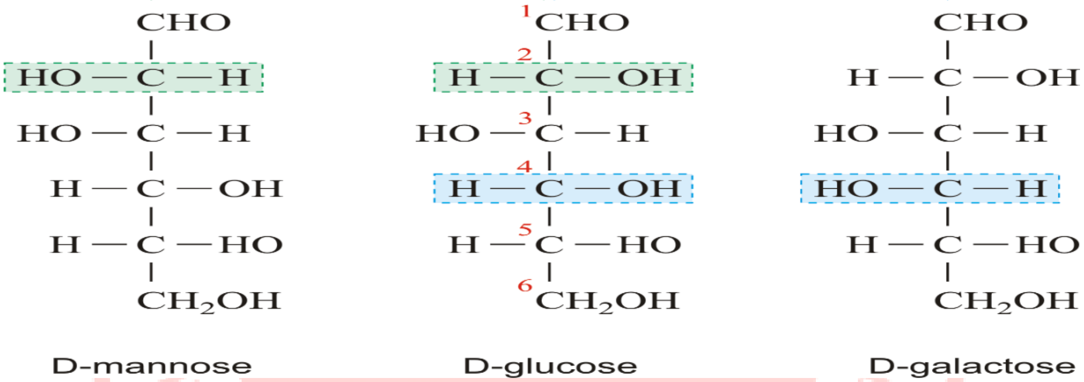


D- GLUCOSE ALPHA-GLUCOPYRANOSE

- **Anomers**. All ring structure exist in two stereoisomeric forms, i.e. alpha-form in which the OH at C_1 in aldoses and C_2 in ketoses lies towards the right and ß-form in which it lies towards left. Thus, glucose, fructose, ribose, etc. all exist in a- and ß-forms. In the aqueous solution, these two forms are in equilibrium through the open-chain form. Such pairs of isomers are called anomers.

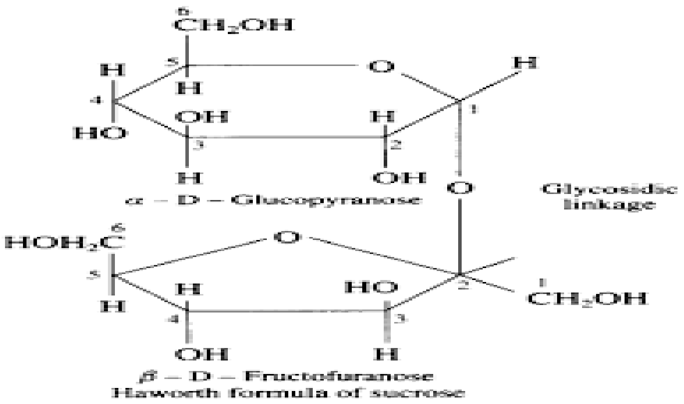


- **Anomeric carbon.** The C_1 carbon atom in aldoses and C_2 carbon atom in ketoses around which the configuration of anomers differs is called the anomeric carbon.
- **Epimers.** Saccharides that differ in configuration at a carbon other than the anomeric carbon are called epimers. For example, glucose and mannose differ in configuration around C_2 and hence, are C_2 - epimers. Similarly, glucose and galactose are C_4 epimers.



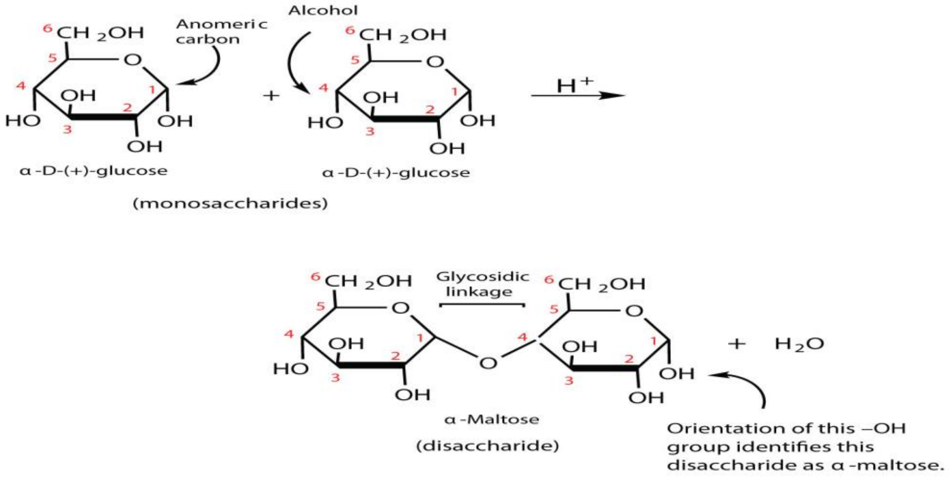
- As carbohydrates contain both hydroxyl and carbonyl groups, carbohydrates can react as alcohols and as aldehydes or ketones. They are converted to esters by acid anhydrides and to ethers in the presence of a base and an alkyl halide or sulfate.
- The primary alcohol group at one end of a carbohydrate molecule and the aldehyde function at the other end are oxidized by nitric acid to carboxylic acid groups, giving dicarboxylic acids called aldaric acids. Aldoses are easily oxidized to monocarboxylic acids (aldonic acids) by mild oxidizing agents, such as bromine water.
- The carbon chain of carbohydrates is cleaved by periodate ion between adjacent hydroxyl groups or between a carbonyl group and an adjacent hydroxyl group.
- **Oxime formation**. Due to the presence of open chain form, glucose has a free -CHO group and hence, forms an oxime. In contrast, glucose pentaacetate because of its cyclic structure does not have a free - CHO group and hence, does not form an oxime.
- **Lobry-De-Bruyn-Ekestein rearrangement** -With base Monosaccharides undergo an interconversion via enediols into the mixture of glucose, fructose, and mannose.
- **Glycosides** when the sugar is treated with an alcohol in the presence of acid. The hemiacetal or hemiketal form in which a carbohydrate exists is converted to an acetal or ketal linkage. Sugar acetals or ketals are called glycosides.

- **Glycosidic linkage** The bonds between two monosaccharide units in disaccharides and polysaccharides are all glycosidic linkages. Glycosidic linkages are found in many natural products joining alcohols or phenols, known as aglycons, to sugars.
- **Sucrose**; In sucrose, glucose is present in the pyranose form and fructose in the furanose form. The glycosidic linkage between C_1 -alpha anomer of glucose unit with the C_2- beta anomer of fructose. Sucrose is a non-reducing sugar. (C-1 ⟹ C-2)

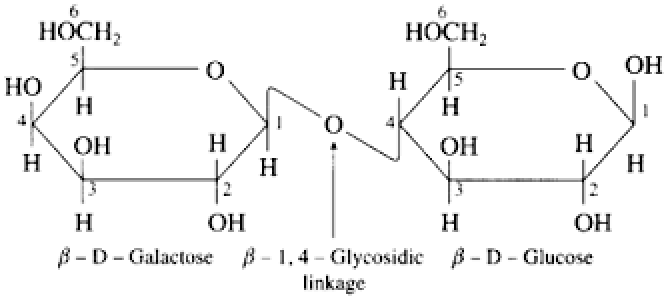


Inverted sugar is obtained by hydrolysis of sucrose is an equimolar mixture of D (+) glucose and D (-)fructose.

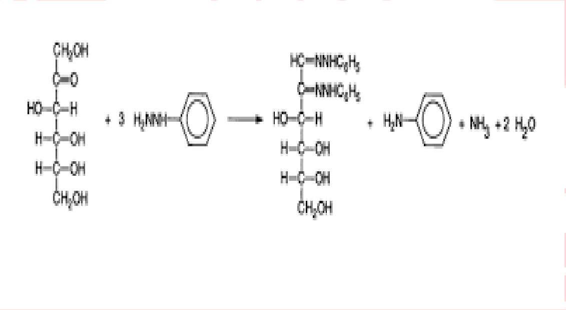
- **Maltose**. Here The glycosidic linkage between C_1 - alpha of the glucose unit and C_4 of the other glucose unit, therefore, it is a reducing sugar. (C-1 ⟹ C-4)



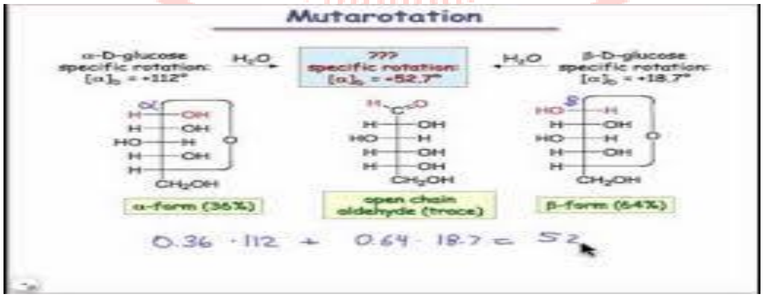
- **Lactose**. Here The glycosidic linkage between C_1 – beta anomer of galactose and the OH of C_4 of the other glucose unit. Therefore, lactose like maltose is reducing sugar. in which one glucose unit has free anomeric -OH Group (reducing form). (C-1 ⟹ C-4)



- **Osazone formation**. All monosaccharides (and reducing disaccharides such as maltose, lactose, etc.) react with three molecules of $C_6H_5NHNH_2$ to form crystalline osazones. Further, all monosaccharides that differ in configuration only at C1 and C2 give the same osazone e.g. glucose, mannose, and fructose form the same osazone.



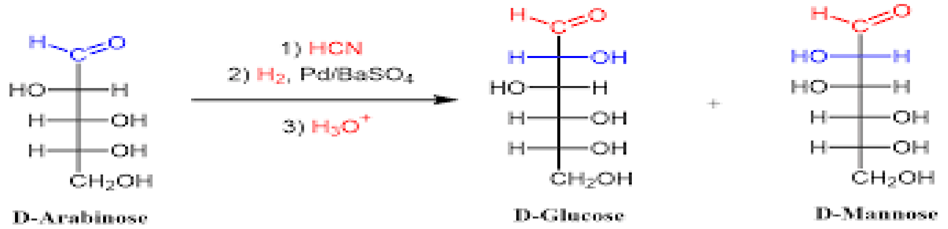
- **Mutarotation.** The specific rotation of freshly prepared solution of a-D-glucose gradually decreases from +112° to 52.7^0 while that of ß-D-glucose increases from 19^0 to 52.7^0 with time. This change in the specific rotation of an optically active compound in an aqueous solution with time, to an equilibrium value, is called mutarotation. All reducing carbohydrates, i.e., monosaccharides and disaccharides (maltose, lactose, etc.) undergo mutarotation in aqueous solution.



- **Cause of Mutarotation**-opening and closing of hemiacetal ring is responsible for the change in a specific rotation.

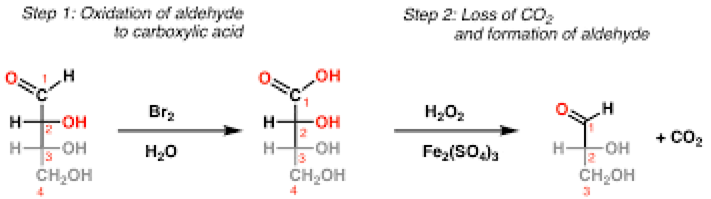
- **Polysaccharides** on hydrolysis give hundreds to thousands of molecules of monosaccharides.
- (1) Starch. $(C_6H_{10}O_5)_n$ where n = 200 - 3000 It is the chief storage polysaccharide of plants. It is a mixture of two components, i.e., water-soluble amylose (20%) and water insoluble amylopectin (80%). Whereas amylose is a linear polymer of a-D-glucose, amylopectin is a highly branched chain polymer of alpha - D glucose.
- (ii) Cellulose. $(C_6H_{10}O_5)_n$ where n = 1000 - 3000 It is a linear polymer of ß-D-glucose and is the chief structural material of all plants. It is also the chief component of cotton, wood, jute etc.
- **The Kiliani-Fischer synthesis** converts an aldose to two epimeric aldoses that have one more stereocenter than the starting compound. Sodium cyanide is used to make epimeric cyanohydrins of the aldose. The cyanohydrins are hydrolyzed to epimeric carboxylic acids, which cyclize to two different lactones. Careful reduction of the lactones produces the hemiacetals of the two epimeric aldoses having lengthened chains.

The Kiliani-Fischer synthesis lengthens the carbon chain of carbohydrates

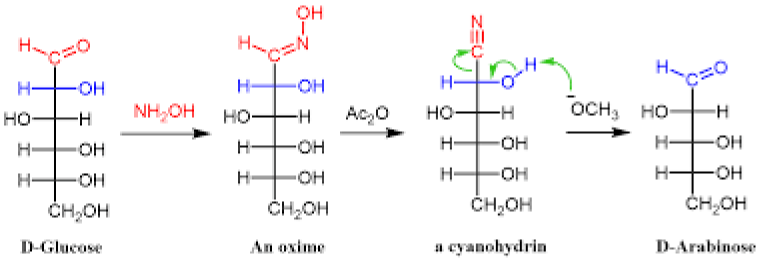


- **Ruff's degradations** is a method for shortening a carbohydrate chain by a single carbon. It involves the oxidization of an aldose to an aldonic acid, followed by its conversion into a shorter aldose.

The Ruff Degradation



- **Wohl degradation** is a method for shortening a carbohydrate chain by a single carbon. It involves the formation of oxime and its dehydration to cyanohydrin by acetic anhydride. Cyanohydrin treated with sodium methoxide gives a shorter aldose.



MULTIPLE-CHOICE QUESTIONS

1. Monosaccharides are classified according to

(a) the number of carbon atoms in the molecule.

(b) whether they contain an aldehyde or a ketone group.

(c) their configurational relationship to glyceraldehyde.

(d) all of the above.

Ans- D

2. Which is a monosaccharide?

(a) Sucrose

(b) Maltose

(c) Galactose

(d) Cellulose

Ans- C

3. Which is a disaccharide?

(a) Glucose

(b) Maltose

(c) Fructose

(d) Cellulose

Ans- B

4. Which of the following is not a monosaccharide?

(a) Ribose

(b) Fructose

(c) Sucrose

(d) Glucose

Ans- C

5. The designation D or L before the name of a monosaccharide

(a) indicates the direction of rotation of polarized light.

(b) indicates the length of the carbon chain in the carbohydrate.

(c) indicates the position of the OH group on the carbon next to the primary alcohol group

(d) indicates the position of the asymmetric carbon atoms in the carbohydrate.

Ans-C

6. The principal sugar in blood is

(a) Fructose

(b) Glucose

(c) Sucrose

(d) Galactose

Ans- B

7. Which of the following statements is false about **α**-D-glucose?

(a) it has a pyranose ring.

(b) it is a hemiacetal

(c) it shows mutarotation.

(d) it is a table sugar

Ans- D

8. **α** -D-Glucose is different from β -D-glucose

(a) in the configuration at C-1

(b) because they are mirror images of each other

(c) because they are enantiomers

(d) because they are geometrical isomers

Ans-A

9. **α** -D-Glucopyranose is a(n)

(a) hemiacetal

(b) hemiketal

(c) acetal

(d) ketal

Ans-A

10. The number of asymmetric carbon atoms in the a-D-glucopyranose molecule is

(a) 2

(b) 3

(c)4

(d)5

Ans-C

11. Which of the following statements is false about an aldohexose?

(a) It is a monosaccharide.

(b) It contains a potential aldehyde group

(c) alpha-D-Glucopyranose is an aldohexose

(d) Fructose is an aldohexose

Ans-D

12. All of the following monosaccharides give the same osazone except

(a) Galactose

(b) Glucose

(c) Fructose

(d) Mannose

Ans-A

13. Mutarotation is a term related to

(a) Interconversion of anomers

(b) Relationship of D- and L- families

(c) Hydrolysis of sucrose

(d) Number of monosaccharides in a carbohydrate

Ans-A

14. The cause of mutarotation is

(a) a change of specific rotation from a (+) to a (-) value.

(b) due to opening and closing of hemiacetal ring .

(c) the reversible change from alpha-D to the beta-D form

(d)all

Ans-D

15. Common table sugar is

(a) Glucose

(b) Sucrose

(c) Fructose

(d) maltose

Ans-B

16. Carbohydrates are-

(a) Polyhydroxy ester

(b) Polyhydroxy aldehyde

(c)Polyhydroxy ketone

(d) Polyhydroxy carbonyl compounds.

Ans-D

17. Which of the following statements is false about sucrose ?

(a) It is also called table sugar.

(b) It may be fermented by yeast to produce alcohol

(c) It reduces Fehling's solution

(d) It does not reduce Tollens' reagent.

Ans-C

18.Which of the following is the general formula of Carbohydrates?

(a) $(C_4H_2O)n$

(b) $(C_6H_2O)n$
(c) $(CH_2O)n$
(d) $(C_2H_2O)n$ COOH
Ans-C

19.Which of the following is an example of C-4 Epimers?
(a) Glucose and Fructose
(b) Glucose and Galactose
(c) Galactose, and Mannose
(d) Glucose, Ribose and Mannose
Ans-B

20. Alpha glucose and beta glucose are

a) Anomer
b) Epimer
c) Enantiomer
d) Tautomer

Ans-A

21. Glucose on oxidation with periodate, gives one mole of formic acid, it exists in…………..

a) Open chain
b) 4 member ring
c) 5 member ring
d) 6 member ring
Ans- D

22 .Glucose when react with 3 moles of phenylhyrazine it forms

a) Osazone
b) Ozone
c) Ozonide
d) None
Ans- A

23. A carbohydrate found in milk is
a) Glucose
b) Galactose
c)Lactose
d)Maltose
Ans- C

24. When glucose react with HI/P it gives
    - a) n-pentane
    - b) n-hexane
    - c) iso pentane
    - d) no reaction

    Ans- B

25. Glucose on oxidation with periodate, gives one mole of formaldehyde, it exists in……form
    - a) Open chain
    - b) 4 member ring
    - c) 5 member ring
    - d) 6 member ring

    Ans- C

26. Open chain Glucose on oxidation with periodate give
    - a) HCOOH+HCHO
    - b) 5HCOOH+HCHO
    - c) 5HCHO
    - d) 5HCOOH

    Ans- B

27. If Glucose on permethylation followed by hydrolysis give 2,3,4,6-tetra-o-methyl glucose, then is in
    - a) Glucofuranose
    - b) Glucopyranose
    - c) Galactopyranose
    - d) None

    Ans- B

28. If Glucose on permethylation followed by hydrolysis give 2,3,5,6-tetra-o-methyl glucose, then is in
    - a) Glucofuranose
    - b) Glucopyranose
    - c) both
    - d) none

    Ans- A

29. Glucose on oxidation with Fehling solution gives

a) gluconic acid

b) glucaric acid

c) n- hexane

d) iso-pentane

Ans- A

30. Fructose on reaction with conc. HNO3 gives

a) oxalic acid

b) tartaric acid

c) tartaric acid + glycolic acid

d) glycolic acid

Ans- C

31 . In maltose linkage between two glucose unit is at

a) C-1 AND C-1
b) C-1 AND C-2
c) C-1 AND C-3
d) C-1 AND C-4
Ans- D

32. Sucrose is a non-reducing sugar due to

(a) presence of α-hydroxyl keto group

(b) its conversion to invert sugar

(c)presence of linkage between both anomeric carbon atoms

(d) none of these

Ans- C

33. Glucose on reaction with oxime form mono oxime it indicates that glucose has ……

a) carbonyl group

b) carboxylic group

c) hydroxy group

d) all

Ans- A

34. In sucrose linkage between glucose AND fructose unit is

- a) C-1 AND C-1
- b) C-1 AND C-2
- c) C-1 AND C-3
- d) C-1 AND C-4

Ans-B

35. Glucose forms osazone with………..moles of phenylhydrazine

a) one

b) two

c) three

d) four

Ans- C

36. If disaccharide is hydrolyzed by **α-** glucosidase then linkage between the monomer is

a) **α**

b) β

c) gamma

d) none

Ans- A

37. The number of isomers of carbohydrates is determined by the formula:

- (a) 2n
- (b) N^2
- (c) 2^n
- (d) 1/2n

Ans- C

38. If disaccharide is hydrolyzed by β-glucosidase then linkage between the monomer is

a) **α**

b) β

c) gamma

d) none

Ans- B

39. Invert sugar is produced on hydrolysis of

(a) Fructose
(b)Maltose
(c) Sucrose
(d) glucose
Ans- C

40. In a disaccharide two monosaccharide units are joined by-
(a) peptide bond
(b) glycosidic linkage
(c) ionic bond
(d)none of these
Ans- B

41. Starch when boiled with dilute acid, finally yields

(a) Glucose
(b) Fructose
(c) Amylose
(d) Amylopectin
Ans-A

42. Invert sugar is-
(a) Optically inactive form of sugar
(b) Equimolecular mixture of glucose and fructose
(c) Mixture of glucose and sucrose
(d) A variety of cane sugar
Ans- B

43. - Amylose and Amylopectin are main constituents of which of the following?

(a) Insulin
(b) Cellulose
(c) Starch
(d) All of the above

Ans- C

44. Which of the following methods are used to determine the Ring size in sugars?

(a) Oxidation with HIO_4
(b) Lactone formation
(c) Haworth and Hirst method
(d) All of the above
Ans- A

45.Which of the following is insoluble in water?

(a) Amylopectin
(b) Cellulose
(c) Starch
(d) All of the above

Ans- D

45.Cellulose has

(a) α -glycosidic linkages
(b) β -glycosidic linkages
(c) Highly branched structure
(d) Both (a) and (c)

Ans- D

46.Kiliani- Fischer synthesis can be used to convert

(a) Aldopentose into aldohexose
(b) Ketopentose into ketohexose
(c) Both (a) and (b)
(d) None of the above

Ans- A

47.The reagent which is used in Ruff-degradation is

(a) H_2O/Fe^{+3}
(b) H_2O/ Fe^{+2}
(c) H_2O_2/ Fe^{+3}
(d) H_2O_2/Fe^{+2}

Ans- C

48. Which of the following type of degradation may be used to convert an aldohexose into an aldopentose?

(a) Ruff- degradation
(b) Wohl degradation
(c) Both (a) and (b)
(d) None of the above

Ans- C

49.- On warming with dilute alkali, fructose give

(a) Glucose
(b) Mannose

(c) Tartaric acid
(d) An equilibrium mixture of glucose, fructose and mannose

Ans- D

50. Glucose on oxidation with nitric acid give

(a) Glucaric acid
(b) Gluconic acid
(c) Saccharic acid
(d) Both (a) and (c)

Ans- A

UNIT II

B.Sc. SEM II

SYLLABUS OF UNIT II

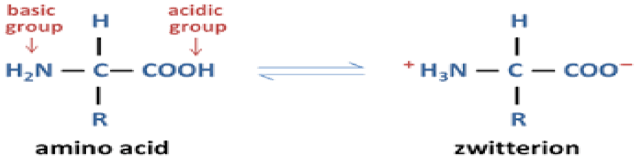
Chemistry of Proteins: Classification of amino acids, zwitter ion structure and Isoelectric point. Overview of primary, secondary, tertiary and quaternary structure of proteins. Determination of primary structure of peptides, determination of N-terminal amino acid (by DNFB and Edman method) and C–terminal amino acid (by thiohydantoin and with carboxypeptidase enzyme). Synthesis of simple peptides (upto dipeptides) by N-protection & C-activating groups and Merrifield solid phase synthesis. Protein denaturation/ renaturation Mechanism of enzyme action, factors affecting enzyme action, Coenzymes and cofactors and their role in biological reactions).

Chemistry of Proteins

The molecules having both an amino group (- NH_2}) and a carboxyl (-COOH) group are called amino acids. Depending upon the position of the NH_2 group with respect to COOH, amino acid classified as α, β, γ-amino acids, etc.

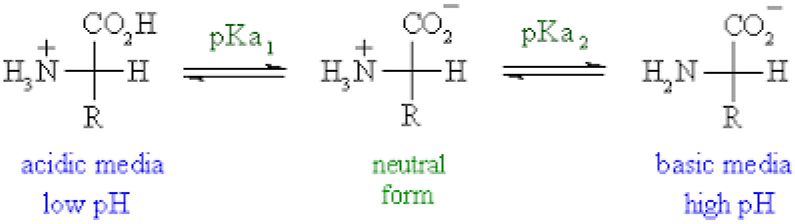
• All naturally occurring a-amino acids, which are the building blocks of proteins, have an amino group located at a-position with respect to the carboxylic group. The a-carbon of all the amino acids (except glycine) is chiral and hence amino acids can exist in two stereoisomeric forms, i.e., R and S. But all the naturally occurring a-amino acids belong to the S-series and have (2S) configuration.

• As - NH_2 and- COOH groups are present within the same molecule, they neutralize each other, and hence amino acids exist as dipolar ions known as Zwitterions.



Because of the dipolar nature they are amphoteric, i.e., they can accept a proton from a stronger acid as well as donate a proton to a stronger base. Further, because of the zwitterionic structure, a-amino acids are high-melting crystalline solids moderately soluble in water.

- The pH at which a particular amino acid exists as a dipolar ion is called the isoelectric point (pI).



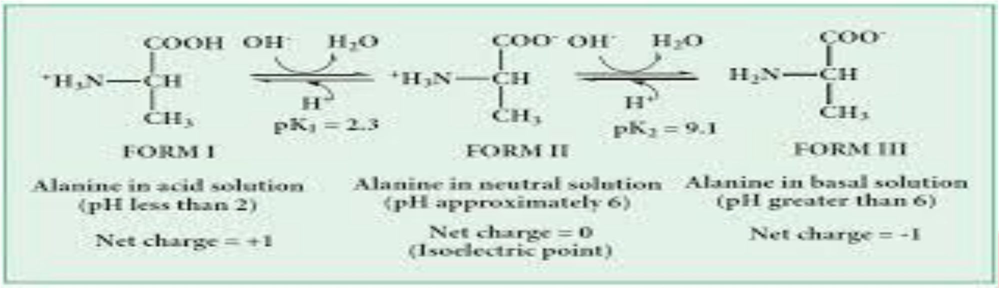
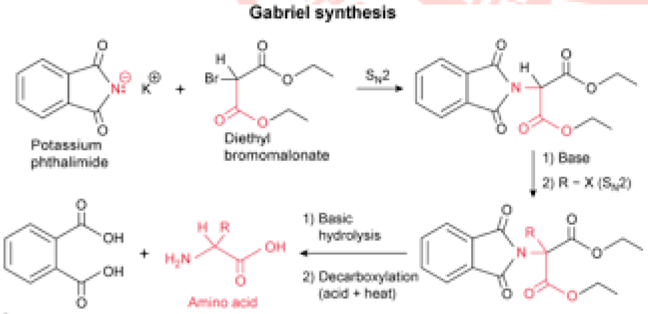


Figure 3.4 ionic forms of alanine

Electrophoresis is the procedure for analyzing mixtures of amino acids and proteins by observing their migration under the influence of a strong electric field. The direction and rate of migration are governed largely by the average charge on the molecules of each type of protein or amino acid. This technique is used for separation of the different amino acids obtained on hydrolysis of a protein.

- a-Amino acids can be synthesized by alkylation of ammonia with a-haloacids, Gabriel phthalimide synthesis, phthalimidomalonic ester synthesis, Strecker synthesis, Erlenmeyer azlactone synthesis.



Curtius reaction, hydantoin synthesis, Darapsky synthesis, reductive amination of a-keto acids and reduction of oximes and hydrazones of a-keto acids.

Out of 20 amino acids required for protein synthesis, human body can synthesize only 10. These ten amino acids (valine, leucine, isoleucine, phenylalanine, methionine, tryptophan, threonine, lysine, arginine and histidine) which the body can synthesize are called **non-essential** or dispensable amino acids.

