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UNIVERSITY OF MUMBAI

Program : M.Sc.

(Choice Based Credit System)

Course : M.Sc. Organic Chemistry

Part – I

Syllabus for Semester III & IV

(To be implemented from the Academic year 2018-2019)

M.Sc. Organic Chemistry

Semester – III

Course Code: PSCHO301

Paper - I (**Theoretical organic chemistry-I**)

Unit 1 **Organic reaction mechanisms** **[15L]**

1.1 Organic reactive intermediates, methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes and ketenes**.** **[5L]**

1.2 Neighbouring group participation**:** Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, π-electrons, aromatic rings, σ-bonds with special reference to norbornyl and **bicyclo[2.2.2]octyl cation** systems (formation of non-classical carbocation) **[3L]**

1.3 Role of FMOs in organic reactivity**:** Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles, the α effect. **[2L]**

1.4 Pericyclic reactions: Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: **[5L]**

Evidence for the concertedness of bond making and breaking

Symmetry-Allowed and Symmetry-Forbidden Reactions –

- The Woodward-Hoffmann Rules-Class by Class
- The generalised Woodward-Hoffmann Rule

Explanations for Woodward-Hoffmann Rules

- The Aromatic Transition structures [Huckel and Mobius]
- Frontier Orbitals
- Correlation Diagrams, FMO and PMO approach

Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene,

1,3,5 hexatriene and allyl system.

Unit 2 **[15L]**

2.1 **Pericyclic reactions** Cycloaddition reactions: Supra and antra facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes. Diels-Alder reactions, 1, 3-Dipolar cycloaddition and cheletropic reactions, ene reaction, retro-Diels-Alder reaction, regioselectivity, periselectivity, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions. **[7L]**

Other Cycloaddition Reactions- [4+6] Cycloadditions, Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions.

Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions.

2.2 Electrocyclic reactions: Conrotatory and disrotatary motions, 4nπ and (4n+2)π electron and allyl systems. **[3L]**

2.3 Sigmatropic rearrangements: H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy-Cope and aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A. **[5L]**

Unit 3:	**Stereochemistry-I**	**[15L]**
3.1	Classification of point groups based on symmetry elements with examples (nonmathematical treatment).	**[2L]**
3.2	Conformational analysis of medium rings: Eight **to** ten membered rings and their unusual properties**,** I-strain, transannular reactions.	**[3L]**
3.3	Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, **perhydroanthracenes**, steroids, and Bredt's rule.	**[5L]**
3.4	**Anancomeric systems,** Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, elimination, molecular rearrangements, reduction of cyclohexanones **(with LiAlH4, selectride and MPV reduction)** and oxidation of cyclohexanols**.**	**[5L]**

Unit 4	**Photochemistry**	**[15L]**
4.1	Principles of photochemistry: quantum yield, electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), electronic energy transfer: photosensitization and quenching process.	**[3L]**
4.2	Photochemistry of carbonyl compounds:π→´π*, n→´π* transitions, Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, and photochemical rearrangements of α, β-unsaturated ketones cyclohexadienones. Photo Fries rearrangement, Barton reaction.	**[8L]**
4.3	Photochemistry of olefins: cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- π- methane rearrangement including aza-di- π -methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes.	**[2L]**
4.4	Photochemistry of arenes**:** 1, 2- , 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.	**[1L]**
4.5	Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions. Chemiluminescence.	**[1L]**

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25 thStereochemistry, P. S. Kalsi, 4 edition, New Age International Ltd
26 Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
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32 Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.

