M. Sc II (Organic Chemistry), Semester-IV

PGOC-401: SYNTHETIC ORGANIC CHEMISTRY

Total Credits: 04 **Total Lectures: 60Hrs**

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Study of transition metal complexes in organic synthesis.
CO 2 : Learn designing of organic synthesis
CO 3 : Use of boron and silicon in organic synthesis.
CO 4 : Study Umpolung in organic synthesis.
CO 5 : Protection and deprotection of hydroxyl, amino, carboxyl, ketone and aldehyde functions as illustrated in the synthesis of polypeptide and polynucleotide.

Course Content:

1. Transition metal complexes in organic synthesis; only Pd, Ni, Co, Pt, Fe, Rh, Ru; Grubb's catalyst, Ziegler Natta catalyst.
2. Use of Boron, Silicon and Tin in organic synthesis.

Ref.2, chapter 47

3. Designing of organic synthesis.
4. Umpolung in organic synthesis.
5. Protection and deprotection of hydroxyl, amino, carboxyl, ketone and aldehyde functions as illustrated in the synthesis of polypeptide and polynucleotide.

Books/References:

1. Modern Synthetic Reactions – H. O. House (Benjamin).
2. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press).
3. Designing of Organic Synthesis – S. Warren (Wiley).
4. Some Modern Methods of Organic Synthesis – W. Carruthers (Cambridge).
5. Organic Synthesis – M. B. Smith.
6. Organometallics in Organic Synthesis – J. M. Swan and D. C. Black (Chapman and Hall).
7. Advanced Organic Chemistry, Part B – F. A Carey and R. J. Sundberg 5^{th} edition (2007).

PGOC-402: CHEMISTRY OF NATURAL PRODUCT

Total Credits: 04 **Total Lectures: 60Hrs**

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Learn biogenesis of terpenoides.
CO 2 : Study biogenesis of alkaloids.
CO 3 : Study biogenesis of steroids.
CO 4 : Study biogenesis and physiological effect of Prostaglandins.
CO 5 : Study biogenesis of Cholesterol, Flavons, Coumarins, Carbohydrates and Proteins.
CO 6 : Synthesis of biotin and Vitamin B2, Synthesis of Vitamin B1, Biological functions of B_6, B_{12}, folic acid and thiamine.

Course Content:

1) Terpenoids
Structure and synthesis of Abietic acid, Zingiberene, Santonin, Cuparenonne and Caryophyllene.

2) Alkaloids
Structure, Stereochemistry, Synthesis and biosynthesis of morphine, reserpine, ephedrine, (+) conin.

3) a) Steroids
Occurrence, Nomenclature, Basic skeleton, Diels hydrocarbon and study of the following Hormones: Androsterone, Testosterone, Estrone, Progesterone, Aldosterone and Cartisone. Biosynthesis of steroids.

b) Prostaglandins
Occurrence, nomenclature, classification, biogenesis and physiological effects, synthesis of PGE2 and PGF2

4) Biogenesis
Alkaloids (pyridine, morphine and indole type) Terpenoids, Cholesterol, Flavones, Coumarins, Carbohydrates and Proteins.

5) Vitamins

Synthesis of biotin and vitamin B2, Synthesis of vitamin B1, Biological functions of B_6, B_{12}, folic acid and thiamine.

Books/ References:

1. The total synthesis of natural products- Apsimon.
2. Alkaloids - Manskey and Holmes.
3. Chemistry of Terpenes - A.A. Newmen.
4. The chemistry of natural products- P. D B.Mayo.
5. Terpenes- Simonson.
6. Aspects of terpenoid chemistry and biochemistry- T.W. Goddwin.
7. Vitamins and Co-enzymes- Woguer.
8. Chemistry of Natural products- P. W. Bently.
9. Steriods - Fieser and Fieser.
10. Organic Chemistry Vol. II and I- I. Finar.
11. The molecules of nature - J.B. Hendrickson.
12. The biogenesis of natural products Peter Bernfield.
13. Total synthesis of steroids- R.T. Slickenstaff A.C. Ghosh and G.C. Wole .
14. The chemistry of natural products- vol. Nakanishi.