The remaining ten amino acids which the body cannot synthesize are called **essential** or indispensable amino acids. The lack of essential amino acids in the diet causes diseases. Depending upon the number of amino and carboxylic groups amino acids are classified into the following three categories:

(1) Neutral amino acids
(2) Acidic amino acids
(3) Basic amino acids

$-COOH > -NH_2$	Acidic	Asp, Glu	Two
$-NH_2 > -COOH$	Basic	Lys, His, Arg	Three
$-NH_2 = -COOH$	Neutral	Others	

Amino acids behave as both amines as well as carboxylic acids. Thus, the amino group can be acylated; the carboxylic acid group can be esterified. Reaction with ninhydrin is analytically important reaction of a-amino acids, although primary amines also undergo the same reaction.

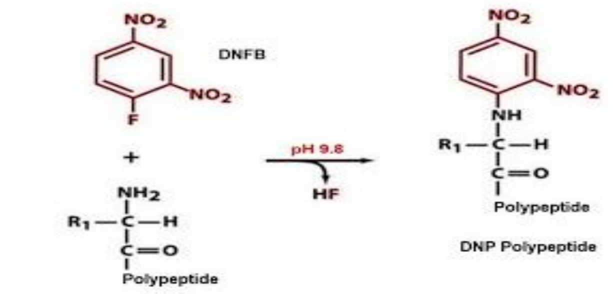
The amides formed by condensation of - NH_2 group of one a-amino acid with COOH group of the other with the elimination of a molecule of H_2O are called peptides. The -CO-NH-bond thus formed is called the peptide bond in which the amide group is flat and the carbonyl and amino groups lie in one plane having H (of NH) and O (of CO) trans with respect to each other. Peptides are generally classified as dipeptides, tripepides.... polypeptides etc. according as two, three or a large number (hundred to thousands) of molecules of a-amino acids are joined together by peptides bonds.

• Peptides can be hydrolyzed to their constituent amino acids by heating them in aqueous acid or base. Amino acid analysis gives the relative number of each amino acid in the peptides which involves hydrolysis of a peptide followed by separation of the resulting amino acids by ion-exchange chromatography.

The end of the peptide chain with a free or derivatized amino group is called N-terminus. When a peptide is written, the N-terminus is usually on the left. The carboxyl group of the N-terminal amino acid links it to the rest of the peptide.

• The end of the peptide chain with a free or derivatized carboxyl group is called C-terminus. When a peptide is written, the C-terminus is usually on the right.

N-terminal amino acid can be determined by Edman degradation or Sanger method.



C-terminal amino acids can be determined either by hydrazinolysis method or by enzymatic (selective) hydrolysis with carboxypeptidase.

• Proteins are extremely complex natural polymers which are essential for growth and maintenance of life. They are present in almost all living cells, being found in almost every part of plants and animals. In nut shell, each living cell is made up of thousands of different proteins. On the basis of molecular structure, proteins are classified as fibrous and globular proteins.

(1) **Fibrous proteins** consist of linear thread-like molecules which tend to lie side by side to form fibres. The polypeptide chains in them are held together usually at many points by H-bonds. Examples are: Keratin in skin, hair, nails and wool, collagen in tendons, fibroin in silk and myosin in muscles. These are insoluble in water and are stable to moderate changes in pH and temperature.

(2) **Globular proteins**. The polypeptide chain in these proteins is folded around itself in such a way so as to give the entire protein molecule a spheroidal shape. This folding occurs due to the following four type of forces: (i) Disulphide bridging (ii) intramolecular H bonding(iii) van der Waals interactions and (iv) dipolar interactions. Unlike fibrous proteins, globular proteins are soluble in water and are sensitive to small changes in temperature and pH. Examples are enzymes, hormones (insulin, thyroglobulin), antibodies, hemoglobin, fibrinogen, albumin, etc

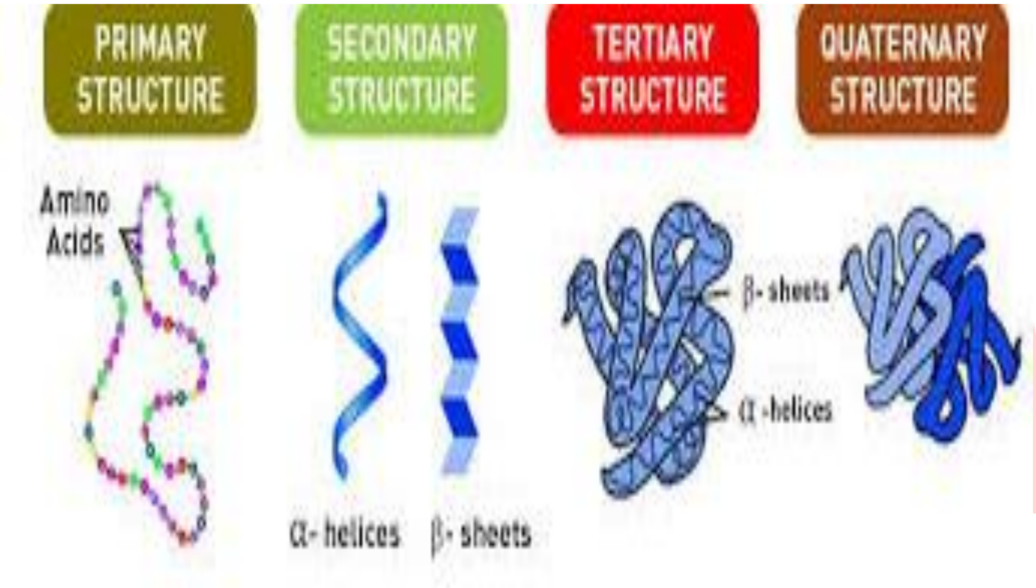
• **Hydrolysis of simple proteins** gives only a-amino acids while conjugated proteins on hydrolysis give a non-protein portion called the prosthetic group in addition to a-amino acids.

Primary structure. The sequence in which the various amino acids are linked to one another in a protein molecule is called its primary structure.

Secondary structure referes to the conformation which the polypeptide chains assume as a result of H-bonding. There are two types of secondary structures:

(i) **alpha-Helix.** If the size of the groups R is large, intramolecular H-bond are formed between c = 0 of one molecule and NH on the fourth amino acid in the polypeptide chain giving right handed a-helical structure to the protein molecule. Examples are a-keratin in hair, nail, wool, skin ez and myosin in muscles.

(ii) B-Flat sheet or B-pleated sheet structure. If the size of the groups R is small, intermolecular H-bonds are formed between c = o of one polypeptide chain the NH of the other chain giving a B-flat sheet structure to the protein molecule. This is an ideal structure and is possessed only by synthetic polyglycine. If, however the size of group is moderate, the polypeptide chains contract a little giving ß-pleated sheet structure to protein molecule, i.e., silk protein fibroin.



• **Tertiary structure** of a protein refers to its complete three dimensional structure.

• **Quaternary structure** refers to the association of two or more polypeptide chains in protein.

• Proteins play different biological functions such as

(1) structural materials (a-keratin in skin, hair, nails, wool etc., collagen in tendons, myosinin muscles and fibroin in silk),

(ii) transport agents (haemoglobin in blood transports oxygen from lungs to all parts of the body).

(iii) enzymes (catalyse all biological reactions),

(iv) metabolic regulators (insulin controls glucose level in the blood, thyroglobulin help in the synthesis of the hormone thyroxine and nucleoproteins (which carry genetic information from parents to the off sprints).

(v) antibodies are globular proteins which protect us from diseases.

On heating g or on treatment with mineral acids, the water- soluble globular proteins undergo coagulation or precipitation with loss of biological activity to give water insoluble fibrous proteins. This process is called denaturation of proteins and the coagulated protein thus formed is called the denatured protein. During denaturation, the secondary and tertiary structure of the proteins change but primary structure remains intact. Examples of denaturation are (1) coagulation of albumins present in the white of an egg when the egg is boiled hard and (ii) formation of cheese from milk on adding lemon juice when the globular milk protein, lactalbumin becomes fibrous.

Enzymes

- Enzymes can be defined as biological polymers that catalyze biochemical reactions.
- Enzymes are essentially biological catalysts which are required to catalyse biological reactions
- Enzymes may be defined as complex non-living organic compounds, produced in living organisms, which are capable of catalyzing specific organic

Characteristics of Enzymes-

- Enzymes are highly specific to the reactions they catalyze.
- They alter or speed up the rates of chemical reactions that occur in a cell.
- They remain unchanged after a chemical reaction.
- They are affected by temperature.
- They are affected by pH.
- They catalyze reversible reactions.

  Distribution

Enzymes are not randomly distributed but are specifically located inside the cells for example

- Digestive Enzymes: (Pancreas and stomach)
- Glycosol :(oxidation of glucose)
- Mitochondria TCA cycle

Enzymes are composed of:

1.APO ENZYME : Protein portion consisting of amino acid chains

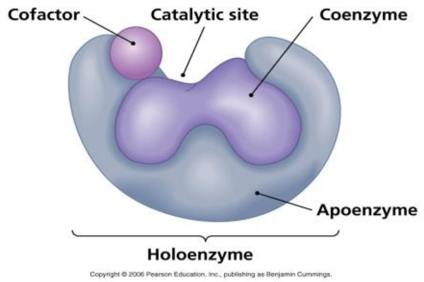
2. CO- FACTORS activate enzymes and are not protein parts.

- HOLOENZYME (conjugated enzyme)

Both cofactors and apo enzymes help to form a conjugated enzyme called holoenzyme

3. SUBSTRATE AND ACTIVE SITE :

- Enzymes operate by binding to a substrate
- The catalytic (active) site is the portion of the enzyme where substrate binding occurs.



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Classification of Enzymes-THERE ARE SIX MAJOR GROUPS OF ENZYMES

1. Oxidoreductases

Enzymes involved in oxidation-reduction reactions. Eg. Alcohol dehydrogenase

2. Transferases

Enzymes involved in transfer of groups from one molecule to another. Eg. Hexokinase

3. Hydrolases

Enzymes that bring about hydrolysis by addition of water. Eg. Lipase

4. Lyases

Enzymes that catalyze the breaking of a chemical bond through means not involving hydrolysis, and forms a double bond or adds a group to a double bond. Eg. Fumarase

5. Isomerases

Enzymes involved in all kinds of isomerization reactions. Eg. Phosphohexose isomerase

6. Ligases

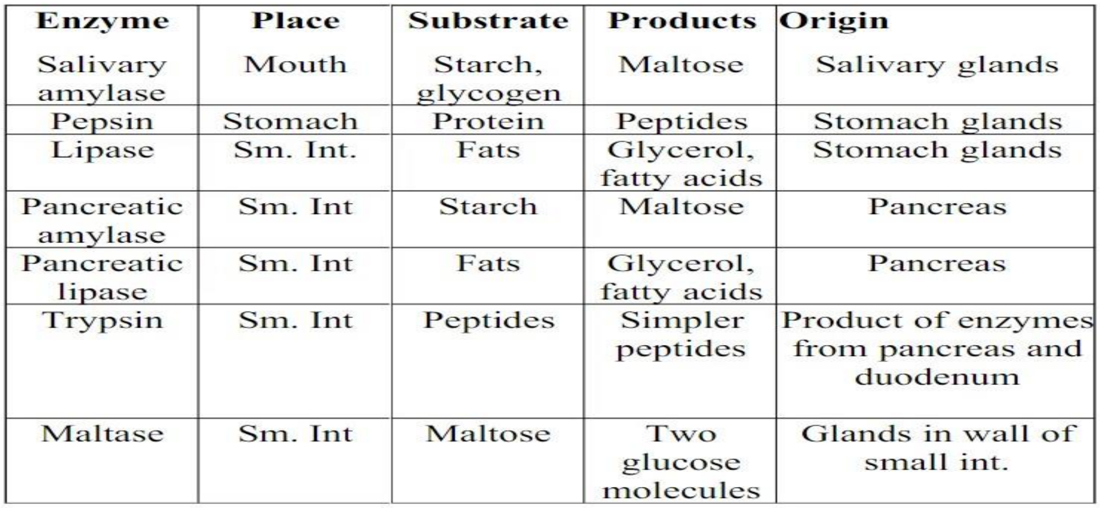
Enzymes catalyzing the joining of two molecules with hydrolysis of ATP. Eg. Glutamine synthetase

Enzymes can be classified in two main groups: on the basis their type of reaction

(2) Hydrolytic enzymes

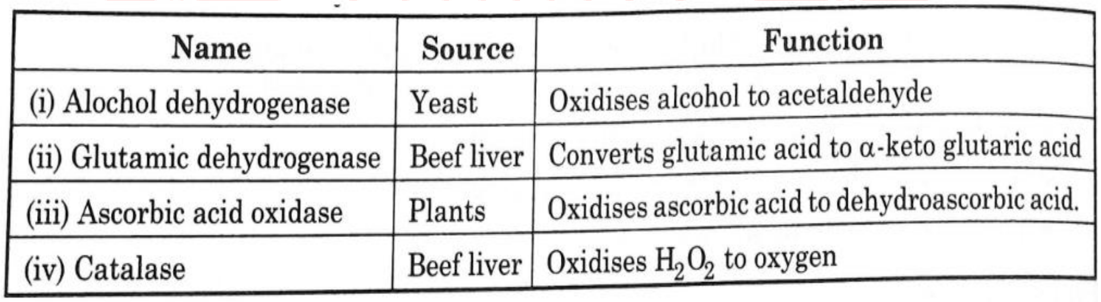
(2) Oxidative enzymes

(1) Hydrolytic enzymes



Enzyme	Place	Substrate	Products	Origin
Salivary amylase	Mouth	Starch, glycogen	Maltose	Salivary glands
Pepsin	Stomach	Protein	Peptides	Stomach glands
Lipase	Sm. Int.	Fats	Glycerol, fatty acids	Stomach glands
Pancreatic amylase	Sm. Int	Starch	Maltose	Pancreas
Pancreatic lipase	Sm. Int	Fats	Glycerol, fatty acids	Pancreas
Trypsin	Sm. Int	Peptides	Simpler peptides	Product of enzymes from pancreas and duodenum
Maltase	Sm. Int	Maltose	Two glucose molecules	Glands in wall of small int.

(2) Oxidative enzymes:



Name	Source	Function
(i) Alochol dehydrogenase	Yeast	Oxidises alcohol to acetaldehyde
(ii) Glutamic dehydrogenase	Beef liver	Converts glutamic acid to α-keto glutaric acid
(iii) Ascorbic acid oxidase	Plants	Oxidises ascorbic acid to dehydroascorbic acid.
(iv) Catalase	Beef liver	Oxidises H_2O_2 to oxygen

Factors affecting the enzyme activity

(1) Specificity: An enzyme catalyses a very few reaction (frequently only one). Therefore, enzymes are highly specific in nature.

(2) Effect of temperature:

The rise in temperature accelerates an enzyme activity but after a certain limit (i.e. 37^0 C) the rate decreases rising with the temperature. Hence, enzyme has maximum activity at optimum temperature (37^0C). Below optimum temperature, the rate of enzymatic reaction decreases and enzyme becomes inactive at 0^0C. On increasing the temperature above optimum temperature, denaturation of protein takes place.

(3) Effect of concentration: The activity of an enzyme increases with increase in the concentration of substrate until a limiting rate is reached (till the active sites of enzyme are fully bound to substrate).

(4) Effect of pH: Enzymes are highly sensitive towards pH. Each enzyme has maximum activity at its optimum pH. For example: Pepsin has maximum activity in acidic medium (lower pH value) and Trypsin has maximum activity in basic medium (high pH value).

Mostly enzyme have maximum activity at neutral pH.

Simple enzyme made up of proteins only.

Complex enzymes = Protein part(Apoenzyme) + Non-protein part (Co-factor) (Co-enzyme)

If non-protein part, i.e., organic molecule is bonded with apo enzyme by covalent bond, it is known as Prosthetic group.

If non-protein part, i.e., organic molecule is bonded with apo enzyme by non-covalent bond, it is known as co-enzyme.

Mechanism of Enzyme action:

Lock and Key theory: Proposed by Emil Fischer in 1894.

Rigid active site of enzyme.

There is no change in the active site before and after a chemical reaction.

Induced Fit Model: Proposed by Danial Koshland in 1958.

Flexible active site of enzyme

Active sites continuously reshape on interaction with the substrate.

Michaelis-Menten equation:

"It is an equation which describes how reaction velocity varies with substrate concentration."

$V_0 = V_{max}\,[S] / K_m + [S]$

Where V_0 is the initial reaction velocity

V max is the maximum velocity

Km is the Michaelis constant

[S] is the substrate concentration

MULTIPLE CHOICE QUESTION

1. Proteins are polymers of ______
   a) α-amino acids
   b) β-amino acids
   c) γ-amino acids
   d) δ-amino acids

Ans- A

2. Which of the following amino acids is optically inactive?
a) Glycine
b) Alanine
c) Lysine
d) Valine
Ans- A

3. What is the one letter code for tyrosine?
a) T
b) Y
c) R
d) S
Ans- B

4. Which of the following amino acids are aromatic in nature?
a) Methionine
b) Isoleucine
c) Proline
d) Histidine
Ans- D

5. Which of the following is a non-essential amino acid?
a) Threonine
b) Glutamine
c) Phenylalanine
d) Valine
Ans- B

6. Which of the following is a neutral amino acid?
a) Glycine
b) Lysine
c) Arginine
d) Histidine
Ans- A

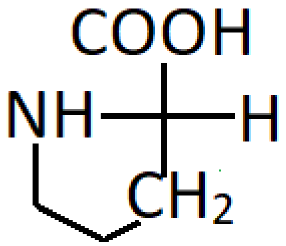
7. Cysteine is a/an ________ amino acid.
a) acidic
b) essential

c) aromatic
d) sulphur containing
Ans- D

8. . What is the one letter code for asparagine?
a) A
b) P
c) N
d) S
Ans- C

9. Which of the following is incorrect regarding tryptophan?
a) It is an essential amino acid
b) It is a basic amino acid
c) It has an aromatic side chain
d) It is a non-polar amino acid
Ans- B

10. The structure shown below is ______



a) Side chain of histidine
b) Side chain of tryptophan
c) Side chain of proline
d) Proline
Ans-D

11. Identify the amino acid with the formula $HOOC-CH_2-CH_2-CH(NH_2)-COOH$.
a) Glutamic acid
b) Aspartic acid
c) Glutamine
d) Asparagine
Ans- A

12. Which out of the following amino acids carries a net positive charge at the physiological pH ?

a) Valine
b) Leucine
c) Isoleucine
d) None of the following
Ans- D

13. Which of the amino acids below is the uncharged derivative of an acidic amino acid?
a) Cystine
b) Tyrosine
c) Glutamine
d) Serine
Ans-C

14. Which of the characteristics below apply to amino acid Glycine?
a) Optically inactive
b) Hydrophilic, basic and charged
c) Hydrophobic
d) Hydrophilic, acidic and charged
Ans- A

15. Which one of the following amino acids may be considered a hydrophobic amino acid at physiological p H of 7.4?
a) Isoleucine
b) Arginine
c) Aspartic acid
d) Threonine
Ans- A

16. Which of the following amino acids is most compatible with an α- helical structure?
a) Tryptophan
b) Alanine
c) Leucine
d) Proline
Ans- B

17. Which of the following factors is **not** responsible for the denaturation of proteins?
(a) Heat
(b) Charge
(c) pH change

(d) Organic solvents

Ans- B

18. Enzymes are

(a) Carbohydrates
(b) Nucleic acids
(c) Globular proteins
(d) Fibrous proteins

Ans-C

19. What name is given to the class of enzymes which catalyse the oxidation of one substrate with simultaneous reduction of another substrate ?

(a) Oxidoreductase
(b) Oxireducants
(c) Reduse oxidise
(d) None of these

Ans-A

20. Which vitamin is essential for proper blood clotting?

(a) Vitamin A
(b) Vitamin D
(c) Vitamin K
(d) Vitamin C

Ans- C

21. Choose the **correct** option of a fat soluble vitamin from the following:

(a) A, D, E, K
(b) B, C, D, K
(c) A, B, D, K
(d) A, B, C, D

Ans- A

22. Water soluble vitamin are

(a) A and B
(b) B and C
(c) C and D
(d) D and E

Ans- B

23- Which of the following bonds is responsible for stabilizing the secondary structure of a protein?

- **(a)** Peptide bonds
- **(b)** Hydrogen bonds
- **(c)** Ionic bonds
- **(d)** Covalent bonds

Ans- B

24-The α-helix and β-sheet are examples of which level of protein structure?

- **(a)** Primary structure
- **(b)** Secondary structure
- **(c)** Tertiary structure
- **(d)** Quaternary structure

Ans- B

25- Which amino acid is often found in turns or bends of protein structures due to its flexible side chain?

- (a) Alanine
- (b) Proline
- (c) Leucine
- (d) Glutamine

Ans-B

26- Tertiary structure of a protein is primarily stabilized by:

- **(a)** Hydrogen bonds
- **(b)** Disulfide bonds
- **(c)** Ionic bonds
- **(d)** Peptide bonds

Ans-B

27- The folding of a protein into its functional three-dimensional structure is often assisted by:

- (a) Chaperone proteins
- (b) Ribosomal RNA
- (c) mRNA
- (d) tRNA

Ans- A

28- The disulfide bridges in proteins are formed between:

- (a) Two cysteine residues
- (b) Two glycine residues

(c) A cysteine and a methionine residue
(d) A cysteine and a proline residue

Ans- A

29-In a β-sheet structure, the hydrogen bonds form between:
(a) Adjacent amino acids in the same chain
(b) Amino acids in different chains
(c) Amino and carboxyl groups
(d) Adjacent amino acids in different chains

Ans- D

30- Collagen, found in connective tissues, is an example of:
(a) Fibrous protein
(b) Globular protein
(c) Transport protein
(d) Enzyme

Ans- A

31- Which of the following is true about fibrous proteins?
(a) They are usually spherical in shape.
(b) They are water-soluble.
(c) They provide structural support.
(d) They are enzymes.

Ans- C

32-Which of the following is NOT a function of proteins?
(a) Enzymatic catalysis
(b) Structural support
(c) Energy storage
(d) Cell communication

Ans- C

33-The R-groups of amino acids play a significant role in determining the:
(a) Primary structure of proteins
(b) Secondary structure of proteins
(c) Tertiary structure of proteins
(d) Quaternary structure of proteins

Ans-C

34- Which one of the following amino acids may be considered a hydrophobic amino acid at physiological pH of 7.4?

(a) Isoleucine
(b) Arginine
(c) Aspartic acid
(d) Threonine

Ans- A

35-which one of the following will perform ninhydrin test?

(a) Carbohydrate
(b) Fats
(c) Amines
(d) Proteins

Ans- D

36-Beta Amino acid on heating gives?

(a) Acyclic diamide
(b) Acrylic acid
(c) Lactum
(d) None of these

Ans- B

37- on heating Alpha amino acid the product formed is:

(a) Lactone
(b) Lactam
(c) Cyclic diamide
(d) None

Ans- C

38-On heating Gamma amino acid the product formed is:

(a) Lactone
(b) Lactam
(c) Cyclic diamide
(d) None

Ans- B

39- Glycine is a unique amino acid because it

(a) has no chiral carbon
(b) has a sulphur containing R group
(c) cannot form a peptide bond

(d) is an essential anta acid

Ans- A

40- A zwitter ion is

(a) an ion that is positively charged in solution
(b) an ion that is negatively charged in solution
(c) (c)a compound that can ionise both as a base and an acid.
(d) (d)a carbohydrate with an electrical charge.

Ans- C

41- Which one of the following compounds form zwitterions?

(a) carbonyl compounds
(b) amino acids
(c) phenols
(d) heterocyclic compounds

Ans- B

42- The α-Helix is held in a coiled conformation partially because of

(a) optical activity
(b) resonance
(c) hydrogen bonding
(d) delocalization

Ans- C

43- Upon hydrolysis, proteins give

(a) amino acids
(b) fatty acids
(c) hydroxy acids
(d) alcohols

Ans- A

44- **α**, β, and y amino acids are distinguished by

(a) heating
(b) hydrolysis
(c) oxidation
(d) treating with alkali.

Ans- A

45-. Biological important amino acids are

(a) Alpha amino acid
(b) Beta amino acid
(c) Gama amino acid
(d) Delta amino acid

Ans- A

46- The main structural feature of protein is
(a) Ether linkage
(b) Ester linkage
(c) peptide linkage
(d) all of the above

Ans- C

47- A reagent used for the detection of protein is
(a) Conc. Nitric acid
(b) Fehling`s solution
(c) Tollen`s reagents
(d) Bayer`s reagent.

Ans- A

48- Protein is an important constituent of over diet. It functions mainly as-
(a) A source of energy
(b) Construction and repairing material
(c) Shock absorber
(d) Reserve food

Ans- B

49- Amino acid are soluble in-
(a) Benzene
(b) Petroleum ether
(c) Diethyl ether
(d) Water

Ans- D

50- At isoelectric point an amino acid behaves as-

(a) Anion
(b) Cation
(c) Zwitter ion
(d) All the above

Ans- C

UNIT III

BSc SEM II

SYLLABUS OF UNIT III

Chemistry of Nucleic Acids: Constituents of Nucleic acids: Adenine, guanine, thymine and Cytosine (Structure only), Nucleosides and nucleotides (nomenclature), Synthesis of nucleic acids, Structure of polynucleotides; Structure of DNA (Watson-Crick model) and RNA (types of RNA), Genetic Code, Biological roles of DNA and RNA: Replication, Transcription and Translation

Chemistry of Nucleic Acids

- Nucleic acid was discovered by Friedrich Miescher in 1869.
- In the early 1880s Albrecht Kossel further purified the substance and discovered its highly acidic properties. He later also identified the nucleobases.
- In 1889 Richard Altmann creates the term nucleic acid.
- In 1938 Astbury and Bell published the first X-ray diffraction pattern of DNA.
- In 1953 Watson and Crick determined the structure of DNA.

Nucleic acids are biopolymers in which the repeating structural unit is a nucleotide. These are found in the nuclei of all living cells in the form of nucleoproteins.

That is why nucleic acids are also called polynucleotides.

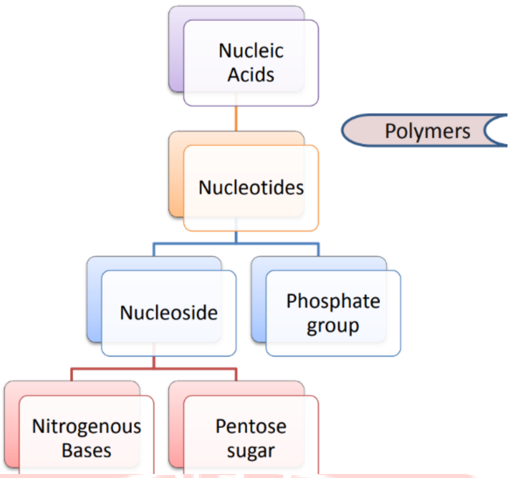
There are two types of nucleic acids:

DNA : deoxyribonucleic acid

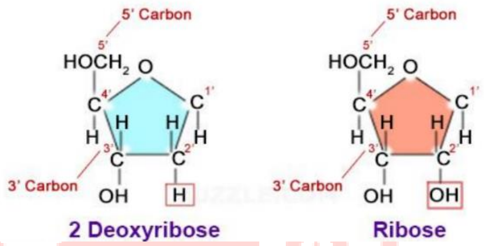
RNA: ribonucleic acid

• **Nucleotides** contain all the three components: a pentose sugar, nitrogenous base and a phosphoric acid group. Their general structure is: Phosphorus-sugar-Base.

• **Nucleosides** contain only two components: a pentose sugar and a nitrogenous base, i.e., purine or pyrimidine. Their general structure is: Sugar-Base.