33 Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34 Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
35 Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
36 Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
37 Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A john Wiley and Sons, Ltd., Publication)

Course Code: PSCHO302

Paper-II

Synthetic Organic Chemistry-I

Unit 1: Name reactions with mechanism and application [15L]

1.1 Mukaiyama esterification, Mitsonobu reaction, Darzen's Glycidic Ester syntheis, Ritter reaction, Yamaguchi esterification, Peterson olefination. **[5L]**

1.2 **Domino reactions**: Characteristics; Nazerov cyclization **[3L]**

1.3 **Multicomponent reactions**: Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, Pictet-Spengler synthesis **[5L]**

1.4 **Click Reactions**: Characteristics; Huisgen 1,3-Dipolar Cycloaddition **[2L]**

Unit 2: Radicals in organic synthesis [15L]

2.1 **Introduction:** Generation, stability, reactivity and structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals. [3L]

2.2 **Radical Initiators**: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide. [1L]

2.3 **Characteristic reactions** - Free radical substitution, addition to multiple bonds. Radical chain reactions, Radical halogenation of hydrocarbons (Regioselectivity),radical cyclizations, autoxidations: synthesis of cumene hydroperoxide from cumene. [4L]

2.4 **Radicals in synthesis**: Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling, C-C bond formation in aromatics: SRNAr reactions. [4L]

2.5 Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation. [3L]

Unit 3: Enamines, Ylides and α-C-H functionalization [15]

3.1 **Enamines:** Generation & application in organic synthesis with mechanistic pathways, Stork enamine reaction. Reactivity, comparison between enamines and enolates. Synthetic reactions of enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines. [4L]

3.2 **Phosphorus, Sulfur and Nitrogen Ylides:** Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination. [6L]

3.3 **α-C-H functionalization:** By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth–Gilbert homologation, Steven's rearrangement. [5L]

Unit 4: Metals / Non-metals in organic synthesis **[15]**

4.1 **Mercury in organic synthesis:** Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics, transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents. [3L]

4.2 **Organoboron compounds:** Mechanism and regiochemistry hydroboration of alkenes and alkynes, asymmetric hydroboration using chiral boron reagents, 9-BBN hydroboration, oxazaborolidine (CBS catalyst) and functional group reduction by diborane. [3L]

4.3 **Organosilicons:** Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes. β-silyl cations as intermediates. Iodotrimethylsilane in organic synthesis. [3L]

4.4 **Silyl enol ethers**: Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions. [2L]

4.5 **Organotin compounds**: Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at the same C atom. [2L]

4.6 **Selenium in organic synthesis:** Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno acetals as α-C-H activating groups [2L]

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- **Organic Electrochemistry,** H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Course Code: PSCHO303
Paper-III
Natural products and Spectroscopy

Unit 1: Natural products-I **[15L]**

1.1 **Carbohydrates:** Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and D-glucosamine (synthesis not expected).Structural features and applications of inositol, starch, cellulose, chitin and heparin**.** [5L]

1.2 **Natural pigments:** General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of β-carotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5-trimethoxyacetophenone. [5L]

1.3 **Insect pheromones:** General structural features and importance. Types of pheromones (aggregation, alarm, releaser, primer, territorial, trail, sex pheromones etc.), advantage of pheromones over conventional pesticides. Synthesis of bombykol from acetylene, disparlure from 6-methylhept-1-ene, grandisol from 2-methyl-1, 3-butadiene**.** [3L]

1.4 **Alkaloids:** Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine. [2L]

Unit 2: Natural products-II **[15L]**

2.1 **Multi-step synthesis of natural products:** Synthesis of the following natural products with special reference to reagents used, stereochemistry and functional group transformations: [8L]

a) Woodward synthesis of Reserpine from benzoquinone
b) Corey synthesis of Longifoline from resorcinol
c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol
d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone and Isobutylene
e) Synthesis of Juvabione from Limonene

f) Synthesis of Taxol.