PGOC-403: GREEN CHEMISTRY

Total Credits: 04 **Total Lectures: 60Hrs**

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Elaborate basic principles of green chemistry.
CO 2 : Understand solvent free microwave assisted organic synthesis.
CO 3 : Use of green reagent in green synthesis.
CO 4 : Study of green catalyst.
CO 5 : Study phase transfer catalyst in green synthesis.
CO 6 : Advantages of PTC reactions to green synthesis.
CO 7 : Learn microwave assisted reactions in water.
CO 8 : Learn microwave assisted reactions in organic solvent.
CO 9 : Understand ultrasound assisted reactions.

Course Content:

1. Introduction to Green Chemistry.

Introduction, Principles, atom economy and scope, Inception to green chemistry, Introduction to alternative approaches, Solvent free reactions-principle, scope, utility of solvent free conditions, controlling solvent free reactions. Phase changes, optimum reaction temperatures, miscibility of reactants and catalysts.

Solvent free microwave assisted organic synthesis: Introduction, solvents free techniques-Reactions on solid mineral support, solid-solid phase transfer catalysts reactions without solvent, support or catalyst. Microwave activation-benefits, limitations, equipments, microwave effects-according to reaction medium and according to reaction mechanism.

2. Approaches to Green Chemistry.

Basic principles of green synthesis:

a) Use of green reagents in green synthesis-dimethyl carbonate, polymer supported reagents-per acids, chromic acids.
b) Green catalysts: Acid catalysts, oxidation catalysts, and basic catalysts.
c) Phase transfer catalyst in green synthesis: Aliquat 336, benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride.

d) Advantages of PTC reactions to green synthesis. Applications of PTC's in C-alkylation, N-alkylation, S-alkylation, darzens reaction, Williamsons synthesis and Wittig reaction.

3. Microwave induced and ultrasound assisted green synthesis.

Introduction to synthetic organic transformations under microwave.

a) Microwave assisted reactions in water: Hoffmann elimination, hydrolysis, oxidation, saponification reactions.

b) Microwave assisted reactions in organic solvents: Esterification reactions, Fries rearrangement, Ortho ester Claisen rearrangement, Diels-Alder reaction, decarboxylation.

c) Microwave solvent free reactions (solid state reactions): Deacetylation, Deprotection, saponification of ester, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, and reductions.

d) Ultrasound assisted reactions: Introduction, substitution, addition, oxidation, reduction reactions.

Books /References:

1. Organic Chemistry, vol-2, I.- L. Finar, ELBS.
2. Stereoselective Synthesis: A practical Approach- M. Nogrudi, VCH.
3. Organic Synthesis in water- Paul A. Grieco Blackie.
4. Green Chemistry, theory and practice- Paul T. Anastas and John C. Warner.
5. New Trends in Green chemistry- V. K. Ahluwalia and M. Kidwai.
6. Organic Synthesis: Special techniques- V. K. Ahluwalia and Renu Aggarwal.

PGOC-404: APPLIED ORGANIC CHEMISTRY

Total Credits: 04 **Total Lectures: 60Hrs**

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Study carbamate pesticides.
CO 2 : Learn organophosphorous pesticides.
CO 3 : General survey and synthesis of insect repellents.
CO 4 : Understand structure and synthesis of Juvenile harmones.
CO5 : Synthesis of Pheromones.
CO 6 : Synthesis of important dyes and intermediates.

Course Content:

1) Agrochemical:

a. Carbamate pesticides: Introduction, carbaryl, Baygon, Aldicarb, Ziram, Zineb
b. Organophosphorus pesticides: Malathion, monocrotophos, dimethoate, phorate, mevinphos
c. Insect repellents: General survey and synthesis
d. Juvenile harmone: introduction structures JHA importance synthesis
e. Pheromones: introduction, examples, and importance in IPM synthesis of juvabione bombycol, grandisol, and disparure

2) Dyes and Intermediates:

Synthesis of important dye intermediates. Commercial processes for Azo dyes, reactive dyes, optical brighteners, thermal sensitive dyes, dispenses dyes.