(1) A pentose sugar, i.e., D-(-)ribose or 2-deoxy-D-(-)ribonse. Both these sugars are found in the furanose form.



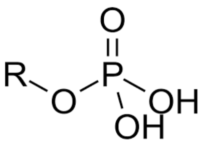
- If the sugar is derived from ribose as deoxyribose, the polymer is DNA (deoxyribonucleic aci
- If the sugar is a compound ribose, the polymer is RNA (ribonucleic acid)

(2) A heterocyclic base: Two types:

(a) Purines [Adenine (A) and guanine (G)],

(b) Pyrimidines [Uracil (U), Thiamine (T) and Cytosine (C)].

(3) Phosphoric acid



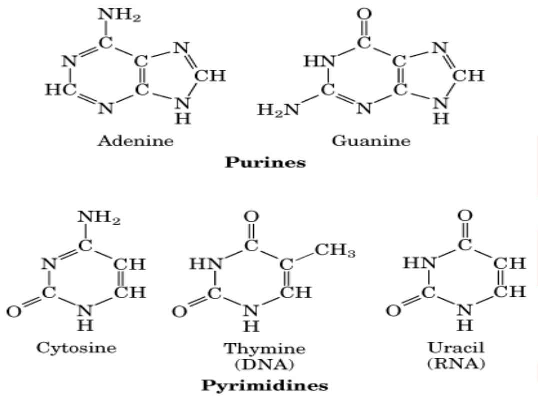
A nitrogenous base, or nitrogen-containing base, is an organic molecule with a nitrogen atom, so has the chemical properties of a base. The main biological function of a nitrogenous base is to bond nucleic acids together. Nitrogenous bases are typically classified as the derivatives of two parent compounds, pyrimidine and purine.

Pyrimidine

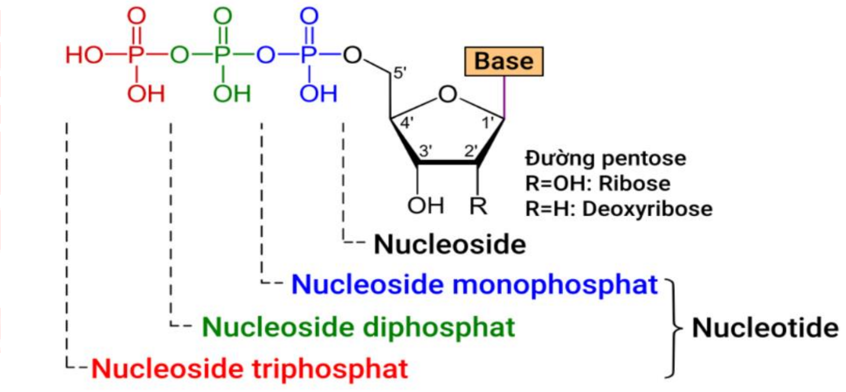
Pyrimidine is an aromatic heterocyclic single ring organic compound similar to pyridine, it has the nitrogen atoms at positions 1 and 3 in the ring.

Purine

Purine is a heterocyclic aromatic organic compound that consists of a two rings in their structure. It is water-soluble.

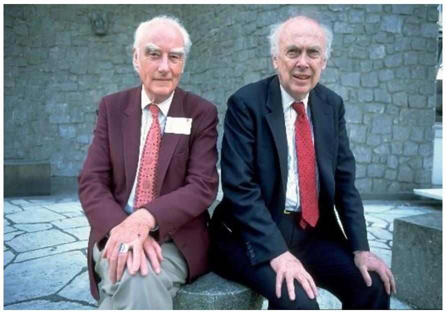


Types of heterocyclic base



(1) **Primary structure**. The primary structure of nucleic acids refers to the sequence in which the four nitrogen bases (A, G, C and T in DNA or A, G, C and U in RNA) are attached to the sugar-phosphate backbone of a nucleotide chain.

(2) **Secondary structure**: (Double helical structure of DNA or Watson and Crick model of DNA).



It was proposed by **J.D. Watson and F.H.C. Crick** in 1953 and for this work Watson and Crick were awarded Nobel Prize in 1962. This model of DNA is based on X-ray photographic technique of Wilkins & Frenklin.

(1) DNA is a polynucleotide, double stranded, Right handedly coiled and helical. The backbone of each strand consists of sugar-phosphate units

(ii) The two strands of DNA double helix are complementary and not identical

(iii) The diameter of helix is about 2.0 nm or 20Å.

(iv) The length of each coil of DNA or the distance between any two successive arns of the helix is 3.4 nm or 34A.

(v) There are 10 Nitrogen base pairs in each turn. The distance between any two adjacent base pairs is 0.34 nm.

(vi) The nitrogen base pairs of two strands are linked together through hydrogen bonds.

(vii) A purine base of one strand is always paired with a pyrimidine base of the other strand.

(viii) Guanine and cytosine are paired with three hydrogen bonds (i.e. C=G) and Adenine and Thymine are paired through two H-bonds (i.e., A=T) These H-bonds are weak and ionizable.

(ix) Unlike DNA, RNA has a single strand.

There are three different DNA types:

- **A-DNA:** It is a right-handed double helix similar to the B-DNA form. Dehydrated DNA takes an A form that protects the DNA during extreme conditions such as desiccation. Protein binding also removes the solvent from DNA, and the DNA takes an A form.
- **B-DNA:** This is the most common DNA conformation and is a right-handed helix. The majority of DNA has a B type conformation under normal physiological conditions.

- **Z-DNA:** Z-DNA is a left-handed DNA where the double helix winds to the left in a zig-zag pattern. It is found ahead of the start site of a gene and hence, is believed to play some role in gene regulation. It was discovered by Andres Wang and Alexander Rich.

(iii)**Tertiary structure**: This is the locations of atoms in three-dimensional space, taking into consideration geometrical and steric constraits. A higher order than the secondary structure in which large scale folding in a linear polymer occurs and the entire chain is folded into a specific 3-dimensional shape.

There are several important differences between RNA and DNA

-RNA is much more abundant than DNA

- the pentose sugar in RNA is ribose, in DNA it's deoxyribose

- in RNA, uracil replaces the base thymine (U pairs with A)

- RNA is single stranded while DNA is double stranded

- RNA molecules are much smaller than DNA molecules

Functions of DNA- DNA controls the synthesis of proteins, the entire structural and functional make up of the cell with self replication.

Functions of RNA- It controls the synthesis of proteins.

There are three types of RNA molecules in a cell that control the biosynthesis of specific proteins.

- messenger RNA (or mRNA), which carries genetic information from the DNA to the ribosomes for protein synthesis.
- ribosomal RNA (or rRNA), plays a crucial role in the protein synthesis within cells, and
- transfer RNA (or tRNA), is responsible for transferring amino acids to the ribosomes during protein synthesis based on the mRNA sequence. RNA controls the process of learning and memory storage.

MULTIPLE CHOICE QUESTIONS

1-The sugar moiety present in DNA is

a. β–D-ribose
b. β–D-2-deoxyribose
c. α–D-2-deoxyribose
d. β–D-3-deoxyribose
Ans- B

2- Nucleic acids are the polymer of
a. Nucleoside

b. Nucleotides
c. Bases
d. Sugars
Ans- B

3- The four nitrogenous bases commonly found if DNA are:

a) Adenine, thymine, cytosine, uracil
b) Uracil, adenine, cytosine, guanine.
c) Uracil, cytosine, guanine, thymine.
d) Adenine, thymine, cytosine, guanine.
e) None are correct
Ans- D

4- The sugar moiety present in RNA molecules is

a. β−D−2−deoxyribose
b. β−D−galacose
c. β−D−fructose
d β−D−ribose
Ans-D

5- The sugar moiety present in DNA and RNA is

a. Hexose
b. Triose
c. Pentose
d. Tetrose
Ans- C

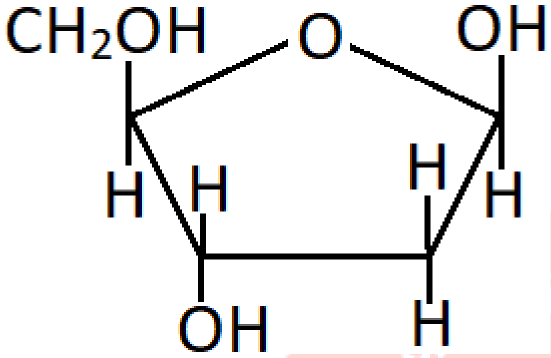
6- 51- The number of hydrogen bonds between Guanine and Cytosine; and between Adenine and Thymine in DNA are:

a. 1, 2
b. 3, 2
c. 3, 1
d. 2, 1
Ans- B

7- RNA on hydrolysis does not yield which of the following?
a) Amino acid
b) Pentose sugar

c) Nitrogen base
d) Phosphoric acid
Ans- A

8-The following compound is a component of which of the following?



a) RNA
b) DNA
c) Adenine
d) Guanine
Ans- B

9-DNA is a polynucleotide.
a) True
b) False
c) not sufficient data
d) mostly false but true in exceptional case.

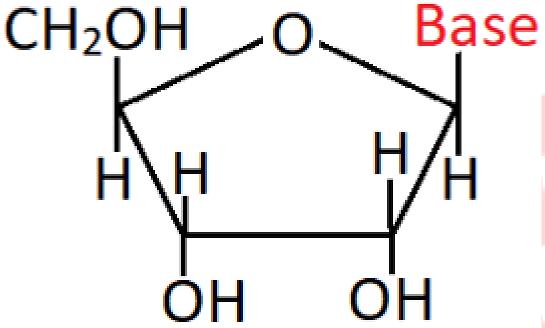
Ans- A

10- Which of the following bases is not present in DNA?
a) Adenine
b) Guanine
c) Thymine
d) Uracil
Ans- D

11- Which of the following bases contain two keto groups?
a) Adenine
b) Guanine
c) Thymine
d) Cytosine
Ans-C

12- Which sugar is present in RNA?
a) β-D-ribose
b) β-D-fructose
c) β-D-galactose
d) β-D-2-deoxyribose
Ans- A

13-The structure shown is that of a _______



a) DNA nucleoside
b) RNA nucleoside
c) DNA nucleotide
d) RNA nucleotide
Ans- B

14-Which of the following statements is correct?
a) Adenine is a pyrimidine
b) DNA is made of amino acids
c) Nucleosides do not contain phosphorous
d) RNA contains thymine
Ans- C

15- Which of the following best describes cytosine?
a) pyrimidine, present in RNA and DNA
b) pyrimidine, present only in DNA
c) purine, present only in RNA
d) purine, present in RNA and DNA
Ans- a

16- The attachment between the base and sugar in a nucleotide is through ______ bond.
a) hydrogen
b) peptide
c) phosphodiester
d) glycosidic
Ans- D

17-Which part of the nucleotide is responsible for the formation of bonds in DNA double helix?
a) Base
b) Sugar
c) Phosphate group
d) Hydroxyl group of sugar
Ans- A

18- Identify the complementary strand of the DNA primary structure ATGCCGATC.
a) AUGCCGAUC
b) TACGGCTAG
c) UACGGCUAG
d) GATCGGCAT
Ans- A

19- Two DNA samples A and B have melting temperatures 305K and 320K respectively. Identify the correct statement based on this information.
a) A and B are complementary strands
b) B has more CG pairs than A
c) A has more CG pairs than B
d) A has more hydrogen bonds than B
Ans- B

20- Most occurring DNA in nature.
a- A- DNA
b- B- DNA
c- Z-DNA
d- Y- DNA
Ans- B

21- The building blocks of nucleic acids are:
a) Amino acids
b) Monosaccharides
c) Nucleotides
d) Fatty acids
Ans- C

22-The two main types of nucleic acids are:
a) DNA and RNA
b) mRNA and Trna
c) rRNA and tRNA
d) DNA and ATP
Ans- A

23-The sugar found in DNA is:
a) Ribose
b) Deoxyribose
c) Glucose
d) Fructose
Ans- b

24-How many hydrogen bonds are there between adenine and thymine in DNA?
a) One
b) Two
c) Three
d) None
Ans-2

25-The backbone of DNA is composed of:
a) Nitrogenous bases
b) Sugars
c) Phosphate groups
d) All of the above
Ans- D

26-Which type of RNA carries amino acids to the ribosome during protein synthesis?
a) Messenger RNA (mRNA)
b) Transfer RNA (tRNA)
c) Ribosomal RNA (rRNA)
d) Small nuclear RNA (snRNA)
Ans- B

27- Which of the following statements about nucleic acids is false?
a) They store and transmit genetic information
b) They are composed of nucleotides
c) They are involved in protein synthesis
d) They do not play a role in cellular energy storage
Ans- D

28-What is the complementary mRNA sequence to the DNA sequence: ATG CTA GCA?
a) TAC GAT CGT
b) UAC GAU CGU
c) UAC GUA CGU
d) AUG CUA GCA
Ans- B

29-Which of the following is not a function of RNA?
a) Carrying genetic information

b) Acting as an enzyme
c) Carrying amino acids during protein synthesis
d) Storing genetic information
Ans- D

30- Which of the following is true about the structure of DNA?
a) It is a single-stranded molecule
b) It has a double helix structure
c) It contains ribose sugar
d) It contains uracil instead of thymine
Ans- B

31-Which scientist(s) is credited with the discovery of DNA?
a) Watson and Crick
b) Friedrich Miescher
c) Rosalind Franklin
d) Gregor Mendel
Ans- B

32- What is the primary function of mRNA?
a) Carrying amino acids during protein synthesis
b) Transferring genetic information from DNA to the ribosome
c) Storing genetic information within the nucleus
d) Initiating DNA replication
Ans- B

33-A-DNA is favored in conditions of:
a) High humidity
b) Low salt concentration
c) Low humidity
d) Neutral pH
Ans- C

34-B-DNA is characterized by how many base pairs per turn of the helix?
a) 10.5
b) 11
c) 12
d) 13.5
Ans- A

35- Which of the following best describes DNA replication?

a) The process of converting RNA into proteins
b) The synthesis of new DNA strands using existing DNA as a template
c) The packaging of DNA into chromosomes during cell division
d) The process of transcribing DNA into mRNA
Answer: b)

36- What is the process of transcription primarily responsible for?
a) Synthesizing proteins directly from amino acids
b) Replicating DNA to form identical copies
c) Producing RNA molecules from a DNA template
d) Editing mRNA before it is translated into proteins
Answer: c)

37- A-DNA is a conformation of DNA that is:
a) Relatively rare
b) Found only in viruses
c) Found only in bacteria
d) Found under physiological condition
Ans- A

38- What is the process by which mRNA is decoded to produce a specific sequence of amino acids?
a) Transcription
b) Translation
c) Replication
d) Transduction
Answer: b

39-rRNA is called
a) Ribosomal RNA
b) Transfer RNA
c) Messanger RNA
d) Replication RNA
Ans-A

40- B-DNA is characterized by which type of groove?
a) Major groove
b) Minor groove
c) Both major and minor grooves
d) None of the above
Answer: c)

41-The sequence of bases in Z-DNA is:
a) Identical to B-DNA
b) Identical to A-DNA
c) Alternating purine-pyrimidine
d) Random
Ans- C

42-The study of DNA conformation and structure is important because:
a) It helps in understanding genetic diseases
b) It aids in drug design
c) It provides insights into evolutionary relationships
d) All of the above
Ans- d

43- If a DNA molecule contains 30% adenine, what percentage of cytosine does it contain?
a) 20%
b) 30%
c) 40%
d) 60%

Answer: c) 40%

44-If a DNA molecule is 100 base pairs long, how many adenine bases does it contain if it has a 25% adenine content?
a) 25
b) 50
c) 75
d) 100
Answer: b) 50

45-What is the length of a DNA molecule containing 1000 base pairs?
a) 3.4 nm

b) 34 nm

c) 340 nm

d) 3400 nm

Answer: c) 340 nm

46- The diameter of the DNA double helix is approximately:
a) 0.34 nm
b) 2 nm
c) 20 nm
d) 200 nm

Answer: b) 2 nm

47-If a DNA molecule contains 35% guanine, what is the percentage of cytosine?
a) 15%
b) 25%
c) 35%
d) 45%
Answer: c) 35%

48-Nucleic acid supercoiling refers to the:
a) Addition of phosphate groups to the DNA backbone
b) Twisting and coiling of DNA strands upon themselves
c) Removal of histone proteins from DNA
d) Separation of DNA into single strands
Ans- B

49-Supercoiling in DNA primarily occurs due to the action of:
a) DNA ligase
b) DNA polymerase
c) Topoisomerases
d) Helicases
Ans-C

50-Which type of supercoiling is introduced during DNA replication to facilitate unwinding of the DNA strands?
a) Positive supercoiling
b) Negative supercoiling
c) Neutral supercoiling
d) Hyper-supercoiling
Ans- B

UNIT IV

B.Sc. SEM II

SYLLABUS OF UNIT IV

Introductory Medicinal Chemistry: Drug discovery, design and development; Basic Retrosynthetic approach. Drug action-receptor theory. Structure –activity relationships of drug molecules, binding role of –OH group, -NH2 group, double bond and aromatic ring. Mechanism of action of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), HIV-AIDS related drugs (AZT- Zidovudine)

Introductory Medicinal Chemistry

Drug: Any substance (other than food) that is used to prevent, diagnose, treat, or relieve symptoms of a disease or abnormal condition. Drugs, when consumed, cause a change in an organism's physiology, including its psychology. Consumption of drugs can occur via inhalation, injection, smoking, ingestion, absorption via a patch on the skin, suppository, or dissolution under the tongue.

The word "drug" is derived from the French word "drogue," which means a dry herb..

Characteristics of an ideal drug:

1. An ideal drug must be non-toxic.

2. An ideal drug must have minimum side effects.

3. An ideal drug must be efficient.

4. The action of an ideal drug should be localized at a particular site in the body.

5. An ideal drug should not make host cells resistant to the drug.

6. An ideal drug should not injure or damage host tissue.

Side effects of drugs:

All drugs can act as poisons if taken in excess. For example:

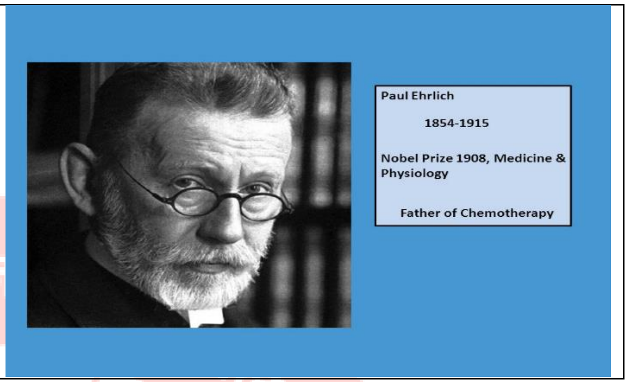
- Overdoses of paracetamol can cause coma and death.

- Overdose of aspirin can cause gastric irritation and bleeding.

- Overdose of antibiotics can inhibit the growth and development of the body of humans and animals.

FATHER OF MEDICINE - Charaka

FATHER OF CHEMOTHERAPY- Paul Ehrlich



Classification of drugs

(A) Classification on the basis of sources

(1) **Synthetic drugs**: Most of the drugs in use today are synthetic in origin. Example: Aspirin, Paracetamol, etc.

(2) Natural drugs: Taxol, quinine, colchicine—plants

Heparin, insulin, thyroid extracts --- animals

Penicillin, streptomycin----microorganism (soil fungi and some bacteria)

(3) semi-synthetic drugs ----- 6-aminopenicillanic acid

(4) bio synthetic --- biosynthetic human insulin

Classification on the basis of therapeutic use-

1. **Antipyretics**: The chemicals used to bring down body temperature in high fever are called antipyretics. The important antipyretics are aspirin, phenacetin and paracetamol.

2. **Analgesics**: The chemicals used for relieving pain are called analgesics. Aspirin, naproxen, ibuprofen, diclofenac sodium, etc., are some important analgesics.

3**. Antiseptics and disinfectants**: The chemicals which kill or prevent the growth of microorganisms are called antiseptics, whereas disinfectants are those chemicals which are capable of killing microorganisms but are not safe to be applied to living tissues.

Some important antiseptics are iodine, dettol, bithional. Chlorine and sulphur dioxide.

4. Tranquilizers: The chemicals used for the treatment of stress, mild and severe mental diseases are called tranquilizers. The important tranquilizers are barbiturates (veronal, amytal, nembutal, etc. chlorodiazepoxide, meprobamate, equanil, etc

5. Antimicrobials: The chemicals used to cure diseases caused by microbes such as bacteria, viruses, fungi, etc., are called antimicrobials The important antimicrobials are Antibiotics and sulpha drugs.

6. Antibiotics: The chemicals which are produced by certain microorganisms and are capable of inhibiting the growth or even destroying infection causing microorganisms in human beings are called antibiotics, Penicillin ampicillin amoxicillin etc, are the important antibiotics.

The antibiotics effective against several different types of harmful microorganisms are called broad spectrum antibiotics. Tetracycline, Chloramphenicol are such antibiotic.

7. Sulpha drugs: These are the derivatives of sulphanilamide. The important sulpha drugs are sulphadiazine, sulphapyridine, sulphaguanidine.

8. Antifertility drugs: The chemicals used for birth control are called antifertility drugs. These control the female menstrual cycle and ovulation, the birth control pill is essentially a mixture of synthetic estrogen and progesterone derivatives. Mifepristone (a synthetic steroid) is used as a 'morning after pill.

9. Antihistamines: The drugs used to combat the effects of allergy are called antihistamines. They check the production of histamines in the body. The commonly used antihistamines are diphenylhydramine, chloropheniramine and promethazine.

10. Antacids: Antacids are those chemical substances which remove the excess acid and raise the pH to an appropriate level in stomach. The important antacids are omeprazole and lansoprazole.

Different routes of drug administration

(1) Oral/swallowed: It is the oldest and bad common mode of administration. Most drugs in this mode are absorbed in small intestine It is safer, more convenient, painless, cheaper mode. Both solid and liquid dosage forms can be given orally

(2) Inhalation: Volatile oils and gases are given by inhalation.

Ex. General anaesthatic, amylnitrite.

This route is potentially dangerous because it is so fast and direct.

(3) Oral/sublingual: The tablet or pellet containing the drug is placed under the tongue or crushed in the mouth and spread over the buccal mucosa

(4) Rectal: Here the drugs are absorbed directly from the rectum. Certain irritant and unpleasant drugs can be put into rectum are suppositories or retention enema for systematic effect.

Ex. Diazepam, paraldehyde and few other drugs are sometimes given rectally,

(5) Epithelial: In this mode drugs are absorbed through the skin.

(6) Parenteral route: It refers to administration by injection into tissue f or blood without having to cross the intestinal mucosa. This route can be employed even in unconscious, uncooperative or vomiting patient.

Sites of drug action:

(1) Enzyme inhibition

(2) Drug-Receptor interaction

(3) Non-specific interaction.

Therapeutic Index: The medicinal value of the drugs is represented by Therapeutic index.

It may be defined as the ratio of Maximum tolerated dose (MTD) to the Maximum curative dose (MCD).

[Therapeutic index= Maximum tolerated dose / Maximum curative dose]

OR

[Therapeutic index = MTD

Therapeutic index or therapeutic ratio is a quantitative measurement of the relative safety of a drug.

For animals in pre-clinical trials. [Therapeutic index= (LD_{50} / ED_{50}

For humans in clinical trials, Therapeutic index = TD_{50} / ED_{50}

where, LD Lethal Dose
ED Effective Dose
TD Toxic dose

Therapeutic index gives idea about drug safety margin.

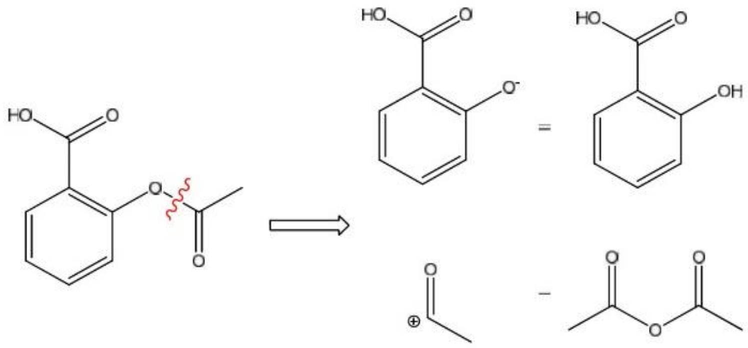
The larger the therapeutic index the safer the drug. Reasonably safe drug must have therapeutic index more than 1.

Retrosynthetic approach

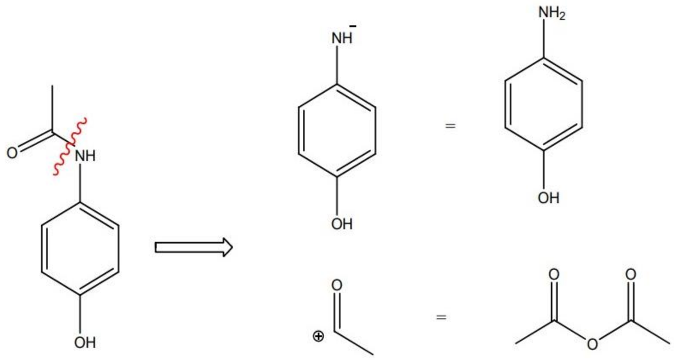
- Retrosynthetic analysis is a technique for solving problems in the planning of organic syntheses.
- This is achieved by transforming a target molecule into simpler precursor structures regardless of any potential reactivity/interaction with reagents.

- Each precursor material is examined using the same method. This procedure is repeated until simple or commercially available structures are reached.
- These simpler/commercially available compounds can be used to form a synthesis of the target molecule

Retrosynthetic approach of Aspirin (common analgesic)



Retrosynthetic approach of Paracetamol (Anti Pyretic)



Drug discovery design and development-

(1) Target Identification: Scientists select a target for a potential new medicine, such as proteins, genes, or RNA, involved in a particular disease. A good target needs to be efficacious, safe, and druggable, meaning it can interact with a drug molecule and elicit a measurable biological response.

(2) Target validation is crucial for identifying disease targets that can be affected by drugs. Techniques include in vitro tools, animal models, and modulation of targets in patients. Lead compounds can be found in nature, created from scratch, identified through high-throughput screening, or produced using biotechnology.

(3) Selection of lead compound (Lead Compound Identification Methods):

- Nature: Historically, scientists discovered important compounds from moldy plants and soil bacteria.
- De Novo: Scientists create molecules using computer modeling.
- High-Throughput Screening: Researchers test thousands of compounds to identify potential leads.
- Biotechnology: Scientists engineer living systems to produce disease-fighting molecules.

(4) Early safety tests: Lead compound, go through a series of test to provide disease an early evaluation of the safety of the lead compound.

Absorption, distribution, metabolism, excretion and toxicological properties of each lead compound is tested.

A successful drug must:

- distributed to the proper site of action in the body
- metabolized efficiently and effectively
- absorbed into the bloodstream
- successfully excreted from the body.
- demonstrated to be not toxic.

Early safety studies are performed via computational models, in living on and in animals

(5) Lead optimization : The aim of this stage of the work is to refine each hit series, trying to produce potent and safe compounds with pharmacokinetic properties that are adequate to examine their efficiency in any in vivo models that are available. Hundreds of different analogues of the initial leads are made and tested by the team of biologists and chemists working concurrently. The biologists evaluate the analyses on biological systems, while the chemists use this information to make additional relations. The compounds that successfully pass become the candidate drug.

(6) Preformation studies: Just after the candidate drug is optimized, the researchers begin to think about how the candidate drug will be formulated, what will be the route of administration, and how it will be manufactured at a large scale. Before processing the new drug into a formulation, a series of studies are conducted on the drug to determine the most suitable and acceptable dosage form.

Preformulation studies include the determination of the physiochemical properties of the drug, such as solubility, partition coefficient, dissociation constant, lipophilicity, dissolution, and determination of solid state properties (particle size, density, flow, compression properties).

(7) **Preclinical testing**: Preclinical testing involves in vitro and in vivo tests

In vitro tests, experiments are conducted in the lab, usually carried out in test tubes and beakers and in vivo studies, tests are conducted in living cell. The objective of these studies is to understand how the drug works and what safety profile.

The Preclinical studies must provide detailed information on preliminary efficiency, toxicity, pharmaco-kinetic and safety.

After preclinical testing, the findings are reviewed and decide whether the drug should testing in people.

Phase 0 clinical trial: In these trials, a single sub-therapeutic dose is given to 10 to 15 human volunteers to quickly weel out drug candidates that are metabolically or biologically ineffective.

Phase 1 Clinical trial: These trials are usually conducted with about 20-100 healthy volunteers.

Phase II clinical trial: These trials are performed on about 100 to 500 patients. Drugs that do not show promising results in phase II are often not pursued in Phase III.

In fact, only 18% drugs in Phase-II proceed to Phase-III.

Phase-III clinical trial: This phase investigates the efficacy of a new drug over 6 to 12 months in a larger patient population (about 1000-5000) to generate significant data about safety, efficacy and the overall benefit-risk relationship of the drug.

- This phase a key in determining whether the drug is safe and effective.
- It also provides the basis of labeling instructions to help ensure proper use of the drug.
- One the phase III trials are complete the sponsoring company analyses all of the data.
- If the data is correct for safety purpose, the company files a new drug application (NDA) to the FDA requesting approval to market the drug.

Structure-Activity Relationship (SAR) of drug molecules

The QSAR approach attempts to identify and quantify the physicochemical properties of a drug and to see whether any of these properties has an effect on the drug's biological activity. If such a relationship holds true, an equation can be drawn up which quantifies the relationship and allows the medicinal chemist to say with some confidence that the property (or properties) has an important role in the pharmacokinetics or mechanism of action of the drug.

It also allows the medicinal chemist some level of prediction. By quantifying physicochemical properties, it should be possible to calculate in advance what the biological activity of a novel analogue might be.

There are two advantages to this.

- Firstly, it allows the medicinal chemist to target efforts on analogues which should have improved activity and, thus, cut down the number of analogues that have to be made.
- Secondly, if an analogue is discovered which does not fit the equation, it implies that some other feature is important and provides a lead for further development

Compounds with similar structures of a pharmacologically active drug are often themselves biologically active.

This information may be used to develop a new drug that has increased activity, a different activity from an existing drug and fewer unwanted side effects.

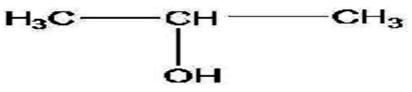
Structure activity relationship is usually determined by making minor changes to the structure of a lead to produce analogues and assessing the effect these structural changes have on biological activity.

(i) Binding role of hydroxyl (-OH) group (Effect of -OH group)

- Due to presence of -OH group into an aliphatic compound, the physiological activity of compound decreases.

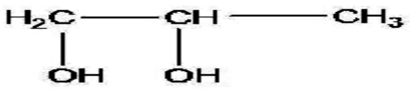
Ex **Activity order -** (a) (more active) > (b) > (c) (less active)

(a)



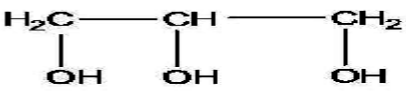
$H_3C-\underset{OH}{\underset{|}{CH}}-CH_3$

(b)



$\underset{OH}{\underset{|}{H_2C}}-\underset{OH}{\underset{|}{CH}}-CH_3$

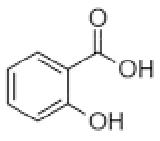
(c)



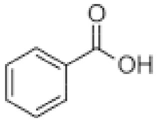
$\underset{OH}{\underset{|}{H_2C}}-\underset{OH}{\underset{|}{CH}}-\underset{OH}{\underset{|}{CH_2}}$

- Due to presence of -OH group into aromatic compounds, the physiological activity of compounds increases.

Ex. Salicylic acid (more active) and benzoic acid (less reactive)



Salicylic acid



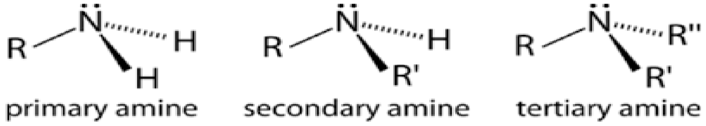
Benzoic acid

(2) Binding role of amino group (Effect of amino group)-

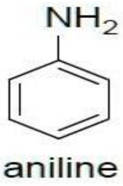
We know that amino group is toxic in nature. The toxic effect of amino group may be reduced by the following processes

(a) Alkylation: Generally, alkylation reduces the toxic effect of amino group.

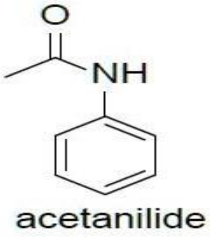
Example.



(b) Acylation: Generally acylation decreases the toxicity or physiological action of a compound containing amino group. Example

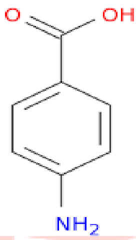


(Toxic)



(Febrifuge)

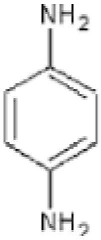
(c) Carboxylation: Generally, carboxylation also decreases the physiological action of amino compounds**. Example:** Aniline (Toxic or Poisonous), p-aminobenzoic acid (PABA) (Component of vitamin B complex)



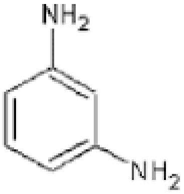
Note: The entrance of a second amino group into the benzene ring increases the toxicity. Example:

1,2-diaminobenzene (o-phenylenediamine), 1,3-diaminobenzene (m-diaminobenzene), 1,4-diaminobenzene (p-diaminobenzene)

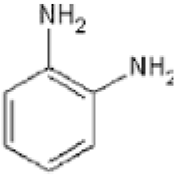
A



B



C



3) Binding role of DOUBLE BOND- The unsaturated compounds are generally more toxic than their corresponding saturated compounds.

Example:

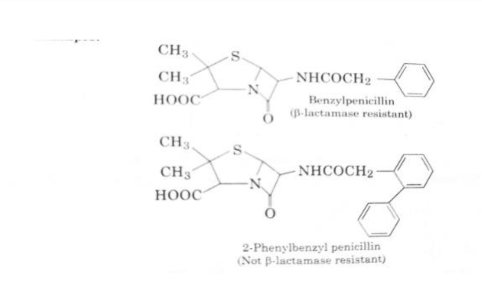
CH2=CH-CH2OH	CH3-CH2-CH2-OH
Allyl alcohol (strong Poisonous)	Propanol (Mild Narcotic)
CH3-CH=CH-CHO	CH3-CH2-CH2-CHO
Crontonaldehyde (more toxic)	Butanol(less toxic)

Caffeine is more Physiologically active than hydroxy-caffeine

(4) Binding role of aromatic rings (effect of aromatic group)-

Due to presence of an aromatic ring, the size and shape of the lead molecule changes. These changes in the size and shape of the molecule affect the activity and efficiency of the compound. Example:

The positive and negative effects of these changes are generally not predictable.

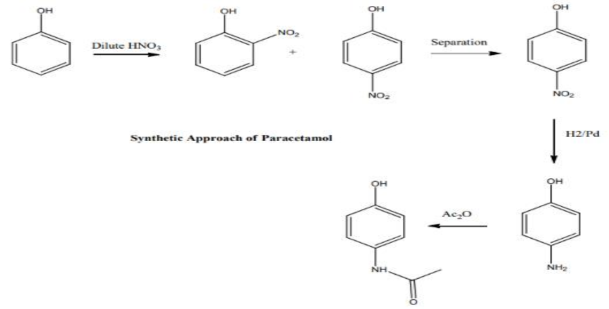


Mechanism of action of the representative drugs

(A) Analgesics, Antipyretics and Anti-inflammatory agents- Antipyretic analgesics are a group of heterogeneous substances including acidic (non-steroidal, Anti-inflammatory drugs, NSAIDs) and non- acidic (paracetamol, pyrazolinones) drugs.

- Antipyretics are the class of drugs which are used to reduce the fever.
- Analgesics are the class of drugs which are used to reduce the pain.
- Antipyretics have no effects on body temperature when it is in the ne range. The most commonly used antipyretics-analgesics are:

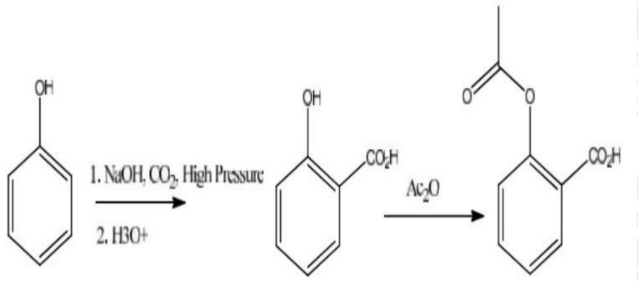
(1) **Paracetamol or Acetaminophen**: It is the most common antipyretic It is the acetyl derivative of p-amino phenol. It's structural formula is



Synthetic Approach of Paracetamol

Aspirin-

- Aspirin is also known as acetyl salicylic acid.
- It is a nonsteroidal Antipyretics and Anti-Inflammatory



Uses of aspirin-

(i) It is an effective analgesic only in case of mild pain, while it is ineffective in case of severe pain.

(ii) It is used in the treatment of fever, pain, rheumatic fever, rheumatoid, arthritis, Kawasaki disease.

(iii) Like its ability to control pain, aspirin's ability to control fever is due to its action on the prostaglandin system through its irreversible inhibition of COX.

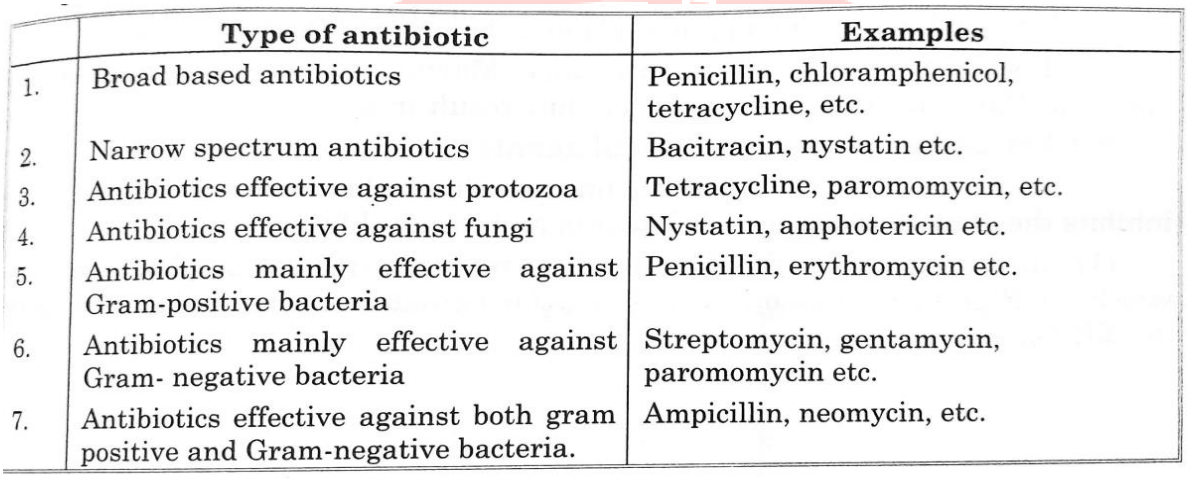
(iii) It's common adverse effect is upset stomach.

(B) Antibiotics : Antibiotics are chemical substances produced by various species of microorganisms, which in low concentration destroy or inhibit the other species of microorganisms. In the present usage the term antibiotic includes chemically related and derived substances. Antibiotics have prevented millions of deaths and radically changed healthcare during the last century

- Penicillin- the first antibiotic in 1928 was discovered by **Alexander Fleming** observed the killing of staphylococci by a fungus (Penicillium notatum). He got a Nobel prize in 1945.

- Penicillin first used in World War II (1942) and saved 12-15% patient

Classification of antibiotics-

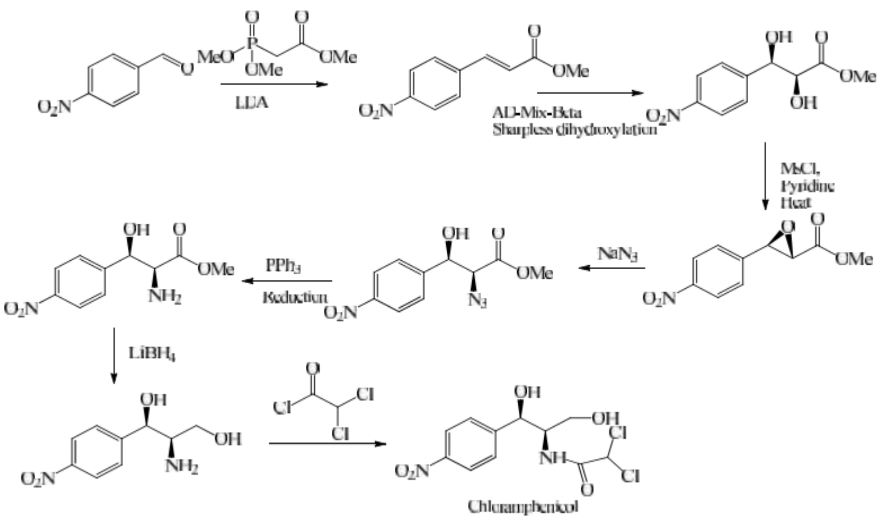


	Type of antibiotic	Examples
1.	Broad based antibiotics	Penicillin, chloramphenicol, tetracycline, etc.
2.	Narrow spectrum antibiotics	Bacitracin, nystatin etc.
3.	Antibiotics effective against protozoa	Tetracycline, paromomycin, etc.
4.	Antibiotics effective against fungi	Nystatin, amphotericin etc.
5.	Antibiotics mainly effective against Gram-positive bacteria	Penicillin, erythromycin etc.
6.	Antibiotics mainly effective against Gram- negative bacteria	Streptomycin, gentamycin, paromomycin etc.
7.	Antibiotics effective against both gram positive and Gram-negative bacteria.	Ampicillin, neomycin, etc.

Classes of antibiotic:

1. β-Lactam antibiotics examples: Penicillins (e.g. amoxicillin), cephalosporins, carbapenems, monobactams, etc.
2. Tetracyclines example: Tetracycline
3. Macrolide antibiotics example: Erythromycin
4. Aminoglycosides examples: Gentamicin, Tobramycin, Amikacin
5. Quinolones example: Ciprofloxacin (a fluoroquinolone)
6. Cyclic peptides examples: Vancomycin, Streptogramins, Polymyxins.
7. Lincosamides example: Clindamycin
8. Oxazolidinoes example: Linezolid (Zyvox)
9. Sulfa antibiotics example: Sulfisoxazole

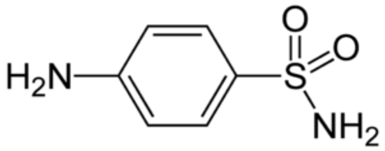
Chloramphenicol is an antibiotic useful for the treatment of a number of bacterial infections. This includes as an eye ointment to treat conjunctivitis. By mouth or injection into a vein, it is used to treat meningitis, plague, cholera and typhoid fever. Its use by mouth or by injection is only recommended when safer antibiotics cannot be used.



C) ANTIFUNGAL AND ANTIBACTERIAL- Antifungal and antibacterial agents are those chemical compounds which inhibits the growth or destroy the bacteria and fungi.

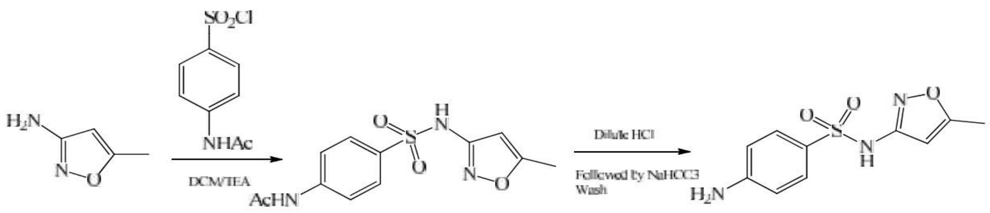
i) Sulphonamide:

- Sulfonamides are generic name for the derivatives of para-amino benzene sulfonamide.
- They are effective chemotherapeutic agents used for the prevention and treatment of bacterial infections in human.
- Sulfonamides are bacteriostatic antibiotics with a wide spectrum action.



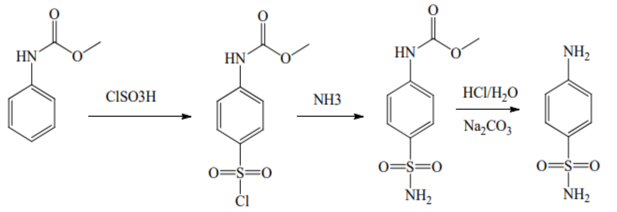
ii) Sulfamethoxazole (SMZ or SMX)

- It is an antibiotic.
- It is used for bacterial infections such as urinary tract infections, bronchitis and prostatitis
- It is effective against both gram negative and positive bacteria such as Listeria monocytogenes and E-coli.



iii) Sulfacetamide:

- Sulfacetamide is 10% typical lotion, is approved for the treatment of acne and seborrhea dermatitis.
- Treatment of urinary tract infection.
- It also has anti-inflammatory properties when used to treat conjunctivitis.



D) Antiviral Agents:

i. The diseases due to viral infections are more frequent. The viral infections are possibly responsible for over 60% of the human illness, whereas only 15% may be due to bacterial infections.

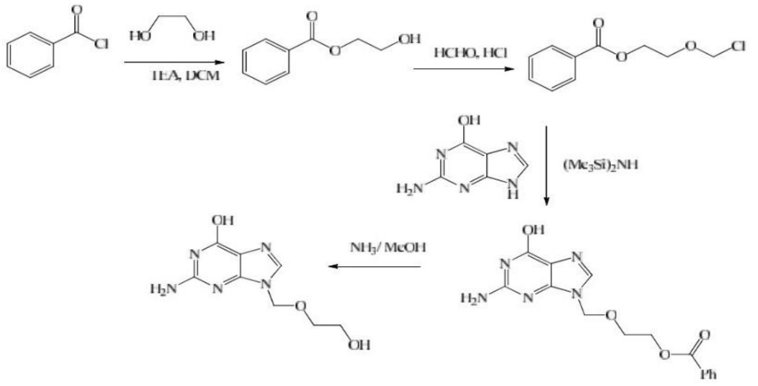
ii. The well know viral diseases include common cold, influenza, bronchitis, hepatitis, herpes gastroenteritis, rabbis, chicken pox, small pox, measles and mumps.

iii. Antiviral drugs are also preventive. They can protect from getting viral infections or spreading a virus to others. Antiviral medicines work differently depending on the drug and virus type. Antivirals can:

- Block receptors so viruses can’t bind to and enter healthy cells.
- Boost the immune system, helping it fight off a viral infection.
- Lower the viral load (amount of active virus) in the body

Acyclovir:

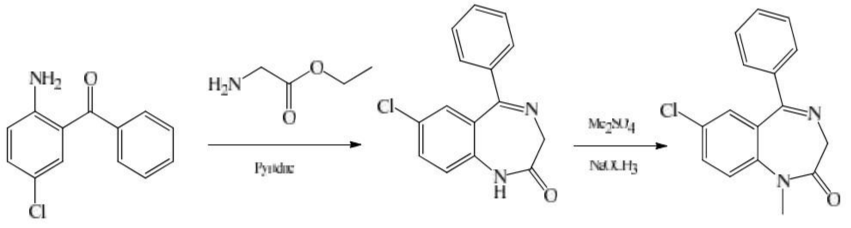
- Acyclovir is an antiviral medication.
- It is primarily used for the treatment of herpes simplex virus (HSV)infections, chicken pox and shingles.
- Chemically acyclovir is 9-[{2-hydroxyethoxy}methyl]-9H-guanine



E) Central Nervous System Agents:

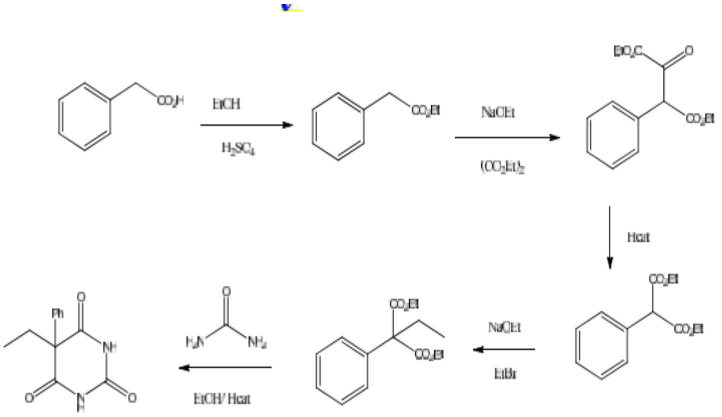
- Central Nervous System (CNS) depressants are medicines that include sedatives, tranquilizers, and hypnotics.
- These drugs can slow brain activity, making them useful for treating anxiety, panic, acute stress reactions, and sleep disorders.
- Drugs that are classified as CNS depressants include: Alcohol. Barbiturates. Benzodiazepines.
- It is commonly used to treat a range of conditions including anxiety, alcohol withdrawal syndrome, muscle spasms, seizures, trouble sleeping and restless legs syndrome.

Diazepam: It is commonly used to treat a range of conditions including anxiety, alcohol withdrawal syndrome, muscle spasms, seizures, trouble sleeping and restless legs syndrome



Phenobarbital

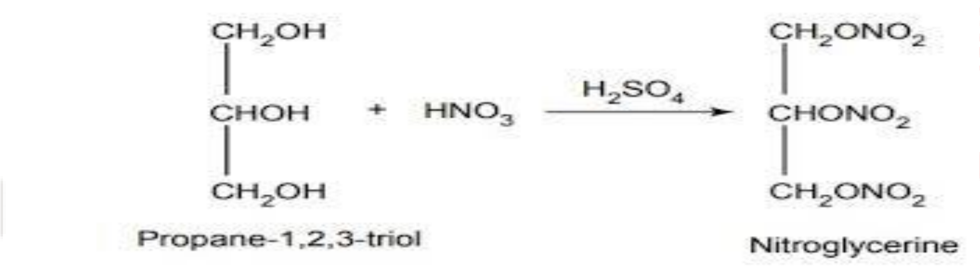
- Phenobarbital, also known as phenobarbitone
- It is used as sedative and hypnotic.



F) Cardiovascular agents:

Cardiovascular agents are medicines that are used to treat medical conditions associated with the heart or the circulatory system (blood vessels), such as arrhythmias, blood clots, coronary artery disease, high or low blood pressure, high cholesterol, heart failure, and stroke.

Nitroglycerine, also known as glyceryl trinitrate (GTN), is a medication used for heart failure, high blood pressure, and to treat and prevent chest pain from not enough blood flow to the heart or due to cocaine. This is taken by mouth, under the tongue, applied to skin, or by injection into a vein.

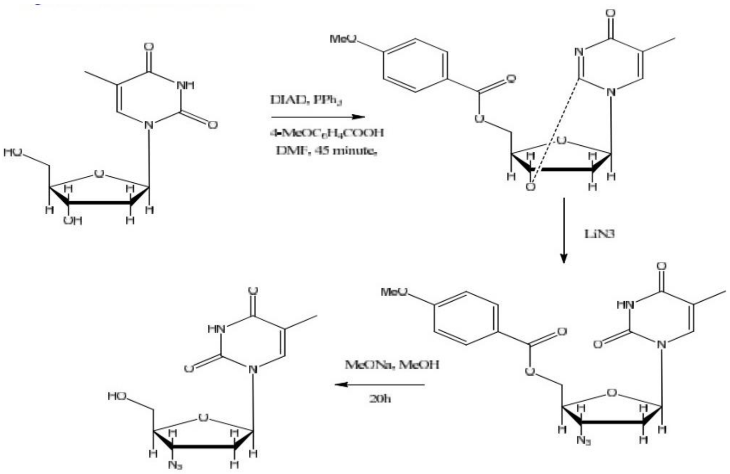


G) HIV-AIDS related drugs Zidovudine (ZDV),

HIV is the virus that causes AIDS. HIV stands for "Human Immunodeficiency virus" There are cells in our body called CD4 cells" or "T cells". These cells help to protect our body from disease. HIV kills these cells.

There are medicines reduce the amount of HIV and increase the T-cells in our body. The medicines used to treat HIV are called "Antiretroviral treatment." Or ART

Zidovudine (AZT): Zidovudine is also known as Azidothymidine (AZT). It is an antiretroviral medicine used to prevent and treat HIV-AIDS. AZT is a thymidine analogue, AZT works by selectively inhibiting HIV reverse transcriptase, the enzyme that the virus uses to make DNA copy of its RNA. Its structural formula is



Drug-receptor interactions-

A receptor is a component that interacts with a drug and initiates biochemical events leading to the drug's effects.
Agonists activate receptors and can differ in affinity and efficacy. Antagonists do not activate receptors and prevent the activation by an agonist.

Drug Action Receptor Theories: After a drug attach to a receptor site, it may initiate or prevent a response. This concept is known as receptor antagonism and is important in medicinal chemistry and drug action mechanisms.

Occupation theory: Developed by Clark and Gaddum, it describes the interaction between a drug and a receptor as a bimolecular interaction. Clark assumed that the effects of a drug were proportional to the fraction of receptors occupied by the drug.

$$A+R \rightleftharpoons AR \qquad \text{i.e. equal to effect}$$

Rate of association = K_1 [A] [R]

Rate of dissociation = K_2 [AR]

At equilibrium,

Rate of forward reaction = Rate of backward reaction

$$K_1 [A][R] = K_2 [AR]$$

dissociation constant, $K = K_1 / K_2 = [A][R] / [AR]$

(2) Rate theory: Rate theory was proposed by Paton and Rang in 1965.According to this theory, the most important factor in determining drug action is the rate at which drug receptor combination takes place. This theory can be explained by the following formula.

Rate of receptor occupation = $K_2 / 1 + [KA] / [A]$

(3) Induced-fit theory: This theory states that, after combination, the substrate introduces a change in conformation of the enzyme, leading to an enzymatically active orientation group. Example: Acetylcholine may interact with the regulating protein and alter the normal forces.