References/ Books:

1. Colour Chemistry – Allan.
2. Chemistry of Synthetic Dyes Vol- 1 to 7.- K. Venkataraman
3. Dyes & their intermediates- Abrahart.
4. The Chemistry of Pesticides and formulations - N. N. Melikov.
5. Chemistry of Pesticides- K. H. Buchel.
6. Pesticides - R. Cleymlin.
7. Text book of Polymer Science- F. W. Billmeyer.
8. Contemporary Polymer Chemistry- H. R. Alcock and F. W. Lambe.
9. Physics & Chemistry of Polymers- J. M. G. Cowie, Blackie.
10. Unit Processes in Organic Synthesis- P. H. Groggins.
11. Perfumary Technology-. B. Biollot & P. V. Wells
12. A formulary of Cosmetic Preparations- M. Ash & I. Ash.

PGOC-405: BIO-ORGANIC CHEMISTRY

Total Credits: 04 **Total Lectures: 60Hrs**

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Study Classification and nomenclature of enzymes.
CO 2 : Learn advantages and limitations of enzymes in organic synthesis.
CO 3 : Study enzyme selectivity-Chemo, region, diastereo and enantio selectivity-Illustration with suitable examples.
CO 4 : Study structure and synthesis of nucleosides and nucleotides.
CO 5 : Study structure of DNA.

Course Content:

1: Enzymes

Definition, Classification and nomenclature of enzymes. Factors affecting the enzyme catalysed reactions. Advantages and limitations of enzymes in organic synthesis-mechanistic aspects of enzyme catalysis -Lock and Key mechanism, Induced-Fit mechanism, Michaelis-Menten Equation, Desolvation and salvation-substitution theory, Three point attachment rule. Factors affecting the enzyme catalysed reactions. Enzyme selectivity-Chemo, regio, diastereo and enantio selectivity-Illustration with suitable examples.

2: Nucleic acids

Introduction, Hydrolysis of nucleic acids, Structure physical and chemical properties of the heterocyclic bases-Adenine, Guanine, Cytosine, Uracil and Thiamine. structure and synthesis of nucleosides and nucleotides. Deoxyribose nucleic acid (DNA): Primary, secondary, tertiary structure of DNA. Structure of RNA. Types of RNA- mRNA, rRNA and tRNA.

Books/ References:

1. Natural products: Chemistry and Biological significance- J.Mann, R.S.Davidson, J.B.Hobbs, D.V., Banthropde & J. B. Harborne, Longm, an, Essex.

PGOC-407: MIXTURE SEPERATION

Total Credits: 02

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Ternary mixture seperation
CO 2 : Study ternary mixture separation on microscale using ether.
CO 3 : To separate the three components from each other using ether.
CO 4 : Determine the type, functional group of each component.
CO 5 : Determine the melting point/ boiling point of the components.

Course Content:

TERNARY MIXTURE SEPARATION:

Separation of at least ten mixtures containing three components. The mixtures should also involve separation of nitro phenols, amino acids, low boiling substances, water soluble substances. Amines, Phenols and acids used should also contain other elements and functional groups. The mixture separation should be carried out on micro-scale using ether.

PGOC-408: ADVANCED PREPARATIONS

Total Credits: 02

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Spectral analysis best on instrumental techniques.
CO 2 : Preparation of organic compounds, their purifications and run TLC.
CO 3 : Determination of physical constant: Melting point, Boiling point.

Course Content:

SINGLE STAGE AND TWO STAGE PREPARATIONS:

At least eight single stage and eight two stage preparations from the following should be carried out. The preparations should be carried out on micro scale.