Multiple choice question

1. Medicinal chemistry deals with

(a) Synthesis of drugs

(b) drug design

(c) Interaction of drug with the body

(d) All of these

Ans- B

2- Neurologically active drug/is/are
- a) Heroin
- b) Aspirin
- c) Phenelzine
- d) All of these

Ans-D

3- Which of the following is used as a painkiller?
- a) Analgesic
- b) Antibiotic
- c) Antipyretic
- d) Antioxidants

Ans- A

4- Which of the following types of drugs are used to reduce fever?
- a) Analgesic
- b) Antipyretic
- c) Antibiotic
- d) Antihistamine

Ans- B

5-Analgesics drug is

a) Chloramphenicol
b) Chloroquine
c) Paracetamol
d) Chlorpheniramine maleate

Ans- C

6- A 0.2 % solution of phenol acts as an…

a) Antiseptic
b) Analgesic
c) Antibiotic
d) Antihistamine

Ans- A

7- Sulphonamides are derivatives of

a) Sulphonic acid
b) Phenol
c) Sulphuric acid
d) Barbituric acid

Ans- A

8- Chloramphenicol is an

a) Antibiotic
b) Antihistamine
c) Antifertility drug
d) Anti-Microbial

Ans- A

9- An example of Tranquilizers drug is

a) Penicillin
b) Promethazine
c) Barbiturate
d) Dettol

Ans- C

10- The antibiotic effective against gram negative bacteria is

a) Novalgin
b) Luminal
c) Streptomycin
d) Bithional

Ans- C

11- The safety of the candidate drug in human are studied in

a) Phase I
b) Phase II
c) Phase III
d) Phase IV

Ans- B

12- ………….. checks the growth of micro- organisms.

a) Anaesthetic
b) Analgesic
c) Antiseptic
d) Antipyretic

Ans- C

13- Which of the following drug is not an antibiotic?

a) Penicillin
b) Amoxilline
c) Acetaminophen
d) tetracycline

Ans- C

14- Which of the following synthetic dye is used as an antiseptic?

a) Phenolphthalein
b) n- Hexylresorcinol
c) Acriflavine
d) Trypan red

Ans -C

15- Which of the following antibiotic is used for tuberculosis?

a) Streptomycin
b) Ampicillin
c) Terramycin

d) Chloromycetin

Ans-A

16- Which of the following is not an antacid?

a) Phenelzine
b) Ranitidine
c) Cimetidine
d) Aluminum hydroxide

Ans- A

17- Which of the following is an analgesic?

a) Novalgin
b) Penicillin
c) Streptomycin
d) Chloromycetin

Ans- A

18- Birth control pills contain

a) Estrogen only
b) Progesterone only
c) Mixture of estrogen and progesterone derivatives
d) Novalgin and paracetamols

Ans- C

19. Drugs that bind to the receptor site and inhibit its natural function are c

(a) antagonists

(b) agonists

(c) molecular targets

(d) enzymes

Ans -A

20. Chloramphenicol is an

(a) antifertility drug

(c) antihistamine drug

(b) antiseptic and disinfectant

(d) antibiotic-broad spectrum

Ans-D

21. Sulphonamide are

a) Antiprotozoal agent
b) Antibacterial agent
c) Antimalarial agent
d) None of these

Ans – B

22 …………….is made by acetylating salicylic acid with acetic anhydride

a) Aspirin
b) Ibuprofen
c) Piroxicam
d) None of these

Ans -A

23. Zidovudine is derivative of

a) Guanosine
b) Thymidine
c) Adenine
d) Uracil

Ans- B

24. MTD is

a) Maximum targated dose
b) Minimum tolerated dose
c) Minimum targated dose
d) Maximum tolerated dose

Ans- D

25. Sulphanilamide is

a) Benzene sulphonyl chloride
b) p- Hydroxy Acetanilide
c) p- amino benzene sulphonamide
d) none of these

Ans-C

26. Drug aspirin is used as

a) Antipyretic
b) Anti- inflammatory
c) Analgesic
d) All of these

Ans- D

27. Which of the following is an antibiotic

a) Paracetamol
b) Aspirin
c) Chlromphenicol
d) Acetaminophen

Ans- C

28. Omeprazole drug was used for the treatment of

a) Acidity
b) Dysentery
c) Meningitis
d) Typhoid

Ans- A

29-Sulphonamide is:

a) Antibacterial
b) Antifungal
c) Antimicrobial
d) All of these

Ans-D

30. Which of the following is an antipyretic drug?

a) Sulphonaminde
b) Aspirin
c) Both
d) None of these

Ans- B

31. The characteristics of a drug is/are

(a) It should be non-toxic
(b) It should not damage host tissues
(c) It should have minimum side effects

(d) All of these

Ans- D

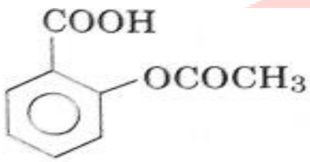
32. The Medicinal value of the drugs is represented by

(a) Refractive Index
(b) Therapeutic Index
(c) Drug Therapy
(d) Both (a) and (b)

Ans -B

33. The structure of aspirin is

(a)



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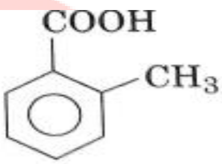

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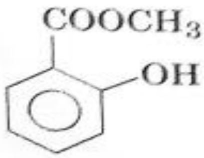

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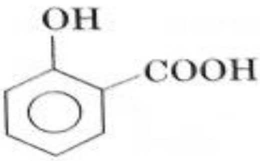


Ans -C

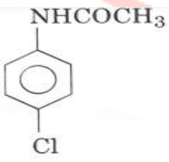
34. Father of chemotherapy is

(a) Paul Ehrlich
(b) Fischer
(c) Newmann
(d) Haworth

Ans -A

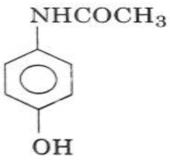
35. The structure of paracetamol is

(a)



(b)

(c)



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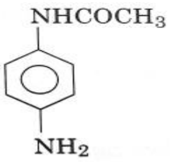


Ans -C

36. AZT (Zidovudine) is used in the treatment of

(a) Malaria

(b) AIDS

(c) Typhoid

(d) Kala-azar

Ans –B

37. The full from "AIDS" is

(a) Acquired Immuno Deficiency Syndrome

(b) Acquired Internal Deficiency System

(c) Acquired Infected Disease Solution

(d) Acquired Immuno Disease Syndrome

Ans- A

38. The full form HIV is

(a) Harmful injection virus

(b) Human infected virus

(c) Human immunodeficiency virus

(d) Human infected deficiency

Ans- C

39. Diazepam is

(a) CNS agent

(b) Antiviral agent

(c) Both (a) and (b)

(d) None of these

Ans- A

40. Therapeutic use of drug nitroglycerine is?

(a) treatment of prostate cancer

(b) treatment of angina

(c) treatment of antidiabetic drug

(d) as an anaesthetic

Ans- B

41. QSAR method involves

(a) Target structure

(b)Ligand X-ray structure

(c) Ligand properties

(d) Target properties

Ans- C

42. Nitroglycerine can be prepared by the nitration of?

(a) Glyceraldehyde

(b) Trinitro glyceraldehde

(c) Glycerol

(d) Trinitroglycerol

Ans- B

43. An antiviral agent is

(a) Sulphonamide

(b) Sulphanilamide

(c) Acylovir

(d) None of these

Ans- C

44. Chloramine-T is used as:

(a) Explosive material

(b) Antiseptic

(c) Neutral

(d) None of these

Ans- B

45. SMZ stands for

(a) Sulphamethoxazole

(b) Sulphanilamide

(c) Sulphacetamide

(d) sulphonamide

Ans- A

46. Which of the following is/are artificial sweetener?

(a) Saccharin
(b) Aspartame
(c) both
(d) None of these

Ans- C

47. Which of the following drug may be used for the treatment of cocci-infection

(a) Sulphanilamide

(b) Aspirin

(c) Paracetamol

(d) Saccharin

Ans- A

48. Sulphacetamide is used for the treatment of

(a) Fever

(b) Pain

(c) Urinary infections

(d) All of these

Ans- C

49.Phenobarbital is

(a) Antiviral agent

(b) CNS agent

(c) Both (a) and (b)

(d) None of these

Ans- B

50. SAR stands for

(a) Skeleton Active Receptor

(b) Stereochemistry And Randor

(c) Structure Activity Relationship

(d) All of these

Ans -C

UNIT V

B.Sc. SEM II

SYLLABUS OF UNIT V

Definition of space lattice, unit cell. Laws of crystallography – (i) Law of constancy of interfacial angles, (ii) Law of rationality of indices and iii) Symmetry elements in crystals and law of symmetry .X-ray diffraction by crystals. Derivation of Bragg equation. Determination of crystal structure of NaCl, KCl and CsCl (powder method)

Solid State

Classification of solids: Solids are of following two types:

I) Crystalline solids: In a crystalline solid, the arrangement of structural units (atoms, molecules or ions) is very regular and extends in three dimensions throughout the crystal. Thus, crystalline solids possess long range order. They are anisotropic in nature, i.e., they possess different magnitudes of physical properties in different directions. They are true solids.

II) Amorphous solids: They do not possess a regular arrangement of structural units throughout the solid and thus possess a short-range order. They are isotropic in nature, Le, they possess the same magnitudes of physical properties in all directions. Amorphous solids are regarded as super cooled liquids or pseudo solids.

Classification of crystalline solids: The crystalline solids may be classified into four categories

(i) Molecular solids

(ii) lonic solids,

(iii) Covalent solids, and

(iv) Metallic solids.

Space lattice: The three-dimensional arrangement of structural units or constituent particles (atoms, molecules or ions) in a crystal called lattice

Unit cell: Unit cell is the smallest three-dimensional group of lattice points, which when repeated in three dimensions in space, gives the whole lattice of the crystal.

Parameters of a unit cell: A unit cell is characterized by the following parameters:

(i) Relative lengths a, b, and c of the three edges along the three axes, i.e., axial distances

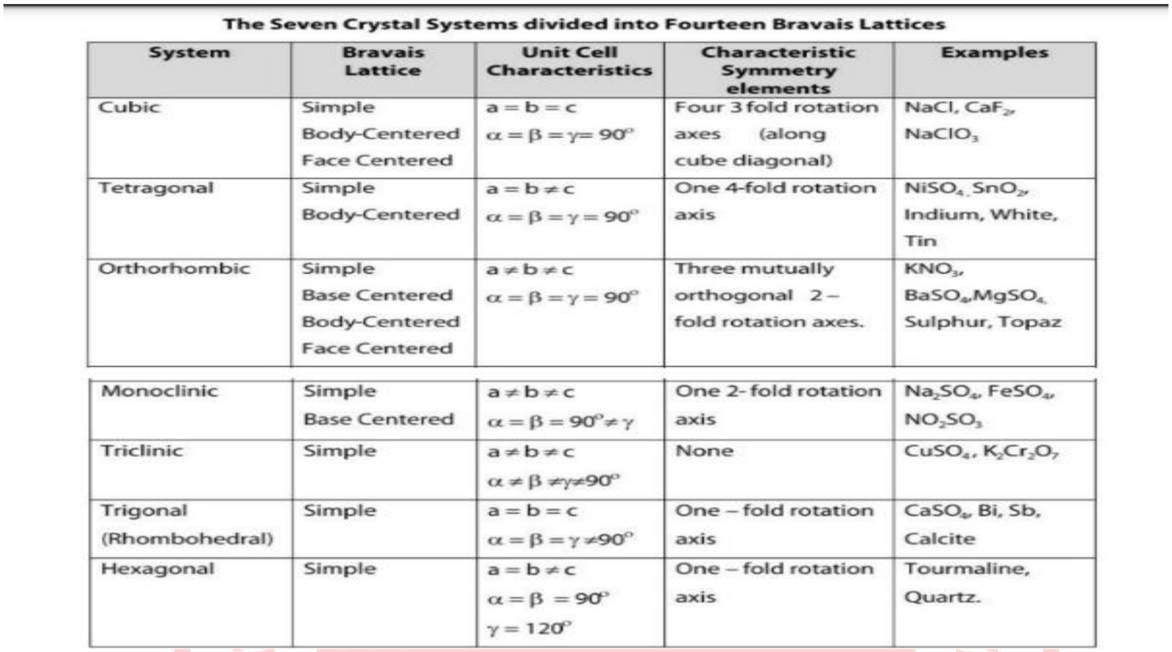
(ii) Axial angles α, β and γ between the pairs of edges (b,c) (c. a) and (a, b) respectively.

Crystallography. It is that branch of science which deals with the study of geometry, properties and structure of crystals.

Steno's Law of constancy of Interfacial angles. The angles between the corresponding faces, called the interfacial angles of the crystals of a particular substance are always the same independent of the shape and size of the crystals.

Goniometer. It is the instrument used to measure the interfacial angles. The simplest is contact goniometer. The other two for more precise work are Reflecting goniometer and X-ray goniometer.

The seven crystal systems or crystal habits: Bravais (1850) showed that the unit cells are of 14 types. Seven of these are primitive and the rest are body-centred and face-centred. The seven primitive unit cells constitute the seven crystal systems. They are known as seven crystal habits or Bravais lattices. Table 1



The Seven Crystal Systems divided into Fourteen Bravais Lattices

System	Bravais Lattice	Unit Cell Characteristics	Characteristic Symmetry elements	Examples
Cubic	Simple Body-Centered Face Centered	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	Four 3 fold rotation axes (along cube diagonal)	NaCl, CaF_2, $NaClO_3$
Tetragonal	Simple Body-Centered	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	One 4-fold rotation axis	$NiSO_4$, SnO_2, Indium, White, Tin
Orthorhombic	Simple Base Centered Body-Centered Face Centered	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Three mutually orthogonal 2 – fold rotation axes.	KNO_3, $BaSO_4$, $MgSO_4$, Sulphur, Topaz
Monoclinic	Simple Base Centered	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	One 2- fold rotation axis	Na_2SO_4, $FeSO_4$, NO_2SO_3
Triclinic	Simple	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	None	$CuSO_4$, $K_2Cr_2O_7$
Trigonal (Rhombohedral)	Simple	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	One – fold rotation axis	$CaSO_4$, Bi, Sb, Calcite
Hexagonal	Simple	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	One – fold rotation axis	Tourmaline, Quartz.

Different types of cubic systems: The cubic systems are of following three types

(1) Simple cubic systems: The unit cell present in a simple cubic system is primitive and consists of constituent particles (atoms, molecules or ions) only at the corner

(ii) Body-centred cubic systems: The unit cell present in these systems is body centred and consists of one structural unit at the Centre of the cube in addition to the structural) units located at all of its corners.

(iii) Face-centred cubic systems: The unit cell present in these systems is face-centred and consists of one structural unit the middle of each of its six faces in addition to a structural unit at each corner,

Types of unit cells: Unit cells may be of following four types:

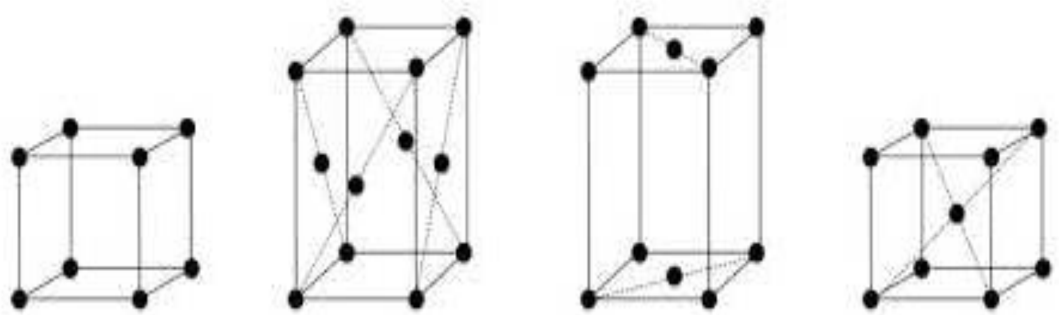
(1) **Simple** when the points are present only at the corners of the unit cell.

(ii) **Face-centred** when in addition to points at the corners, they are also present at the face-centre.

(iii) **End centred** when in addition to points at the corners, there are points at the end faces of the unit cell.

(iv**) Body-centred** when in addition to points at the corners, there is one point present at the body centre.

The simple unit cell is called **primitive** while the others are called **non-primitive**. Corresponding to 7 crystal systems, there are 14. Bravais lattices. (Table -1)



Different type of unit cell

Number of particles per unit cell: The number of particles per unit cell can be calculated with the help of the following rules

(1) A particle present at the corner contributes only 1/8 to a particular cubic unit cell.

(2) A particle present at the centre of a face contributes only ½ to a particular cubic unit cell.

(3) A particle present at the body centre contributes 1 to a particular cubic unit-cell.

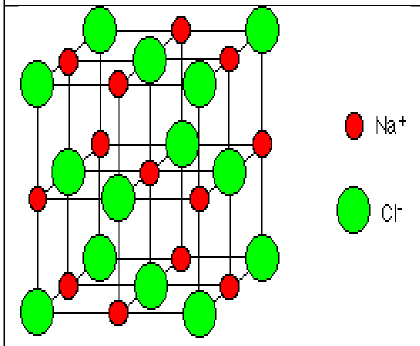
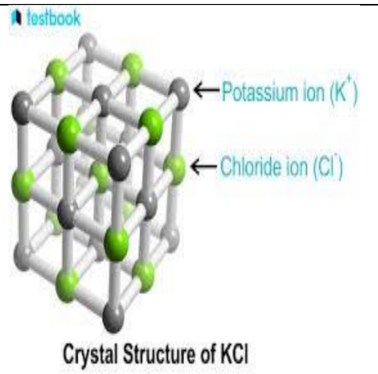
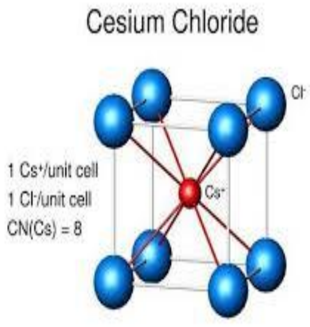
(4) A particle present of the centre of an edge contributes ¼ to a particular cubic unit cell

Thus, the number of atoms per unit cell-

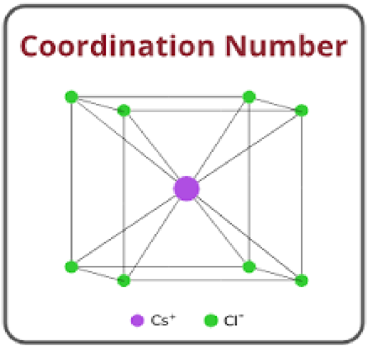
in a simple cubic system = 1/8 * 8 (at corners) = 1

in a body-centred cubic system= 1/8 * 8 (at corners) + 1 (at body centre) = 2

in a face-centred cubic system= 1/8 * 8 (at corners) +1 /2 *6 (at face centre) =4

NaCl	KCl	CsCl
		

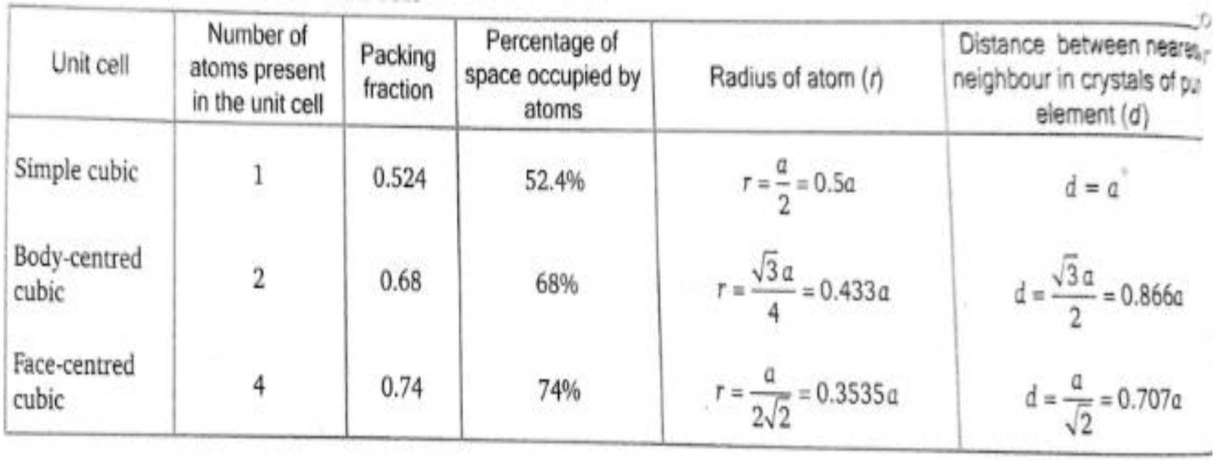
Coordination number: The number of nearest neighbour with which a given particle is in direct contact in a crystal is called the coordination number.



List of Compounds with their coordination no. Table 2

S.No.	Solid	Coordination number
1.	NaCl	6 : 6
2.	KCl	6 : 6
3.	CsCl	8 : 8
4.	$CaTiO_3$	12 : 6 : 2
5.	TiO_2	6 : 3
6.	SiO_2	4 : 2
7.	CaF_2	8 : 4
8.	Na_2O	4 : 8
9.	ZnS (B)	4 : 4
10.	ZnS(W)	4 : 4

Packing fraction and other characteristics: The fraction of no total volume of the unit cell occupied by the atoms present in it is called packing fraction. The packing fractions and some other important characteristics of different types of cubic unit cells are summarized in given Table-3



Unit cell	Number of atoms present in the unit cell	Packing fraction	Percentage of space occupied by atoms	Radius of atom (r)	Distance between neares neighbour in crystals of pu element (d)
Simple cubic	1	0.524	52.4%	$r = \frac{a}{2} = 0.5a$	$d = a$
Body-centred cubic	2	0.68	68%	$r = \frac{\sqrt{3}a}{4} = 0.433a$	$d = \frac{\sqrt{3}a}{2} = 0.866a$
Face-centred cubic	4	0.74	74%	$r = \frac{a}{2\sqrt{2}} = 0.3535a$	$d = \frac{a}{\sqrt{2}} = 0.707a$

Density of a crystal: Density of a cubic crystal is given by

$p = Z*M/a^3* N_a$

where, Z = Number of atoms (in case of crystals of elements) per unit cell or number of formula units (in case of ionic crystals) per unit cell M=atomic mass (in case of crystals of elements) or formula mass (in case of ionic crystals), a = edge length of the unit cell, and N_a = Avogadro's number

Elements of symmetry.

1)Centre of symmetry. It is an imaginary point within the crystal so that any line passing through this point intersects the opposite faces of the crystal at equal distances.

2)Plane of symmetry. It is an imaginary plane passing through the crystal such that it divides the crystal into two parts in such a way that one part is the mirror image of the other.

3)Rotation axis of symmetry. It is an imaginary line passing through the crystal such that when the crystal is rotated about this line, similar appearance occurs more than once in one complete revolution (i.e. through 360°). If similar appearance occurs twice, it is called two-fold axis or diad axis. Similarly, similar appearance three times, four times, six times etc., the axes are called three-fold (triad), four-fold (tetrad), six-fold (hexad) respectively. These are called proper axes of rotation.

4) **Rotation-Reflection axis**. If the crystal is first rotated about the n-fold axis and then reflected through plane perpendicular to axis, it is called overline n: -fold rotation reflection axis

5) **Rotation-inversion axis**. If the crystal is first rotated about the n-fold axis and then inverted through the Centre of symmetry, it is called n- fold rotation-inversion axis.

The above two types are called improper axes of rotation.

Law of Symmetry. The crystals of a particular substance always possess the same elements of symmetry. Example- a cubic crystal always has 23 elements of symmetry (planes = 9, axes= 13 and centre of symmetry = 1).

Planes and Faces of a crystal: Any plane passing through a large number of lattice points is called the crystal plane. The plane surfaces of a crystal are called the faces of the crystal.

Crystallographic axes and Axial ratios: The three lines coinciding with or parallel to the edges of crystal and meeting at a point are called crystallographic axes. A unit or standard plane is so selected that cuts all the crystallographic axes respectively. The ratio $a: b: c$ is called axial ratio. The angles between the axes opposite to the intercepts are represented by α, β, and γ

Hauy's Law of Rational Indices: The intercepts made by any plane or face of a crystal are either same as those for the unit plane or simple whole number multiples of those of the unit plane or one or two intercepts may be infinity if the plane or the face is parallel to one or the two axes i.e. does not cut one or the two axes.

Weiss Indices. The coefficients of the intercepts of any plane expressed in terms of those of the unit plane are called Weiss indices of that plane e.g. for the plane making intercepts na, n'b and n"c, the Weiss indices are (n, n’, n")

Miller Indices. The reciprocals of the coefficients of the intercepts made by the given plane (expressed terms of those of the unit plane) expressed as integers (by multiplying with the LCM of the denominators) are called the Miller indices of the given plane. For example, if the intercepts made by a plane are 2a, 2b, 3c,

Then reciprocals of coefficients are $\frac{1}{2}, \frac{1}{2}, \frac{1}{3}$ .To express as integers, multiply with LCM viz 6, we (332) In general, they are written as (hkl).

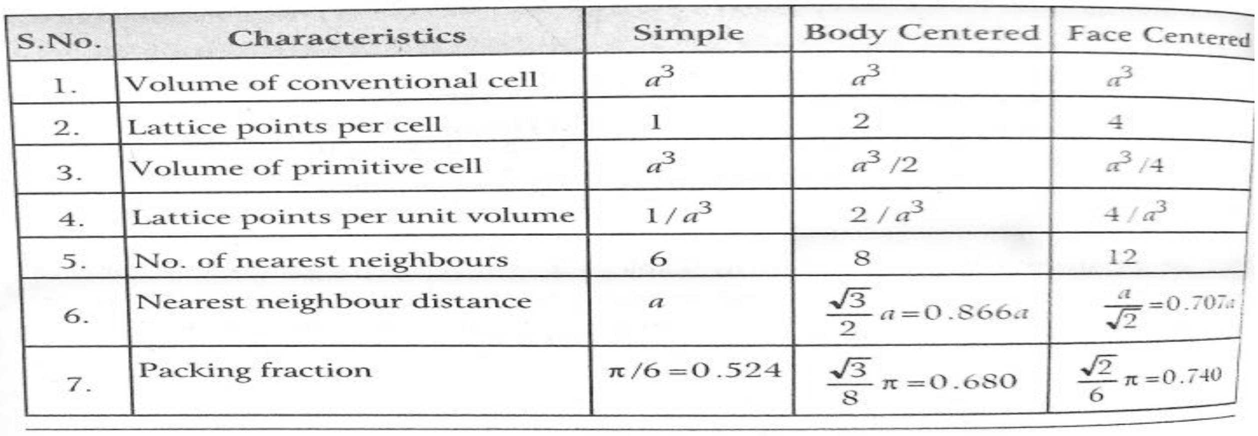
Distance of separation between (hkl) planes. In general

$$1/ d_{hkl} = \sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}$$

For a cubic lattice, a = b = c Hence $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$

- 5-fold, 7-fold, 8-fold or higher axes of symmetry are non-exist because their unit cells cannot be close packed without leaving gap in between.

Characteristics of cubic lattice Table -4



S.No.	Characteristics	Simple	Body Centered	Face Centered
1.	Volume of conventional cell	a^3	a^3	a^3
2.	Lattice points per cell	1	2	4
3.	Volume of primitive cell	a^3	$a^3/2$	$a^3/4$
4.	Lattice points per unit volume	$1/a^3$	$2/a^3$	$4/a^3$
5.	No. of nearest neighbours	6	8	12
6.	Nearest neighbour distance	a	$\frac{\sqrt{3}}{2}a = 0.866a$	$\frac{a}{\sqrt{2}} = 0.707a$
7.	Packing fraction	$\pi/6 = 0.524$	$\frac{\sqrt{3}}{8}\pi = 0.680$	$\frac{\sqrt{2}}{6}\pi = 0.740$

X-Ray Diffraction by Crystals-Study of Internal structure

(1) Laue's method. X-rays on striking a crystal penetrate and then scattered by the electrons. A symmetrical diffraction pattern is obtained thereby showing a regular arrangement of the constituent particles.

(1) Bragg's method. X-rays incident at an angle θ to the atomic plane of the crystal penetrate and then scattered from different equidistant atomic planes producing diffraction maxima at different values of θ (as it is increased gradually) satisfying Bragg's equation viz.

$$2\,d \sin\theta = n\lambda$$

Where d = distance of separation between the successive atomic planes

λ = wavelength of X-ray used

n = 1,2,3 etc. represent Ist order, 2nd order, 3rd order diffraction maxima.

Verification of Bragg's equation.

(1) By finding the values of θ for 1st, 2nd, 3rd maxima from the atomic planes (hkl), the values of λ and d a remaining constant, the values of sin θ are found to be in the ratio 1: 2:3

(if) Using cubic crystal (e.g. that of NaCl), the edge (a) is calculated using Bragg's equation as follows

$$d_{hkl} = \frac{n\lambda}{2\sin\theta} \text{ and}$$

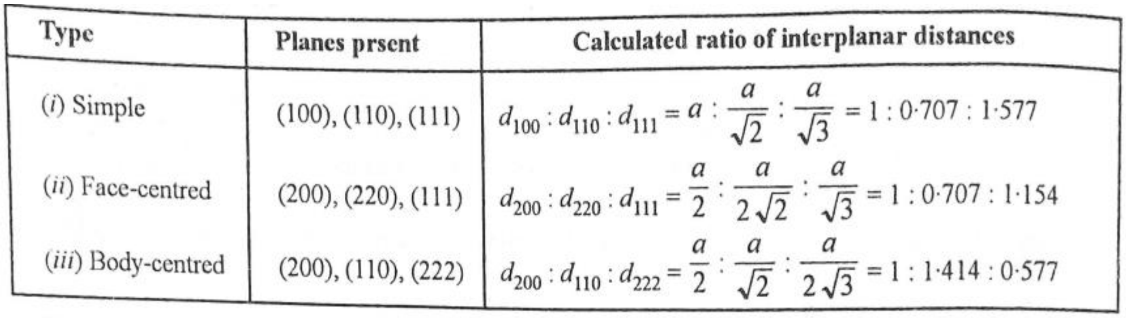
$$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$$

Edge is also calculated from density (p) of the NaCl crystal as follows:

$$a = \left(\frac{4M}{\rho N0}\right)^{1/3} \quad (M=\text{Mol. mass, } N_0=\text{Avogadro No .})$$

The values thus calculated agree fairly well.

To determine the type of cubic lattice. Miller indices of different planes present in the three types of cubic lattices and the calculated values of the ratios of interplanar distances of these planes (using $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$) are given below in Table-5



Type	Planes prsent	Calculated ratio of interplanar distances
(*i*) Simple	(100), (110), (111)	$d_{100} : d_{110} : d_{111} = a : \frac{a}{\sqrt{2}} : \frac{a}{\sqrt{3}} = 1 : 0{\cdot}707 : 1{\cdot}577$
(*ii*) Face-centred	(200), (220), (111)	$d_{200} : d_{220} : d_{111} = \frac{a}{2} : \frac{a}{2\sqrt{2}} : \frac{a}{\sqrt{3}} = 1 : 0{\cdot}707 : 1{\cdot}154$
(*iii*) Body-centred	(200), (110), (222)	$d_{200} : d_{110} : d_{222} = \frac{a}{2} : \frac{a}{\sqrt{2}} : \frac{a}{2\sqrt{3}} = 1 : 1{\cdot}414 : 0{\cdot}577$

Experimentally, the ratio is determined using Bragg's method (viz $d = \frac{n\lambda}{2\sin\theta}$) Comparing with the calculate ratio, the type of lattice can be found.

Powder method. Instead of taking single crystal (as done in Bragg's method), in this method the sampletaken in powdered form in a thin glass tube which is rotated. It is surrounded by a circular film. A beam ofrays focused on the sample is scattered producing a diffraction pattern. Each set of (hkl) planes gives rise diffraction cone meeting the photographic film at two points equidistant from the centre. Knowing the distance (x) of the line on the film from the centre, the interplanar spacing can be calculated.

Theoretically expected X-Ray diffraction patterns of cubic lattices. Combining equation

$d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$ and $2\, d_{hkl} \sin\theta = n\lambda$, we can derive that $\sin^2\theta = \frac{\lambda^2 (h^2+k^2+l^2)}{4a^2} = (h^2 + k^2 + l^2)$ where A = constant. For all possible planes ie. 100, 110, 111,200,210, 211, 220, 300 (or 221)310, 311, 222, 320 etc., $\sin^2\theta$ is calculated. The values not possible give the missing lines. For example,

(1) In primitive cubic lattice, $\sin^2\theta \neq 7$ A, 15 A etc. because for integral values of h, k, 1, $h^2 + k^2 + 1^2 \neq 7, 15$ etc. Hence after every six equally spaced lines there is a gap.

(i) In face-centred cubic lattice. Reflections from planes take place for which h, k, I values are either all odd or all even

(ii) In body-centred cubic lattice. Reflections are not observed from planes for which (h + k + l) is odd. Here the lines are found to be equally spaced.

Crystal structures of NaCl, KCl and CsCl. NaCl and KC1 both have face-centred cubic structures. However their diffraction patterns are different. This is mainly because X-rays are scattered by electrons. In $Na^+ Cl^-$ number of electrons in Na^+ ion is less than in Cl^- ion but in K'CI", both K^+ and Cl^- have equal number electrons.

OBJECTIVE TYPE QUESTIONS

1. The packing fraction of f.c.c. cube is:

(a) 0.52

(b) 0.74

(c) 0.68

(d) 0.58

Ans.b

2. The Miller indices of plane which cuts the intercept of 1, 2 and 3 along the three axes are:

(a) 6, 4, 3

(b) 6, 3, 2

(c) 2, 3, 2

(d) 2, 3, 4

Ans.b

3. The radiation used for powder method is:

(a) Continuous

(b) Monochromatic

(c) Partly continuous and partly monochromatic

(d) None of the above

Ans.b

4. Brillouin zone is defined as:

(a) Regular arrangement of atoms in space

(b) A zone interrupted by grain boundaries

(c) Smallest volume enclosed by parallel planes in a crystal lattice

(d) The Weigner Seitz cell in the reciprocal lattice.
Ans.d

5. Packing fraction of simple cubic lattice is:

(a) $2A / Na^3$

(b) A / a^3

(c) $A / 2Na^3$

(d) A / 4Na3
Ans.a

6. Spacing between adjacent planes for a cubic lattice is

(a) $d = ((h^2 + k^2 + l^2)^{1/2}/a$

(b) $d = a/(h^2 + k^2 + l^2)^{1/2}$

(c) $d = \{a/(h^2 + k^2 + l^2)\}^{1/2}$

(d) $d = a^3$
Ans.b

7. The number of atoms per unit cell in simple cubic lattice is:

(a) 1

(b) 2

(c) 4

(d) 8
Ans.a

8. The number of atoms per unit cell in hexagonal closed packed structure is:

(a) 2

(b) 4

(c) 6

(d) 8

Ans.c

9. The number of nearest neighbours in f.c.c. lattice is:

(a) 6

(b) 8

(c) 10

(d) 12

Ans.d

10. An orthorhombic crystal has axial vectors in the ratio 0.424: 1:0.367. The Miller indices of those crystals plane whose intercepts are in the ratio 0.212: 1: 0.183 will be:

(a) 2:1:2

(b) 1:1/2/ :1/2

c)1: 0: 1/2

d) 1/3:1 : 1/2

Ans.a

11. The number of atoms per unit cell in b.c.c. lattice is:

(a) 1

(b) 2

(c) 4

(d) 8

Ans.b

12. The atoms radius of simple cubic is

(a) a/√2

(b) √3/4 * a

(c) a/2√2

(d) a/2

Ans.d

13. If a=10.5 Å, b = 9.2Å, c = 5.0Å, α = 42°, β=80°and γ= 93°, then the crystal a = 10.5lambda structure is:

(a) Triclinic

(b) Cubie

(c) Orthorhombic

(d) Trigonal

Ans.a

14. For Face centred cubic lattice, the value of coordination number is:

(a) b

(b) 8

(C) 12

(d) 10

Ans.c

15. b.c.c. lattice is:

(a) Reciprocal of itself

(c) Reciprocal of f.c.c.

(b) Reciprocal of s.c.c.

(d) none of these

Ans.b

16. The number of molecules per unit cell in f.c.c. crystal is:

(a) 4

(d) 12

(c) 3

(d) 1

Ans.a

17. The Miller' indices of a plane parallel to Y-Z plane in f.c.c. are:

(a) (1000)

(b) 110

(c) (100)

(d) (200)

Ans.c

18. Number of lattice points per unit cell in a b.c.c. lattice is:

a) 2

b) 4

c)6

d)8

Ans.a

19. The distance between the adjacent atomic planes is $CaCO_3$ is 0.3nm. The smallest angel of bragg diffraction for 3.03 nm. X-ray is :

a) 2.9°

b) 1.45°

c) 0.29°

d) 5.8°

Ans.a

20. Number of lattice Points per unit cell in f.c.c lattice is :

a) 2

b) 4

c) 6

d) 8

Ans.b

21. Bragg's law:

(a) $2\ d\ \sin\theta = n\lambda$

b) $2d\cos\theta = 2\lambda$

c) $d\sin\theta = n\lambda$

d) $d\cos\theta = n\lambda$

Ans.a

22. Bragg's equation $2d\sin\theta = n\lambda$ has no solution for wavelength if:

a) $\lambda > d$

b) $\lambda > 2d$

c) $\lambda < d$

d) $\lambda < 2d$

Ans.d

23. The basic structure of NaCl is:

(a) h.c.p.

(b) f.c.c.

(c) b.c.c.

(d) None of these

Ans.b

24. Number of Bravais lattice is:

(a) 8

(b) 32

(c) 14

(d) None

Ans.c

25. The distance between (110) planes of NaCl is:

a) a/2

b) $a/\sqrt{2}$

c) $a/\sqrt{3}$

d) a

Ans.b

26. Maximum packing fraction in a cubic crystal is:

(a) 0.74

(b) 2

(c)4

(d) 8

Ans.a

27. The Bravais lattice may be grouped into:

(a) 5

(b) 14

(c) 7

(d) 9

Ans.c

28. The distance between nearest neighbours in an b.c.c. lattice, in terms of lattice constant a, is:

(a) a

(b) $\sqrt{3}a/2$

(c) $a/\sqrt{2}$

(d) a/2

Ans.b

29. The total number of atoms per unit cell in diamond structure is:

(a) 4

(b) 6

(c) 8

(d) 12

Ans.a

30. The number of nearest Cl^- ion around each Na^+ ion in NaCl crystals is:

(a) 5

(b) 6

(c) 8

(d) 12

Ans.d

31. The nearest neighbour distance in a simple cubic lattice is:

(a) a

(b) a / √2

(c) a /√3

(d) √2a /3

Ans.a

32. There are seven types of crystals. The number of types of Bravais space lattice they can give rise to, is:

(a) 7

(b) 14

(c) 21

(d) 28

Ans.b

33. The packing factor of diamond cubic crystal structure is:

(a) 60%

(b) 56%

(c) 90%

(d) None of these

Ans.d

34. The Bravais lattice of CsCl crystal is:

(a) Simple cubie

(b) f.c.c.

(c) b.c.c.

(d) None of the above

Ans.b

35. The amorphous solid has a _____order in its structure.

(a) Zero range

(b) Large range

(c) Short range

(d) None of these

Ans.c

36. For simple cubic lattice, the interplanar separation ratios $d_{100}/ d_{110} / d_{111}$=_______

(a) 1: 1/ √2: 1/√3

(b) 1:1/ √2:√3

(c) 1:√2:1/√3

(d) 1:1/ √2: 2/√3

Ans.a

37. The one which is not.compatible with crystal symmetry is:

(a) One-fold symmetry

(b) Three-fold symmetry

(c) Five-fold symmetry

(d) Six-fold symmetry

Ans.c

38. The Miller indices of the plane making equal intercepts on the x, y and z axis are:

(a) 111

(b) 000

(c) 110

(d) 101

Ans.a

39. The lattice constant 'a' related with the density p of the crystal material as:

(a) $a = ((nM)/(Np))^{1/3}$

(b) $a = ((nM)/(Np))^{3}$

(c) $a = ((np)/(NM))^{3}$

(d) $a = ((nM)/(Np^{))- 1/3}$

Ans.a

40. The Lattice density of (100) plane in a simple cubic lattice of lattice constant 2.5 Å is:

(a) $2.5 * 10^{19}$ lattice point/m²

(b) $1.6 * 10^{29}$ lattice point/m²

(c) $2.5 * 10^{-19}$ lattice point/m²

(d) $1.6 * 10^{19}$ lattice point / m^2

Ans. D

41. $a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$, then the crystal structure is:

(a) Triclinic

(b) Cubic

(c) Orthorhombic

(d) Trigonal

Ans. a

42. In a tetragonal lattice a = b = 2.5Å, c = 1.8Å,.Then the lattice spacing between (1,1,1) plane is:

(a) 1.62 Å

(b) 12.6 Å

(c) 1.26 Å

d) 16.2 Å

Ans. c

43. In crystal diffraction, diffracted beams are found only when reflected waves from various planes of atom:

(a) interfere constructively

(b) interfere destructively

(c) do not interfere

(d) None of these

Ans. A

44. Which is the Bragg's equation for second order X-ray diffraction?

(a) $3d \sin\theta = \lambda$

(b) $d\sin\theta = \lambda$

(c) $2d\sin\theta = n\lambda$

(d) None of these

Ans. b

45. How many molecules are there in the unit cell of NaCl?

(a) 2

(b) 4

(c) 6

(d) 8

Ans. b

46. Powder method of crystal analysis was devised by:

(a) Laue

(b) Bragg

(c) Debye and Scherrer

(d) None of these

Ans. c

47. If G is magnitude of a reciprocal lattice vector and d is interplanar spacing of the corresponding set of lattice planes, then:

(a) $G \propto d$

(b) $G \propto 1/d$

(c) $G \propto d^2$

d) $G \propto 1/d^2$

Ans. b

48. An X-ray analysis of a cubic crystal is carried out using X-rays of wavelength 0.58Å. Bragg's reflections are observed at glancing angles of 6.45°, 9.15° and 11.1°. Find the interplanar spacing of the crystal:

(a) $1:\sqrt{2}:\sqrt{3}$

b) $1:1/\sqrt{2}: 1/3$

(c) 0.6:0.6:2.0

(d) $1:\sqrt{2}:1/\sqrt{3}$

Ans. b

49. Which of the following compound has 8:8 coordination number_________

(a) CsCl

(b) NaCl

(c) MgO

(d)Al2O3

Ans. a

50. Which solid structure has a definite and sharp melting point?

(a) All types of solids

(b) No type of solid

(c) Amorphous solids

(d) Crystalline solids

Ans. d

UNIT VI

&

UNIT VII

B.Sc. SEM II

UNIT VI and VII SYLLABUS

Introduction to Polymer Monomers, Oligomers, Polymers and their characteristics, Classification of polymers: Natural synthetic, linear, cross linked and network; plastics, elastomers, fibres, Homopolymers and Co-polymers, Bonding in polymers : Primary and secondary bond forces in polymers ; cohesive energy, and decomposition of polymers. Determination of Molecular mass of polymers: Number Average molecular mass (Mn) and Weight average molecular mass (Mw) of polymers and determination by (i) Viscosity (ii) Light scattering method (iii) Gel permeation chromatography (iv) Osmometry and Ultracentrifuging. Silicones and Phosphazenes –Silicones and phosphazenes as examples of inorganic polymers, nature of bonding in triphosphazenes.
VII -Kinetics and Mechanism of Polymerization: Polymerization techniques, Mechanism and kinetics of copolymerization, Addition or chaingrowth polymerization, Free radical vinyl polymerization, ionic vinyl polymerization, ZieglerNatta polymerization and vinyl polymers, Condensation or step growth-polymerization, Polyesters, polyamides, phenol formaldehyde resins, urea formaldehyde resins, epoxy resins and polyurethanes.

Introduction to Polymer

Polymer, polymerization and repeat unit: A polymer is a large molecule of high molecular mass formed by the repeated combination of large number of small molecules called **monomers**.

> **The polymerisation** is the chemical combination of several similar or different molecules to form a single large molecule called a polymer.
> **The structural unit** which on repetition gives the entire chain of a polymer molecule is called the repeat unit of the polymer.

Functionality: The number of bonding sites present in a monomer is referred to as its functionality.

Degree of polymerization: The number of repeating units present in a polymer is referred to as the degree of polymerization of the polymer.

Classification of polymers:

(i) Based on the origin

(a) **Natural polymers**. The polymers which occur in nature are called natural polymers, Starch, cellulose, proteins, and nucleic acids are natural polymers.

(b) **Synthetic polymers**: These are synthesised in the laboratory. Polythene, polystyrene, PVC, Teflon, nylon, etc., are such polymers.

(ii) Based on structure:

(a) **Linear polymers**: In these polymers, the monomeric units are joined together to form long straight chains. They possess high densities, high tensile strength and high melting point. High-density polythene is a linear polymer.

(b) Branched-chain polymers: These polymers are consist of side chains attached to the main chain. They possess low density low tensile strength and melting point. Low-density polythene is such a polymer.

(c) Cross-linked polymers: In these polymers, the adjacent polymeric chains link together through side chains to form a three-dimensional network structure. These are hard, rigid and brittle, Bakelite, melamine formaldehyde resins, etc. are such polymers.

Types of polymer based on structure

(iii) Based on the type of repeating structural units:

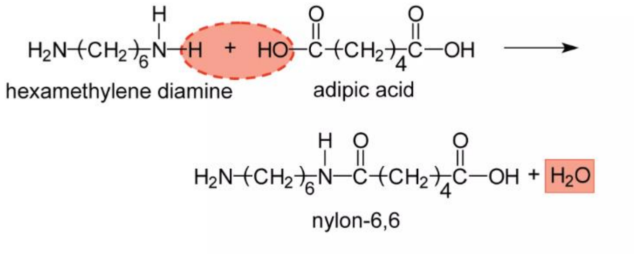
(a) **Homopolymers:** These polymers, are made up of only one type of monomers. For example, polyethene, polystyrene, etc.

(b) **Copolymers**: These polymers, are made up of two or more than two types of monomers. For example, styrene-butadiene rubber.

(iv) Based on method of Polymerisation:

(a)Addition polymers: The polymers formed by addition polymerisation are called addition polymers. Ex- Polythene and polypropylene etc.

(b) Condensation polymers: The polymers formed by condensation polymerisation are called condensation polymers. Nylon 66, terylene, etc.



(v) Based on Molecular Forces

(a) Elastomers: In these polymers, the polymeric chains are held together by the weakest intermolecular forces. Ex- Natural rubber.

(**b) Fibers:** In fibers strong intermolecular forces exist between the polymeric chains. Nylon-6.

(vi) Based on thermal behaviour

(a) Thermoplastics: In these polymers, the intermolecular forces are intermediaries to those of elastomers and fibers. Polythene, polypropylene, PVC, etc., are such polymers.

(b) Thermosetting polymers: The polymers which on heating change irreversibly into hard, rigid, and infusible material are called thermosetting polymers. For example, phenol-formaldehyde resins, melamine-formaldehyde resins, etc.

Molecular mass of polymers: The number average (Mn) mass and weight average (Mw) molecular mass of a polymer defined as

$$M_n = \frac{\sum M_i N_i}{\sum N_i}, \quad M_w = \frac{\sum M_i^2 N_i}{\sum M_i N_i},$$

where, Ni represents the number of molecules having molecular

mass M, For synthetic polymers, Mw is always greater than Mn.

Polydispersity Index (PDI): it is defined as

PD1= Mw/Mn

For natural polymers, PDI is unity. For synthetic polymers, PDI is greater than unity.

Methods of polymerization

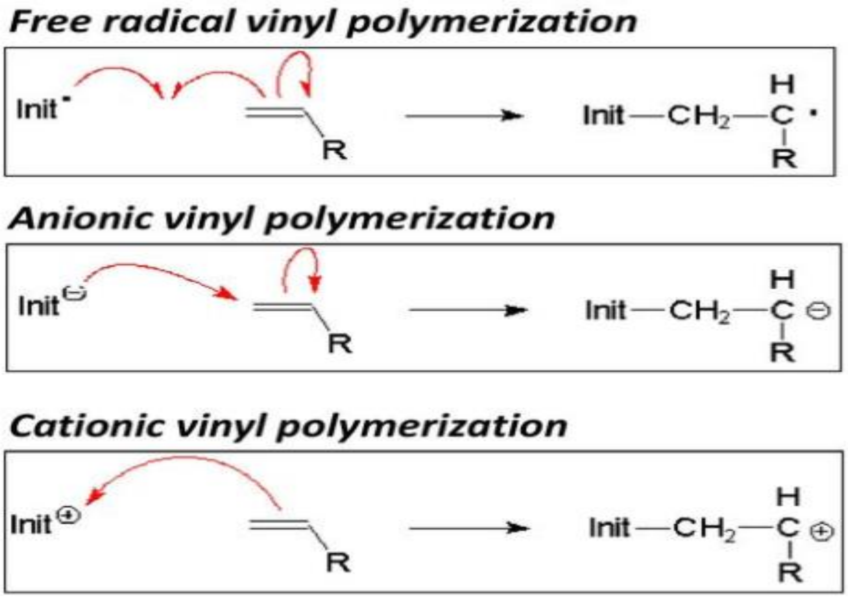
(I) Condensation: It takes place when the monomers are bifunctional or polyfunctional. Polymerization occurs through a series of step condensation reactions between the product of the previous and bi- or poly-functional monomer. The repeating unit in this type of polymerization differs from the monomer molecule due to the elimination of small molecules like H_2O, NH_3, and CO_2. This type of polymerization is used in the manufacture of polyesters polyamides, polyurethanes, etc.

(II) Addition polymerisation: It involves the addition of molecules of the same or different type of monomers and takes place through a chain reaction mechanism via certain active species i.e. free radicals, carbocations or carbanions. There are 3 types of addition polymer-

(i)Free radical addition polymerisation: It is largely used for the polymerisation of alkenes, dienes, and their derivatives. The active species are free radicals that are generated by initiators such as t-butyl peroxide, benzoyl peroxide, etc. polymerization process involves three steps- 1) initiation, 2) chain propagation and3) chain termination.

(ii) **Anionic polymerization** refers to a type of polymerization process that is dependent on the reactivity of anions to initiate and propagate the polymerization reaction. The process is initiated by the removal of a proton from a monomer by a strong base or organometallic compound. Initiators include Lewis base, nucleophiles such as hydroxide, cyanide, alkoxide, amides, butyl lithium or a carbanion.

(iii) **Cationic polymerization** refers to a type of chain growth polymerization mechanism in which the formation of a carbocation intermediate initiates the polymerization reaction. The process is initiated by the reaction of the cation with a monomer, resulting in the formation of a reactive carbocation. Initiators include Lewis acid, electrophilic agents such as HCl, H2SO4, HBr, HClO4.

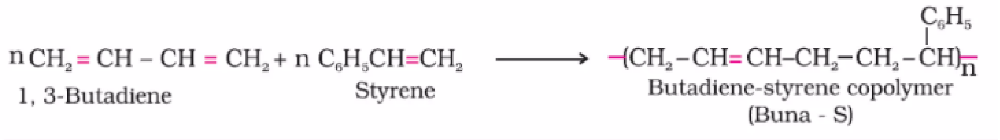


Free radical vinyl polymerization

Anionic vinyl polymerization

Cationic vinyl polymerization

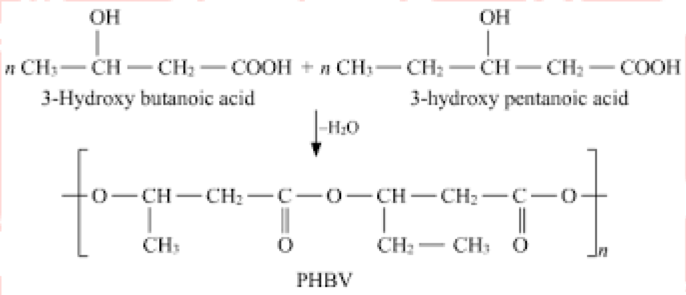
(III) Copolymerisation: When two or more than two different types of monomers undergo polymerisation, the process is called Copolymerisation and the polymer thus formed is called copolymer. The copolymer consists of multiple units of each monomer used in the same chain. Its composition not only depends on the proportion of monomers but also their reactivity. The properties of copolymers are quite different from those of homopolymers derived from each of the combining monomers. Styrene,methyl methacrylate, styrene-butadienerubber,etc. are such polymers.



$$n\,CH_2=CH-CH=CH_2 + n\,C_6H_5CH=CH_2 \longrightarrow -\!\!(CH_2-CH=CH-CH_2-CH_2-\overset{C_6H_5}{\overset{|}{C}H})_n\!\!-$$

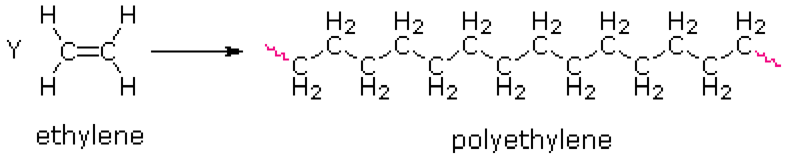
Biopolymers and biodegradable polymers: The naturally occurring such as polysaccharides, proteins and nucleic acid are essential for bile process are called biopolymers.

All the biopolymers are biodegradable as they disintegrate by enzymatic hydrolysis and to some extent by oxidation. The synthetic is not biodegradable as they are almost inert to degradation reaction occurring in nature. Therefore, management of polymeric waste has become a serious problem, in order to combat this problem, biodegradable synthetic polymers have been developed. An important biodegradable polymers is aliphatic esters, Some important biodegradable polymers are PHBV, poly glycolic acid) and poly (lactic acid) nylon -2-nylon -6 etc.

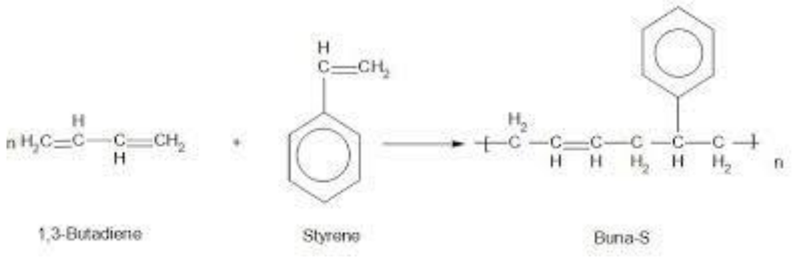


Some commercially important polymers

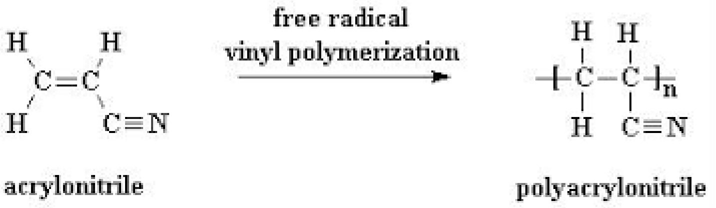
Polyolefins: Polythene, polypropylene, polystyrene, etc., are some important polyolefins, which are used in the preparation of house-bald wares, ropes, toilet articles, radiocabinets, packaging materials.



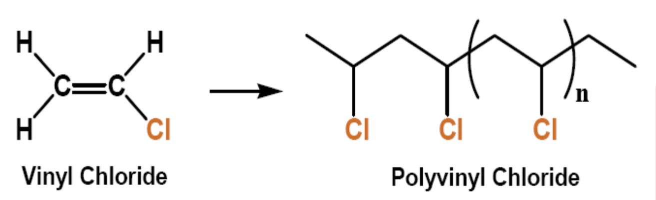
Polydienes: The polymers of this class are synthetic rubbers such as neoprene, Buna-S, etc. They are used for making, shoe soles, motor tyres, etc.



Polyacrylates: These are obtained from acrylic monomers. polymethmethylacrylate, polyacrylonitrile, etc. are such polymers. PMMA is used for making lenses, aircraft windows, whereas poly acrylonitrile in used for making acrylic fibres.