Single Stage Preparations:

1. Acetophenone → Ethyl Benzene
2. Anthranilic acid → ortho Iodobenzoic acid
3. Diels-Alder reaction using Anthracene and Maleic anhydride
4. Benzyl cyanide → p-Nitro benzyl cyanide
5. Bromobenzene → p-Nitro bromobenzene
6. 2-Naphthol → 2,2'-Dihydroxybinaphthyl
7. Glycine → Hippuric acid
8. Salicylic acid → 5-Nitrosalicylic acid
9. Resorcinol Resacetophenone
10. 2-Methoxynephthalene →1-Formyl-2-methoxynaphthalene
11. p-Xylene →Ter-phthalic acid
12. o-Nitrotoluene + Benzaldehyde $\xrightarrow{\text{Base}}$ condensation

TWO STAGE PREPARATION

At the end of course student will be able to –

CO 4 : Spectral analysis best on instrumental techniques.
CO 5 : Preparation of organic compounds, their purifications and run TLC.
CO 6 : Determination of physical constant: Melting point, Boiling point.
CO 7 : Use of different separation techniques.

Course Content:

Two Stage Preparations:

1. Benzophenone → Oxime → Benzanilide
2. Benzoin → Benzil → Benzilquinoxaline
3. Benzaldehyde + Acetophenone → Benzalacetophenone → Epoxide
4. 4-Nitrotoluene → 4-Nitrobenzoic acid → 4-Aminobenzoic acid
5. Resorcinol → 4-methyl-7-hydroxycoumarin → 4-methyl-7-acetoxy -coumarin
6. Phenol →Salicyaldehyde →Coumarin
7. Cyclohexanone → Phenylhydrazone →1,2,3,4- tetrahydrocarbazole
8. Acetanilide → p-Nitroacetanilide → p-Nitroaniline
9. Hydroquinone → Quinone → 1,2,4- Triacetoxybenzene
10. Cyclohexanone → Oxime → Caprolactum
11. Hydroquinone → Diacetate → 2,5-Dihydroxy acetophenone
12. 4-Chlorophenol → 4-Chlorophenyl acetate → 5-Chloro-2-hydroxyacetophenone

Interpretation of NMR, IR and Mass Spectra of about 15 compounds. Minimum 2 three stage preparations to demonstrate how to develop a synthetic sequence.

PGOC-409: LAB COURSE/ PRACTICALS

Total Credits: 02

Course Learning Outcomes :

At the end of course student will be able to –

CO 1 : Students should carry out a small research project.

CO 2 : Students should familiar with literature survey, research methodology, identification of products by analytical and spectral methods.

CO 3 : Students should go through preparation of organic compounds, their purifications and run TLC

CO 4 : Students should familiar with different separation and purification techniques i.e. Recrystallization, distillation, fractional distillation, chromatography and solvent extraction.

Course Content:

PROJECT AND PRACTICALS:

1. Students should carry out a small research project. This should make them familiar with literature survey, research methodologies, Identification of products by analytical and spectral methods and familiarity with chromatographic techniques.

2. Students who are not assigned the project should carry out at least 12 experiments and students who are assigned project work should carry out at least 6 experiments to illustrate the principles of organic reaction mechanism, stereochemistry or selectivity of reagents.

Suggested reagents and reactions –

$LiAlH_4$ (reduction of ethyl benzoate to benzyl alcohol), $NaBH_4$ (reduction of anisaldehyde to p- methoxy benzyl alcohol), SeO_2, NBS(bromination of p-nitrotoluene), Grignard Reaction (preparation of triphenyl carbinol or diphenyl methyl carbinol), Wittig Reaction (preparation of ethyl cinnamate from benzaldehyde), Cannizzaro's reaction (on benzaldehyde) Asymmetric reduction, Phase transfer catalyst isolation of natural products (like Eugenol from cloves, Limonene from orange peels, Trimyristin from nutmeg etc.), photochemical reaction, Peracid and lead tetra acetate oxidation, rearrangement reactions, synthesis of heterocyclic compounds like Hydantoin, thiohydantoin, pyrazolone, Biginelli reaction (synthesis of 4-aryl-3,4-dihydropyrimidinone).