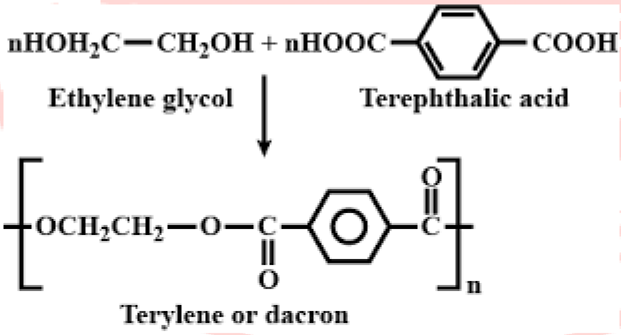


Polyhalo-olefins: These are the polymers of halogen substituted alkenes PTFE (Teflon), PCTEE, PVC, etc, are important polymers of this type. Teflon is used for making non-sticky kitchen utensils, whereas PVC is used for making raincoats, records, shower curtains, shoe soles, etc.

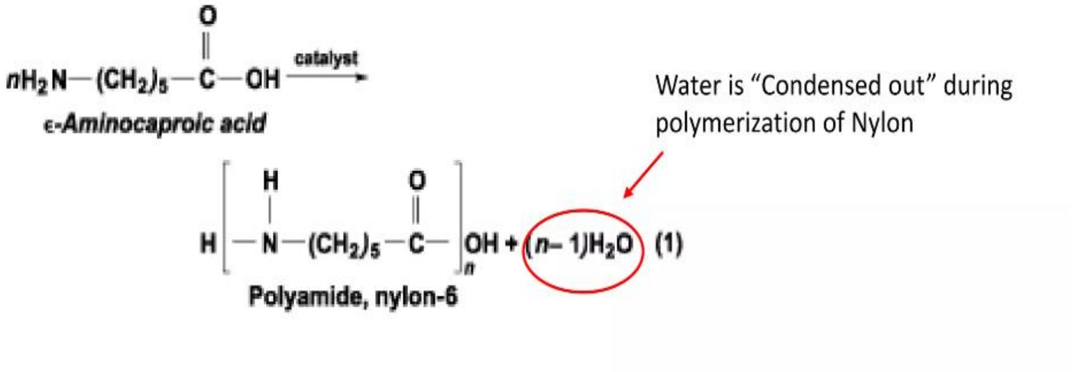


Condensation polymers:

Polyesters: These contain ester linkages and are prepared by the condensation polymerisation of dicarboxylic acids with diols, Terylene (Dacron), glyptal, etc. are such polymers. Terylene is used in the manufacture of textiles, whereas glyptal is used in the manufacture of paints and lacquers.

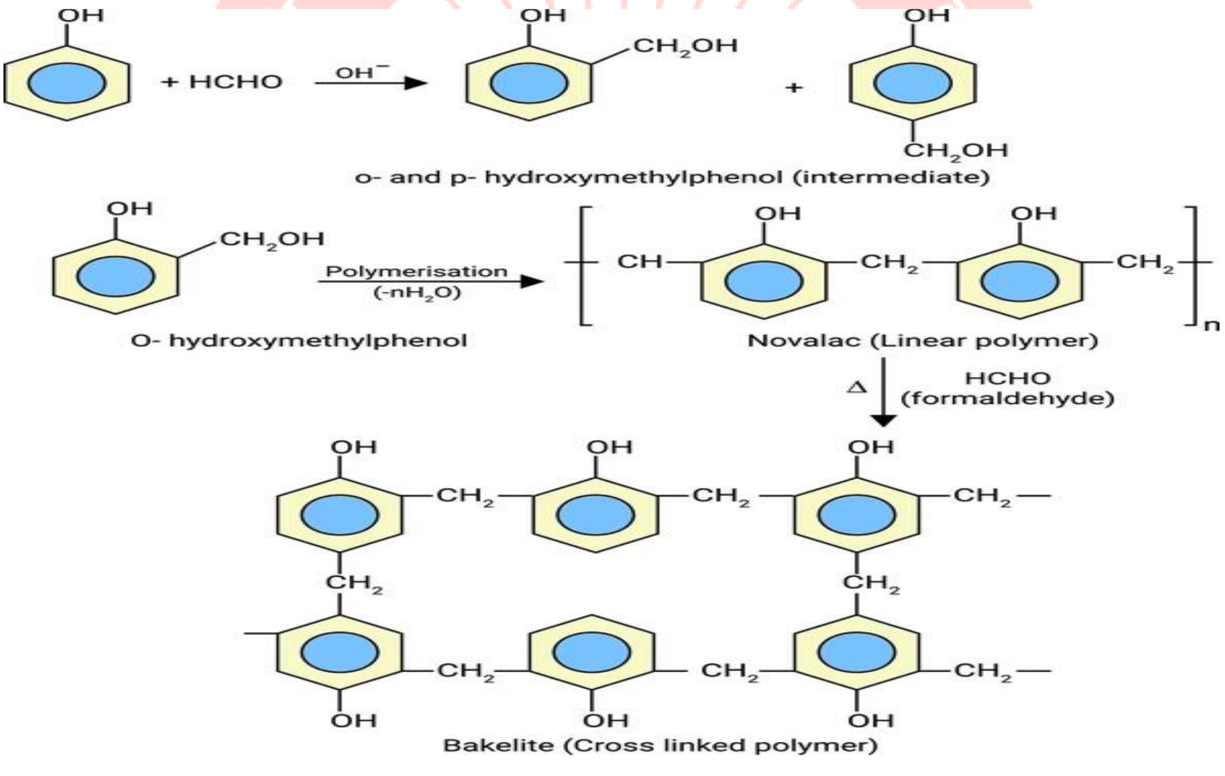


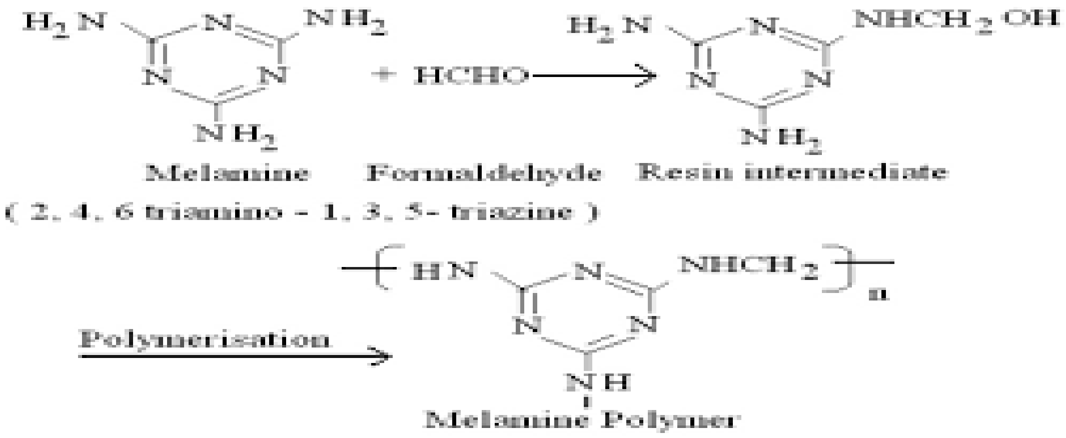
Polyamides: These possess amide linkage (CO - NH -) and are formed by the condensation polymerisation of dibasic acids with diamines or of amino carboxylic acids. Nylon 66, nylon 610, nylon 6, are some important polyamides. They are used in making threads, ropes, bristles, textiles, etc.



Water is “Condensed out” during polymerization of Nylon

Formaldehyde resins: Phenol-formaldehyde resins (bakelite), melamine-formaldehyderesins, etc., are some important polymers of this class. These are thermosetting polymers Bakelite is used for making combs, electric switches, tabletops, etc., whereas melamine-formaldehyde resin is used for making non-breakable plastic crockery.

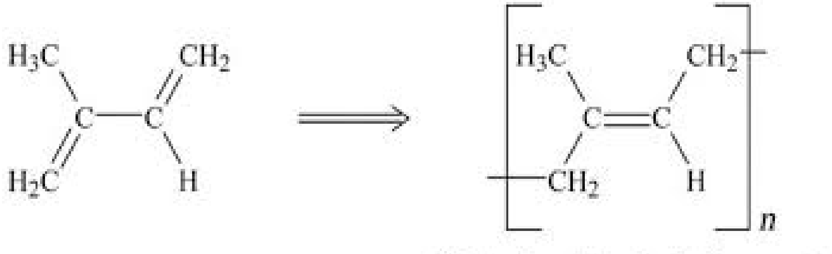




It is used in the manufacture of unbreakable crockery

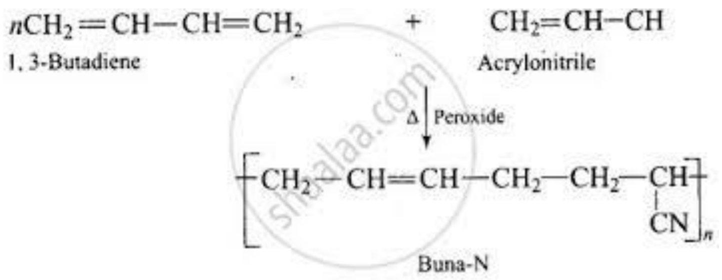
Natural rubber: It is obtained from the tree Heveobrasiliensis. It is a polymer of Isoprene (C_5H_8) Natural rubber is a cis-isomer, The trans-isomer is called gutta-percha.

Natural rubber is a gummy material with poor elasticity. In order to improve its usefulness, it is subjected to vulcanization which involves the introduction of -s-s- polysulphide cross- links. The vulcanized rubber can be stretched only to a limited extent and is superior to unvulcanized rubber. It is used in the manufacture of tyres, gaskets, shock absorbers, foam rubber, etc.



Isoprene Natural rubber (polyisoprene)

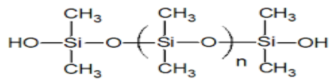
Synthetic rubbers: These are synthesized by the polymerisation of a large number of conjugate dienes. Some important synthetic rubbers are SBR (Buna-S), nitrile rubber (Buna-N), butyl rubber (GR-1), polysulphide rubber (GR - P), etc. They are used for a variety of purposes.

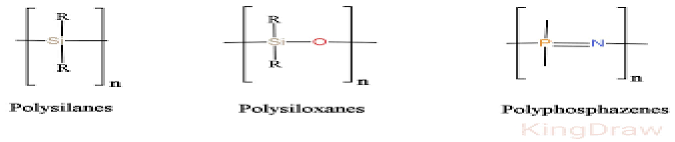


Inorganic polymer

Silicone polymer $[R_2SiO]n$

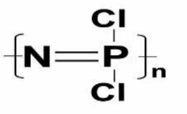
- Silicone polymer is also known as Polysiloxane.
- It is a synthetic polymer,
- Those substances whose molecules consist of polymeric chains are made up of polymerized Siloxane having alternative Silicon and Oxygen atoms (-R2Si-O-SiR2-) where, R is an alkyl chain.
- Since the backbone is of Silicon rather than Carbon atoms. Thus, it is considered an inorganic polymer.
- They are thermally stable have low surface energy and are resistant to water.



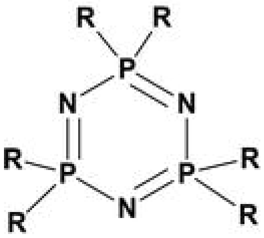


Polyphosphazenes $[PNCl_2]n$

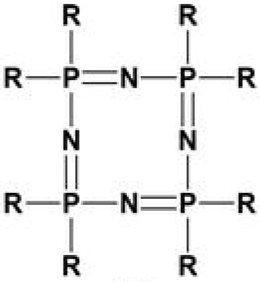
- Polyphosphazenes are polymers with an inorganic backbone consisting of alternating phosphorus and nitrogen atoms, separated by alternating single and double bonds, and organic substituents (R) covalently bonded to the phosphorus atoms as side groups.
- $[PNCl_2]n$ are known as phosphonitrilic chloride. Out of many types $[PNCl_2]_3$ is the most important member of this group.
- They are fire, oil and radiation resistance, having high refractive index, transparent for ultraviolet and visible and hydrophobic, therefore used in land vehicles and aerospace components.
- They have also been used in biostable biomedical devices.



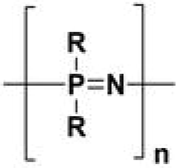
Where n may be 3 to 7



(a)



(b)



(c)

Properties of hexachlorocyclotriphosphazene

- It is elastomeric and thermoplastic
- It has flexible backbone.
- It hydrophilicity or hydrophobicity is tunable.

MULTIPLE TYPE QUESTIONS

1. Polymers are giant molecules made up of small molecule, these small units are called:

(a) Monomer

(b) Dimer

(c) oligomer

(d) None

Answer. (a)

2. The number of repeating units in a given polymer is called

(a) Degree of polymerization

(b) Functionality of polymer

(c) Average mass of polymer

(d) Repeat mass

Answer. (a)

3. Which of the following is used as an initiator in the chain growth polymerization?

(a) conc. H_2SO_4

(b) Benzoyl peroxide

(c) Alkali

(d) Hydrogen

Answer. (b)

4. Formation of terylene is a typical example of.

(a) Addition polymerization

(b) Condensation polymerization

(c) Esterification

(d) Ziegler-Natta polymerization

Answer. (b)

5. Polystyrene is a -

(a) Addition polymer

(b) Condensation polymer

(c) Monomer

(d) Dimer

Answer. (a)

6. A typical polyester is:

(a) Nylon 6,6

(b) Orlon

(c) Epoxy

(d) Terylene

Answer. (d)

7. Polymethyl methacrylate is a typical

(a) Polyester

(b) Polyether

(c) Polyamide

(d) Polyalkene

Answer. (d)

8. Tetrafluoroethylene on polymerisation gives:

(a) PCTFE

(b) PMMA

(c) Teflon

(d) Plexiglass

Answer. (d)

9. Epoxy resins are basically:

(a) Poly epoxy compounds

(b) Poly esters

(c) Poly ethers

(d) Polyamides

Answer. (c)

10. Poly caprolactum is an example of:

(a) Polyesters

(b) Styrene plastics

(c) Acrylic plastics

(d) Polyamide plastics

Answer. (d)

11. Teflon was discovered by:

(a) Roy J. Plumkett

(b) Carothers

(c) H.F. Mask

(d) F.A. Kolthaff

Answer. (a)

12. Addition polymerization is also known as-

(a) chain growth polymerisation

(b) step growth polymerisation

(c) coordination poymerisation

(d) none

Answer. (a)

13. Condensation polymerization is also known as

(a) chain growth polymerisation

(b) step growth polymerisation

(c) coordination poymerisation

(d) none

Answer. (b)

14. Orlon is prepared by the polymerisation of

(a) Vinyl cyanide

(b) Vinyl alcohol

(c) Vinyl chloride

(d) none of the above

Answer. (a)

15. Teflon is prepared by the polymerization of

(a) Butadiene

(b) Vinyl cyanide

(c) Vinyl chloride

(d) Tetrafluoroethylene

Answer. (d)

16. Bakelite is obtained from:

(a) Phenol and formaldehyde

(b) Adipic acid and hexamethylene diamine

(c) terephthalate and ethylene glycol

(d) Neoprene

Answer. (a)

17. Nylon-6,6 is obtained from:

(a) Adipic acid and hexamethylene diamine

(b) Tetrafluoroethylene

(c) Vinyl cyanide

(d) Vinylbenzene

Answer. (a)

18. Neoprene is a polymer of which monomer

(a) Chloroprene

(b) Isoprene

(c) Isobutene

(d) Isopentene

Answer. (a)

19. Which of the following is a thermosetting polymer?

(a) Bakelite

(b) Nylon-6,6

(c) Polyethylene

(d) Teflon

Answer. (a)

20. Which of the following is an example of a condensation polymer?

(a) Nylon-6, 6

(b) Teflon

(c) Polypropylene

(4) Orlon

Answer. (a)

21. Which of the following polymers contain nitrogen.

(a) PVC

(b) Teflon

(c) Nylon

(d) Terylene

Answer. (c)

22. Sebacic acid reacts with hexamethylene diamine to form

(a) Bakelite

(b) Nylon-6, 10

(c) Terylene

(d) Nylon-6, 8

Answer. (b)

23. Ethylene glycol reacts with dimethyl terephthalate to form

(a) Nylon-6, 6

(6) Teflon

(c) Dacron

(d) Orlon

Answer. (c)

24. Natural rubber is a polymer of

(a) Propene

(b) Isoprene

(c) chloroprene

(d) ethene

Answer. (b)

25. The monomers for Buna-S are 1,3-butadiene and

(a) Ethylene glycol

(b) Adipic acid

(c) Styrene

(d) Caprolactum

Answer. (c)

26. Which of the following statements is not true ?

(a) Natural rubber is a hydrocarbon

(b) Natural rubber is made of isoprene units

(c) Natural rubber is a polymer of 1, 3-Butadiene

(d) Natural rubber can be vulcanized.

Answer. (c)

27. Natural rubber is:

(a) All trans polyisoprene

(b) Chloroprene

(c) Buna-S

(d) All cis polyisoprene

Answer. (d)

28. Starch is a polymer of:

(a) Glucose

(b) Fructose

(c) Both

(d) None

Answer. (a)

29. Copolymers can be formed by:

(a) Condensation polymerisation

(b) Addition polymerisation

(c) Both (a) and (b)

(d) None

Answer. (c)

30. Heating of rubber with sulphur can do:

(a) form S-S linkage

(b) hardening of the rubber

(c) Vulcanisation

(d) all of these

Answer. (d)

31. $(PNCl_2)_3$molecule possess .... ring

a) Three member
b) Four member
c) Five member
d) Six member

Answer: d

32. At high temperatures the polymeric material becomes highly viscous and starts flowing, the temperature is called:

(a) T_m

(b) T_g

(c) T_f

(d) None of these

Answer. (c)

33. In emulsion polymerisation, the monomer is dispersed in the aqueous phase as a uniform emulsion, is stabilized by:

(a) Surfactants

(b) Protective colloids

(c) Buffer solutions

(d) All of these

Answer. (d)

34. - Rubber is heated with sulphur for its modification .This process is called

a) Sulphonation
b) Vulcanization
c) Sensitization
d) None of the above

Answer: b

35. Which of the following geometrical structure can not be a crystalline polymer?

(a) Isotactic and syndiotactic

(b) Atactic

(c) Linear

(d) Branched.

Answer. (d)

36. Soft bakelite is used for-

(a) Making electrical goods

(b) Making glue for wooden furniture

(c) Unbreakable crockery

(d) Fibres

Answer. (a)

37. Polymerization of butadiene and styrene give:

a) Buna-N
b) Buna-S
c) Neoprene rubber
d) none of the above

Answer: b

Answer. (c)

38. The inhibition of the chain reaction in presence of atmospheric oxygen is due to its :

(a) Biradical nature

(b) Strong oxidising nature

(c) Ease to combine with the polymer

(d) Greater active mass

Answer. (a)

39. If an a-functional monomer reacts with a b-functional monomer, the functionality of the product molecule

(a) a + b

(b) a + b + 2

(c) a + b - 2

(d) a + b / 2

Answer. (c)

Q40-The commercial name of polyacrylonitrile is :

a) Dacron
b) Orlon
c) Polythene
d) nylon

Answer. (a)

41- Elastomer is/are

a) Buna-N
b) Buna-S
c) Neopropene
d) All

Answer. (d)

42.Free radical polymerisation is initiated-

(a) Thermally

(b) Photochemically

(d) Chemically

(d) All of these

Answer. (d)

43. Which of these are used as free radical initiator ?

(a) conc.H_2SO^4

(b) Benzoyl peroxide

(c) lewis acid

(d) All of these

Answer. (b)

44. Living polymer is an example of

(a) Cationic polymer

(b) Free radical polymer

(c) Anionic polymer

(d) Condensation polymer

Answer. (c)

Silicones have .... repeating units of

a) R_2SiO
b) RSiO
c) R_2SiO_2
d) $RSiO_2$

Answer: a

The most common phosphazene has formula

a) (PNCl)n
b) $(PNCl_2)_n$
c) $(PNCl_3)_n$
d) $(PNCl_4)_n$

Answer: b

46. Ziegler-Natta polymerisation is an example of

(a) Anionic polymerisation

(b) Cationic polymerization

(c) Free radical polymerisation

(d) Coordination polymerization

Answer. (d)

47. - Silicones are the polymers of.......

a) Silicone
b) Silanes
c) Silones
d) Siloxanes

Answer: d

48. Which of the following is highly crystalline in nature?

(a) Nylon 6

(b) Polyethylene

(c) Poly tetra floro ethylene

(d) Polystyrene

Answer. (a)

49.Which of the following is not a type of polymerization process?

a) Addition polymerization

b) Condensation polymerization

c) Substitution polymerization

d) Copolymerization

Answer. (c)

50. Polymer used in bullet proof glass is:

(a) PMMA

(b) Lexan

(c) Nomex

(d) Kevlar

Answer. (a)

51. The weight average molecular mass of a macromolecule is greater …… than the number average molecular mass:

(a)Greater

(b)lesser

(c)equal

(d) none of these

Answer: (a)

52.Vulcanisation is discovered by-

(a) Ziegler-Natta (b) Charles Goodyear

(c) W.H. Carothers (d) J. Flory

Answer: (b)

53. Bisphenol-A is generally used to prepare-

(a) Alkyd resin (b) Polyamides

(c) Epoxy resin (d) Polyester

Answer: (b)

54. Kevlar fibre is an example of-

(a) Polyester (b) Polyurethane

(c) Aramides (d) Resin

Answer: (c)

55- Which of the following is not a free radical initiator-

(a) Benzoyl peroxide/hv (b) Hydrogen peroxide/hv

(c) Diazomethane/hv (d) Ethane/hv

Answer: (d)

56- Ziegler and Natta have been awarded by Nobel prize due to their work on-

(a) Free radical polymerization (b) Ionic Polymerization

(c) Coordination polymerization (d) None of them

Answer: (c)

57- Polymer have :

a) Absolute molecular weight

b) Average molecular weight
c) Low molecular weight
d) Absolute melting point

Answer: (c)

58- Trans form of polyisoprene is:

a) Guttapercha
b) Hydrochloric Rubber
c) Buna –N
d) Synthetic Rubber

Answer: (a)

59- Epoxy resins are:

(a) Thermoplastic polymers (b) Thermosetting polymers
(c) Homopolymers (d) Addition polymers

Answer: (b)

60- Epoxy resins are obtained by the reaction bisphenol A and ------------in presence of a base:

(a) Glycine (b) Cyanohydrin
(c) Epichlorohydrin (d) Adipic acid

Answer: (c)

61- Which of the following is not an example of natural biodegradable polymer?

(a) Collagen (b) Polyvinyl alcohol
(c) Lignin (d) Natural Rubber

Answer: (b)

62. Identify the biodegradable polymer of the following:

(a) PVC (b) Polypropylene
(c) Polystyrene (d) Polylactic acid

Answer: (d)

63. Which of the following can be used as a chain inhibitors?

(a) Phenols (b) amines

(c) quinones (d) All of these

Answer: (d)

64.Cationic polymerization may occurs in presence of

(a) Protonic acids (b) Lewis acids

(c) Trace of water as initiator (d) All of these

Answer: (d)

65. In cationic polymerization, which of the following types of alkenes are preferably polymerized ?

(a) Alkenes containing electron donating groups

(b) Alkenes containing electron withdrawing groups

(c) Both &(a) & (b)

(d) Alkenes containing at least three double bonds.

Answer: (a)

66. Monomers containing electron withdrawing substituent do not polymerize under cationic conditions because the presence of E W Groups-

(a) destabilizes the carbocation intermediates

(b) stabilizes the carbocation intermediates

(c) causes steric hinderance

(d) none of the above

Answer: (a)

67. Anionic polymerization may occur in the presence of

(a)KNH2

(b) LiNH2

(c)n- butyl lithium

(d) all of these

Answer: (d)

68. In anionic polymerization, chain initiation step is;

(a) Electrophilic addition

(b) nucleophilic addition

(c) both a & b

(d) all of these

Answer: (b)

69. If a monomer is of low reactivity and the chain transfer reagent is of high reactivity then

(a) Addition polymerization will occur

(b) free radical polymerization will occur

(c) no polymerization will occur

(d) both a & b

Answer: (c)

70. Homopolymers are made from:

a) Only one type of monomers
b) Two different type of monomers
c) Three different type of monomers
d) Several different type of monomers

Answer: (a)

71. Ziegler Natta catalyst is:

a) $TiCl_4$ and $(C_2H_5)_3Al$
b) $TiCl_4$ and C_2H_6
c) $TiCl_4$ and$CH_2=CH_2$
d) None of the above

Answer: a

72. Besides chain initiation, chain propagation and chain termination other steps in polymerization can be

(a)chain transfer

(b)- inhibition

(c)- retardation

(d)none of these

Answer: (b)

73. Which of the following polymer is least soluble in organic solvent.

(a)HDPE

(b) PVC

(c) Polystyrene

(d) Polycarbonate

Answer: (a)

74. Strongest molecular forces are present in:

(a) Elastomers

(b) fibers

(c) Thermoplastic

(d) Thermoset

Answer: (b)

75. The Polymer used in contact lenses-

(a) Silicon Polymer

(b) Epoxy resin

(c) PMMA

(d) Phenolic resin

Answer: (c)

76. High chlorine content in PVC makes it:

a) Flame retardant.
b) Resistant to photochemical degradation
c) Low dielectric constant
d) Resistant to decolouration

Answer: (a)

Q77-Which of the following polymer is used for dental treatment?

a) PMMA
b) Acrylic resins
c) Phenolic resins
d) Both (a)and (b)

Answer: (d)

Q78-Which of the following is true for phenolic resin

a) Good chemical and thermal resistance

b) No moisture absorbtion

c) Highly inflammable

d) All of these

Answer: (a)

Q79 - Ziegler Natta catalyst is used in preparation of :

a) Low density polythene
b) High density polythene
c) Polyvinyl chloride
d) Teflon

Answer: (b)

Q80-Tm melting point of polymer is ?

a) less than Tg

b) more than Tg

c) equal to Tg

d) none of these

Answer: b

Q81-Which of the following is not an example of free radical vinyl polymerization ?

a) Poly acrylonitrile

b) poly styrene

c) SBR

d) Bakellite

Answer: d

Q82-Which of the following polymer is used for making unbreakable crockery?

a) Bakellite
b) Melamine-formaldehyde resin
c) Nylon-66
d) Nylon-6,10

Answer: b

Q82-Polyurethane are usually prepared by reaction between

a) diol and dioic acid
b) diol and di-isocyanate
c) diol and diamides
d) dioic acid and dichlorides

Answer: b

Q83-which of the following statement is incorrect

a) Glyptal is a thermoplastic polymer
b) Glyptal is a thermosetting polymer
c) Bakellite is a thermosetting polymer
d) Glyptal is used in the manufacturing of paints and lacquers

Answer: a

Q84-Which of the following is/are addition polymerization?

a) Vinyl polymerization
b) Diene polymerization
c) Heteromultiple bond polymerization
d) All of these

Answer: d

Q85- Addition polymerization takes place by .... mechanism

a) Free radical polymerization
b) Cationic polymerization
c) Anionic polymerization
d) All of these

Answer: d

Q86-The number average molecular mass (Mn) and weight molecular mass (Mw)may be determined by:

a) Viscosity
b) Light scattering
c) Osmometry
d) All of these

Answer: d

Q87- In polymerization, the number average molecular mass is represented by :

a) M_n
b) M_w
c) M^n
d) M^{n+}

Answer: a

Q88- Teflon, polystyrene and neoprene are all:

a) Monomers
b) Co-polymers
c) Homoploymers
d) Condensation Polymers

Answer: c

Q89-Condensation Polymer of ....produce melamine resins.

a) Propylene
b) Phenol and formaldehyde
c) Phenol and acetaldehyde
d) Urea and formaldehyde

Answer: d

Q90-Which of the following ia a natural polymer?

a) Silk (b) Wool

c)Starch d)All of the above

Answer: d

Q91- Ziegler Natta catalyst is used in preparation of :

a) Low density polythene
b) High density polythene
c) Polyvinyl chloride
d) Teflon

Answer: b

Q92-Which of the following is a chain growth polymer ?

a)Starch b) Nucleic acid

c)Polystyrene d)protein

Answer: c

Q93-Natural Rubber is :

a) Cis-1,4-poly isoprene
b) Trans-1,4-poly isoprene
c) Both (a) and (b)
d) None of the above

Answer: a

Q94-BUNA -N is:

a) Synthetic fiber
b) Natural fibre
c) Synthetic Rubber
d) Natural Polymer

Answer: a

Q95- A Polymer have :

a) Absolute molecular weight
b) Average molecular weight
c) Low molecular weight
d) None of the above

Answer: (b)

Q96-For the preparation of Nylon 6 the monomer used are

a) Adipic acid + Hexamethylene diamine
b) Acetic acid+ Hexamethylene diamine
c) Caprolactam
d) Acetic acid+ Vinyl chloride

Answer: (C)

Q97-Which of the following is not a stage of addition polymerization

a) Initiation
b) Propogation
c) Termination
d) Recrystalliztion

Answer: (d)

Q98- The monomer of Polystyrene is:

a) $CH_3-CH=CH_2$

b) $CH_2=CH-Cl$
c) $C_6H_5-CH=CH_2$
d) $CH_2=CH-CHO$

Answer: (c)

Q99-High Density Polythene (HDPE) can be prepared from ethylene by :

a) Ziegler-Natta Catalyst
b) Heating with Peroxide
c) Condensing in sealed tube
d) Condensing in Styrene

Answer: (a)

Q100- Which of the following is a linear polymer?

a) Nylon-6
b) Bakellite
c) Low Density Polythene
d) Melamine-formaldehyde

Answer: (a)

Q101- Which of the following type of polymers are known for their high crystallinity

a) Isotactic
b) Syndiotactic
c) Atactic
d) None of these

Answer: (a)

VIII

B.Sc. SEM II

SYLLABUS OF UNIT VIII

Synthetic Dyes: Colour and constitution (electronic Concept), Classification of dyes, Chemistry and synthesis of Methyl orange, Congo red, Malachite green, crystal violet, phenolphthalein, fluorescein, Alizarin and Indigo.

Synthetic dyes

Colour. The matter appears coloured when it interacts with the incident light, which may be fully or partly absorbed and partly reflected. In this case, the colour depends upon the colour of the reflected light. Electromagnetic radiation with a wavelength 400 nm and 800 nm is directly detected by the human eye is known as visible light.

When visible light strikes an object, it can be -

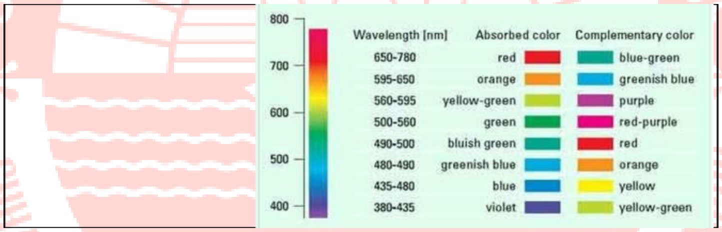
Totally absorbed – which makes the object appear **black**

No absorption and total reflection – which will make the object appear **white**

Partly absorbed and rest reflected – which leads to the sensation of colour to the eye.

Thus the transmitted light can strike the retina of the eye causing the sensation of colour.

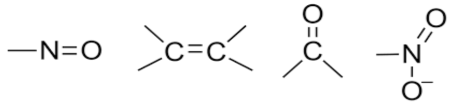
- The colour of the matter is the complementary colour of the absorbed part of the light. For example, when a substance absorbs blue colour it will appear yellow, which is the complementary colour of blue.
- If a compound is colourless, it does not mean that it does not absorb any radiation. In such a case, absorption takes place outside the visible range of radiation i.e. either the infrared or the ultraviolet radiation is absorbed.



Wavelength [nm]	Absorbed color	Complementary color
650-780	red	blue-green
595-650	orange	greenish blue
560-595	yellow-green	purple
500-560	green	red-purple
490-500	bluish green	red
480-490	greenish blue	orange
435-480	blue	yellow
380-435	violet	yellow-green

• **Theories of colour.** The following three theories have been proposed to explain colour:

1. **Otto-Witt's theory:** According to this theory the colour of any compound is due to the presence of certain groups containing multiple bonds. Such groups are called chromophores (Greek: chroma=colour, phoros=bearing) examples of chromophores are



2. The compound containing the chromophore groups is called the chromogen. The greater the number of chromophores in the molecule, the deeper will be the colour of the compound.

3. There are certain groups (auxochromes) that themselves are not chromophores but enhance the intensity of the colour when introduced into a coloured compound. For example, OH, NH_2 NHR, NR_2, Cl, Br, I, etc. The auxochrome plays its role only in the presence of a chromophore.
4. Bathochromic groups cause redshift while hypsochromic groups cause a blue shift in the colour of a compound. In the dye industry, colour deepening means the colour changes from yellow- orange- red- purple- blue- green- black. It means that the bathochromic groups cause deepening while hypsochromic groups cause lightening of the colour of a compound.
5. **Valence bond theory:** According to this theory when a beam of light falls on a compound, the wavelength of photons absorbed depends upon the energy difference between the ground state and the excited state. The larger the difference, the smaller is the wavelength of light absorbed. When the wavelength of light absorbed becomes longer and generally goes in the visible range, the Compound appears coloured. The more extended the conjugation in a molecule, smaller is the energy difference between the ground state and the excited state and hence longer is the wavelength of absorbed light.

6. **Molecular orbital theory**: When a molecule absorbs light, the electrons are excited from the bonding (or non-bonding) orbitals to anti-bonding orbitals. Different energy absorptions for electronic transitions within a molecule are possible depending upon the nature of bonding. The electronic transitions with their relative energies are mainly of the following types:

$$\sigma - \sigma^* > \sigma - \pi^* > n - \sigma > \pi - \pi^* > n - \pi^*$$

Out of all the transitions, only π-π* and n-π* transitions occur in the UV range. The π-π* transition requires minimum energy and hence occurs at longer wavelengths and such transition is always less intense. Further, π-π* transitions are more intense than n-π* transitions and hence are responsible for colour. Simple alkenes such as ethylene absorb at 175 nm (E_{max} 15,000). But in 1,3-butadiene due to the presence of two double bonds in conjugation, the π-π* absorption band shifts to 217 nm with simultaneous increases in the E to 21,000 and 1,3,5-hexatriene shows a strong (π-π*) transition absorption band at 258 nm having epsilon max of 35,000. Further, in the case of aromatic compounds, as the number of fused rings increases, the position of absorption approaches the visible region.

William Henry Perkin is known as the father of dyes.

In 1856 Perkin accidentally discovered mauvine—the first commercialized synthetic dye—and introduced a new era in the chemical industry.

Dyes: A coloured substance can be called a dye, if it can be applied in solution or dispersion to a substance such as textile fibres (cotton, silk, wool, nylon, polyester), paper, leather, hair, fur, plastics, wax, a cosmetic base giving it a coloured look. A dye must satisfy the following conditions:

- It should be suitably coloured,
- It should get fixed on the textile,
- When fixed, it should be fast to light, and resistant to the action of water, soap, detergents, etc.
- It should be resistant to organic solvents during dry cleaning.

Classification of dyes:

Dyes are classified as follows**:**

1. **Based on the source.**
   Natural and synthetic dyes. Indigo and alizarin are two natural dyes. Nowadays, to get a variety of shades, many synthetic dyes are used, the majority of which are obtained from coal-tar and hence these are called coal-tar dyes.

2. Based on their constitution. Depending upon their chemical constitution and the functional groups present, these are classified as: azo dyes, nitro dyes, nitro dyes, triphenylmethane dyes, anthraquinone dyes, indigoid dyes, phthalein dyes, acridine dyes, etc.

3. Based on their application.

(a) Acid dyes are sodium salts of azo dyes containing sulphonic or carboxylic acid groups. These are applied to the fabric from their acid solution. For example: orange 1, orange II. methyl orange and congo red.

(b) Basic dyes are salts of bases having amino or alkylamino groups as auxochromes. For example, azo dyes (such as aniline yellow, butter yellow and chrysodine G) and triphenylmethane dyes (such as malachite green and crystal violet).

(c) Direct or substantive dyes are water-soluble dyes which are directly applied to the fabric from an aqueous solution. These involve H-bonding between the dye and the fabric. e.g. Congo red and Martius yellow.

(d) Dispersive dyes are water-insoluble dyes which are applied to the fabric from a dispersion of the finely divided dye in a soap solution in the presence of some stabilizing agent such an phenol, cresol or benzoic acid. Such dyes are: celliton fast pink 8 and celliton fast blue B

(e) Vat dyes are water insoluble dyes which cannot be applied directly to the fabric Such dyes are initially reduced to a soluble colourless form (leuco form) in large vats using a reducing agent such as an alkaline sodium hydrosulphite. In alkaline medium, the leuco form develops an affinity for cellulose fiber due to which these dyes are mainly used for dying cotton fibers. The cotton fiber to be dyed is soaked into this alkaline solution which is then oxidized to the insoluble form by exposure to air or some oxidizing agent such as chromic acid or perboric acid. A well-known example of vat dye is indigo.

(f) Fiber-reactive dyes contain a reactive group which reacts directly with the hydroxyl or amino group of the fiber. The colour of the dyed fabric is fast and has a long life. e.g. derivatives of 2,4-dichloro-1,3,5-triazine.

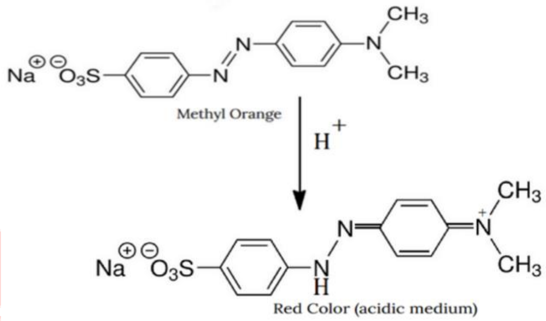
(g) Ingrain dyes These are obtained by coupling reaction of phenols, naphthols, and arylamines adsorbed on the surface of a fabric, with a diazonium salt. The colour is not so fast due to the adsorption of the dye on the surface only, e.g. para red.

(h) Mordant dyes can not dye the fabric directly, but require some mordant. Here, the mordant acts as a binding agent between the
fibre and the dye. Metal ions are used as mordants for acid dyes but tannic acid is used as the mordant for basic dyes. The same dye can form lakes of different colours depending upon the type of the mordant used. For example, alizarin gives rose-red shade with Al^3 ions, blue shade with Ba^{+2}ions, and red with Cr^{-6} violet with Mg^{+2}

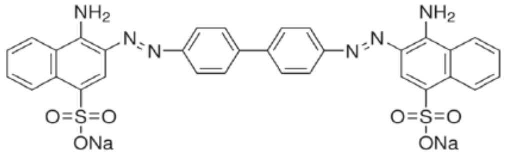
(i)Azo dyes have aromatic systems linked to the azo (- N =N-) group as the chromophores and NH_2, NR_2 OH, OR, etc, as the auxochromes. e.g. Methyl Orange and Congo red.

Examples of some important dyes

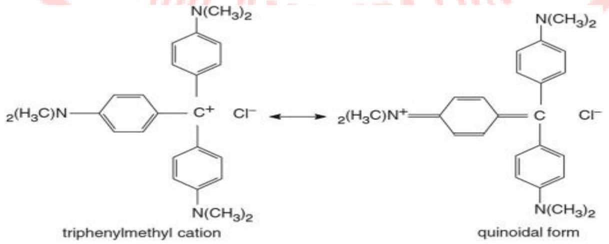
- **Methyl orange** is a monoazo dye and is synthesized by coupling of N,N-dimethylaniline with diazotised sulphanilic acid. Methyl orange is rarely used for dying purposes because its colour is not stable to washing and light. It is a very good indicator used in acid-base titrations. It changes its colour from yellow in basic to red in acidic solutions. In the basic solution, the chromophore is an azo group while in the acidic solution, the chromophore is the p-quinonoid.



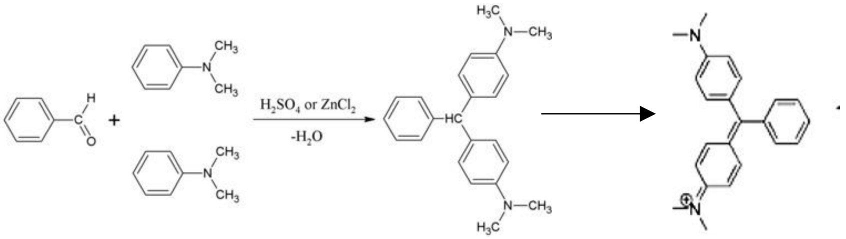
- **Congo red** is a bis azo dye and is synthesized by coupling of tetrazotised benzidine(4,4'-diaminodiphenyl) with two molecules of naphthionic acid. Congo red is a direct dye which gives the red colour to cotton. It is not a good dye because the colour changes when the acid is added. It is used as an indicator which is blue in acidic solution (below pH 3) and red in basic solution (above pH 3).



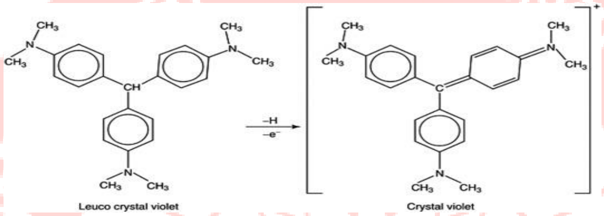
- **Triphenylmethane dyes** are derivatives of triphenylmethane containing - NH_2, NR_2 and OH groups in the ring which are generally colourless (leuco bases). These leuco bases on oxidation get converted into colourless carbinol bases which readily change from colourless benzenoid form to the coloured quinoid form in the presence of acids due to salt formation.



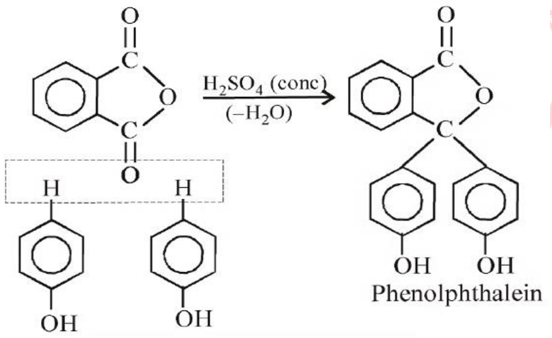
- **Malachite green.** Condensation of two molecules of N,N-dimethylaniline with one molecule of benzaldehyde at 373K in presence of conc. H_2SO_4} gives the leuco base which on oxidation with PbO, in a solution of CH_3COOH and HCl produces a carbinol base. The carbinol base reacts with HCl to give malachite green dye. Malachite green can be applied to wool and silk directly but for cotton it needs tannin as a mordant.



- **Crystal violet** is obtained by heating N,N-dimethylaniline with $COCl_2$ (phosgene). Initially formed Michler's ketone condenses further with dimethylaniline to give crystal violet. The colour of crystal Violet depends upon pH of the solution. The colour is purple in weakly acidic solution, green in strongly acidic and yellow in still more acidic solution.

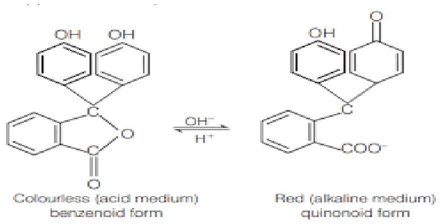


- **Phenolphthalein.** Condensation of two molecules of phenol with one molecule of phthalic anhydride in presence of conc. H_2SO_4 gives phenolphthalein. It is not used as a dye but is a very good indicator in acid-base titrations. It is insoluble and hence colourless in acid but becomes soluble and gives a deep red colour (pink when light) in basic medium because of the resonance to give quinonoid structure. In presence of excess of alkali, it again becomes colourless due to the loss of the quinonoid structure and resonance.

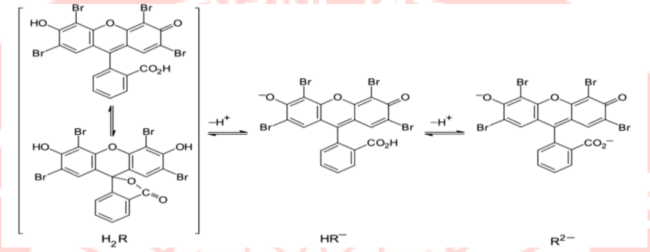


- **Fluorescein**. Condensation of two molecules of resorcinol with one molecule of phthalic anhydride on heating at 473K or 383-393K in the presence of oxalic acid gives fluorescein. It is a red powder insoluble in water but dissolves in alkalis to give a brown solution which produces a very strong yellowish green fluorescence.

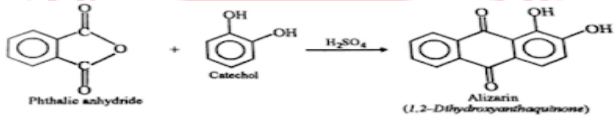
  The sodium salt of fluorescein is called Uranine which is used to dye wool and silk yellow from an acid bath.



• **Eosin** is prepared by bromination of fluorescein in glacial acetic acid. Eosin is used to dye wool and silk red with a yellow fluorescence. Eosin in the form of lead lake is called Vermilionette which is used for poster printing and making of red inks.



• **Alizarin dye** is prepared by sulphonation of anthraquinone with fuming H_2SO_4 at 413K followed by the fusion of the sodium salt with a calculated quantity of sodium or potassium chlorate at 453- 473K under pressure. Alizarin is obtained after acidification of the product with dil. HCl. It is a ruby red crystalline compound insoluble in water and alcohol but highly soluble in alkalies to give purple solution. Oxidation of alizarin with Mn and H_2SO_4 leads to the formation of purpurin. while reduction of alizarin with Zn dust and NH_4OH gives anthrarobin. Alizarin is a mordant dye. The colour of the lake depends upon the metal ion used. AI^{+3} gives a red lake, Fe^{+3} gives violet-black and Cr^{+6} gives brown-violet.



Synthesis of Alizarin dye from catechol

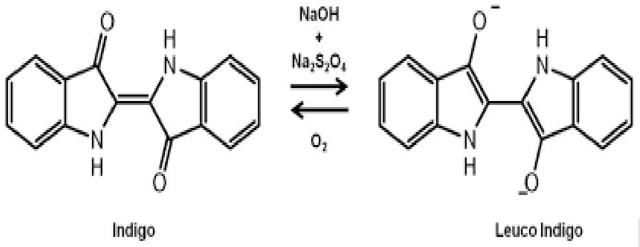
- **Indigo** is officially called as indigotin and is found naturally as indican which is the glucoside of indoxyl in Indian plant, indigofera tinctoria and the European plant, isatis tinctoria. Acid or enzymatic hydrolysis of indican yields indoxyl which on aerial oxidation gives indigotin. Indigo can be synthesized by the following three methods:

1. Heumann's first indigo synthesis (1890).

2. Heumann's second indigo synthesis (1896).

3. From aniline and ethylene oxide (1943).

On agitation with alkaline sodium hyposulphite in large vats, insoluble indigotin is reduced to soluble leuco form, called indigotin white. The cloth to be dyed is soaked in th is alkaline solution and then exposed to air to get the original blue colour on the cloth due to oxidation .



MULTIPLE CHOICE QUESTION

1. Visible light consists of electromagnetic radiation of wavelength
(a)200-400nm

(b)400-800nm

(c)300- 500nm
(d)500-650nm
Ans. (b)
2. Quinonoid theory of color is given by.
(a) Otto
(b)Armstrong
(c) W.H.Perkin
(d) All of the above
Ans. (b)

3. Which following is not a chromophore?
(a) – NH2
(b) - NO is an example
(c)- NO2
(d) -N=N-
Ans. (a)

4. Which of the following is an example of basic dye?
(a) Alizarin
(b) Malachite

(c) Indigo
(d) Orange-I
Ans. (b)

5. Roots of the madder plant contain:
(a) Indigo
(b) Saffron (yellow)
(c) Alizarin
(d) Crystal violet
Ans. (c)

6. The dye which is also used in medicine

(a) Crystal violet
(b) Congo red
(c) Methyl orange
(d) Alizarin
Ans. (a)

7. Optical brighteners are also
(a) White dye
(b) Enhancing dye
(c) Azo dye
(d) Nitro dye
Ans. (a)

8. The function of optical brighteners is:

(a) to absorb UV light and re-emit visible light.
(b)to absorb visible light and re-emit UV light
(c) to absorb I.R. light and emit UV light.
(d) None of the above.
Ans. (a)
9. Phenolphthalein is used as an indicator and gives pink colour in :

(a) acidic medium
(b) basic medium
(c) neutral medium
(d) all of these
Ans. (b)
10. Which dye is used as an indicator in complexometric titration using EDTA:

(a) Methyl orange
(b)Eriochrome black-T
(c) Phenolphthalein
(d) Methyl red
Ans. (b)

11. Which of the following is a chromophore?
(a) - NO2
(b)-OH
(c) – NH2
(d) -Cl
Ans. (a)

12. The water-solubility of dyes can be increased by introducing
(a)- SO3Na groups
(c) -OH groups
(b) -COOH groups
(d) All of these
Ans. (b)

13. The reason why materials appear coloured is
(a) The selective absorption of spectral colours
(b) The interaction between the light and the electrons of the dye molecules
(c) The composition of the white light from various spectral colours
(d) All of these
Ans. (b)

14. Which dyes will fixed to the fibre by chemical reaction?

(a) vat dyes
(b) Disperse dyes
(c) acid dyes
(d) None of these
Ans. (c)

15. Which of the following is an auxochrome?

(a) -N=O

(b) - N =N-
(c) - NO2
(d) – OH

Ans. (d)

16. A substance which appears orange-colored absorbs the radiation in the range (nm)
(a) 400-435
(b) 480 – 490
(c) 500-560
(d) 605-750
Ans. (b)

17. Colour lake formed by alizarin with Mg2+ ions (mordant) is
(a) brown black
(b) rose red
(c) violet
(d) red
Ans. (c)

18. Saturated hydrocarbons give the transitions:
(a) $\pi-\pi^*$,
(b) $n-\pi^*$,
(c) $\sigma-\sigma^*$,
(d) $n-\sigma^*$

Ans. (c)

19. Colour of a compound is best explained by
(a) Molecular orbital theory
(b) Valence bond theory
(c) Witt's theory
(d) None of these
Ans. (a)

20. carbonyl compounds give the transitions:
a) $\pi-\pi^*$,
b) $n-\pi^*$,
c) $\sigma-\sigma^*$,
d) *both a and b*
Ans. (d)

21. Chromophore-Auxochrome theory was proposed by:
a) Armstrong,
b) Otto –
c) Witt

d) Otto –Witt

Ans. (d)

22. Flouroscien is a type of
   a) Azo dye
   b) Nitro dye
   c) Phthalein dye
   d) None of the above

Ans. (c)

23. Malachite green is obtained by the condensation of

(a) benzaldehyde and N,N-dimethylaniline
(b) Formaldehyde and dimethyl aniline
(c) benzaldehyde and N-methylaniline
(d) Formaldehyde and N-methyl aniline

Ans. (a)

24. An azo dye can be prepared by the coupling of benzene diazonium chloride and

(a) Benzene

(b) Phenol

(c) Nitro benzene

(d) Chlorobenzene

Ans. (b)

25. A mordant is a substance, which is:

(a) Coloured

(b) Fixes dye on the fabric

(c) Leuco base of a dye

(d) All of these

Ans. (b)

26. VAT dyes are generally applied to the fabric in the form of:

(a) Leuco base

(b) Mordant dyes

(c) Dispersed dyes

(d) Oxidized base

Ans. (a)

27. A human being can see in:

(a) UV region

(b) Visible Region

(c) IR Region

(d) all of these

Ans. (b)

28. Dyes which can be applied to cellulosic fiber from a water solution are called

(a) Ingrain dyes

(b) Substantive dyes

(c) Mordant dyes

(d) Vat dyes

Ans.b

29. Which of the following is not a necessary characteristic of a dye?

(a) It must be highly soluble in water

(b) It must be fast to soap, detergent and sunlight

(c) It must have a suitable colour

(d) It must be able to fix the fibre

Ans.a

30. The dyes which are applied to the fabric in the colourless reduced state and then oxidised to coloured state are called:

(a) Azo dyes

(b) Dispersed dyes

(c) Basic dyes

(d) Vat dyes

Ans. (d)

31. In the case of Alizarin, the use of Al^{3+} ions as a mordant imparts which colour to the fabric?

(a) Rose Red

(b) Blue

(c) Green

(d) Purple

Ans. (a)

32. Phthalic anhydride is treated with catechol in the presence of conc. H_2SO_4 at 453K, a product is obtained which is:

(a) Phenolphthalein

(b) Fluorescein

(c) Alizarin

(d) Indigo

Ans. (c)

33. For a coloured compound to behave as a dye, it must contain:

(a) Auxochrome

(b) chromophore

(c) both a & b

(d) None of these

Ans. (c)

34. β-carotene has______ conjugated double bonds:

(a) 5
(b) 8
(c) 11
(d) 13

Ans. (c)

35. Which of the following ketone acts as an intermediate in the synthesis of crystal violet dye?

(a) Acetone

(b) Butanone-2

(c) Michler's Ketone

(d) Michael Ketone

Ans. (c)

36. Alizarin dye is a class of:

(a) Anthraquinone dye

(b) Indigotin dye

(c) Phthalein dye

(d) Azo dye

Ans. (a)

37. The first process in the application of Vat dye is

(a) Oxidation

(b) Bleaching

(c) Vatting

(d) Chlorination

Ans.c

38. A vat dye is dissolved using alkaline solution of:

(a) Sodium chloride

(b) Sodium hydrosulphite

(c) Calcium hydroxide

(d) Caustic soda

Ans.b

39. Acid dyes are mainly applied on

(a) Cotton

(b) Linen

(c) Wool

(d) None of these

Ans.c

40. _______dye is called as ice colours:

(a) Azoic

(b) Vat

(c) Sulphur

(d) Acid

Ans.a

41. Red ink is prepared from:

(a) Phenol

(b) Aniline

(c) Congo red

(d) Eosin

Ans.d

42. An insoluble coloured compound formed by the action of metallic salts on dye is known as:

(a) Lake

(b) Mordant

(c) Dye intermediate

(d) None of these

Ans.a

43. Which of the following is a dye ?

(a) Methyl orange

(b) Orange-I

(c) Aniline yellow

(d) All of these

Ans.d

44. Which of the following is a vat dye and often used in dyeing jeans?

(a) Indigo

(b) Alizarin

(c) Picric acid

(d) Crystal violet

Ans.a

45. Which colour is obtained in basic medium of methyl orange?

(a) Red

(b) Blue

(c) Orange

(d) Yellow

Ans.d

46. Methyl orange belongs to the class of:

(a) Acidic dye

(b) Basic dye

(c) Mordant

(d) Vat dye

Ans.a

47. An auxochrome group is:

(a) - OCH_3

(b) – N $(CH_3)_2$

(c) - OH

(d) All

Ans.d

48. Which of the following is not a chromophoric group?

(a) Nitro

(b) Carboxyl

(c) Nitroso

(d) Azo

Ans.b

49. Congo red is:

(a) nitro dye
(b) monoazo dye
(c) bis azo dye
(d) triaryl methane dye

Ans. C

50. Malachite green is:

a) Nitro dye

(b) Nitroso dye

(c) Azo dye

(d) Triaryl methane dye

Ans. d