2.2 **Prostaglandins:** Classification, general structure and biological importance. Structure elucidation of **PGE1**. [2L]

2.3 **Lipids:** Classification, role of lipids, Fatty acids and glycerol derived from oils and fats. [2L]

2.4 **Insect growth regulators:** General idea, structures of JH2 and JH3 . [1L]

2.5 **Plant growth regulators:** Structural features and applications of arylacetic acids, gibberellic acids and triacontanol. Synthesis of triacontanol (synthesis of stearyl magnesium bromide and 12-bromo-1-tetrahydropyranyloxydodecane expected). [2L]

Unit 3: Advanced spectroscopic techniques-I **[15L]**

3.1 **Proton NMR spectroscopy:** Recapitulation, chemical and magnetic equivalence of protons, First order, second order, Spin system notations (A2, AB, AX, AB2, AX2, AMX and A2B2-A2X2 spin systems with suitable examples). Long range coupling (Allylic coupling, 'W' coupling and Coupling in aromatic and heteroaromatic systems), Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents. [7L]

3.2 **^{13}C –NMR spectroscopy:** Recapitulation, equivalent and non-equivalent carbons (examples of aliphatic and aromatic compounds), ^{13}C- chemical shifts, calculation of ^{13}C- chemical shifts of aromatic carbons, heteronuclear coupling of carbon to ^{19}F and ^{31}P. [4L]

3.3 Spectral problems based on UV, IR, ^{1}HNMR and ^{13}CNMR and Mass spectroscopy . [4L]

Unit 4: Advanced spectroscopic techniques-II **[15L]**

4.1 **Advanced NMR techniques:** DEPT experiment, determining number of attached hydrogens (Methyl/methylene/methine and quaternary carbons), two dimensional spectroscopic techniques, COSY and HETCOR spectra, NOE and NOESY techniques. [10L]

4.2 Spectral problems based on UV, IR, ^{1}HNMR, ^{13}CNMR (Including 2D technique) and Mass spectroscopy [5L]

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Course Code: PSCHOEC-I 304

Paper-IV

Medicinal , Biogenesis and green chemistry

Unit 1: Drug discovery, design and development [15L]

1.1 Introduction, important terms used in medicinal chemistry: receptor, therapeutic index, bioavailability, drug assay and drug potency. General idea of factors affecting bioactivity: Resonance, inductive effect, bioisosterism, spatial considerations. Basic pharmacokinetics: drug absorption, distribution, metabolism (biotransformation) and elimination. Physical and chemical parameters like solubility, lipophilicity, ionization, pH, redox potential, H-bonding, partition coefficient and isomerism in drug distribution and drug-receptor binding. Procedures in drug design: Drug [7]

1.2 discovery without a lead: Penicillin, [8L]
Librium. Lead discovery: random screening, non-random (or targeted) screening. Lead modification: Identification of the pharmacophore, Functional group modification. Structure-activity relationship, Structure modification to increase potency and therapeutic index: Homologation, chain branching, ring-chain transformation, bioisosterism, combinatiorial synthesis (basic idea).

Unit 2: Drug design, development and synthesis [15L]

2.1 Introduction to quantitative structure activity relationship studies. QSAR parameters: - steric effects: The Taft and other equations; Methods used to correlate regression parameters with biological activity: Hansch analysis- A linear multiple regression analysis. Introduction to modern methods of drug [5L]

2.2 design and synthesis- computer- [3L]
aided molecular graphics based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design.

2.3 Concept of prodrugs and soft drugs. (a) Prodrugs: Prodrug design, types of [3L]
prodrugs, functional groups in prodrugs, advantages of prodrug use. (b) Soft drugs: concept and properties. Synthesis and application of the following

2.4 drugs: Fluoxetine, cetrizine, [4L]
esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.

Unit 3: Biogenesis and biosynthesis of natural products [15L]

3.1 Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis. [3L]

3.2	Acetate pathway: Biosynthesis of malonylCoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides.	[4L]
3.3	Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic amino acids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isoflavonoids. Mevalonate pathway:	[4L]
3.4	Biosynthesis of mevalonic acid, monoterpenes – geranyl cation and its derivatives, sesquiterpenes – farnesyl cation and its derivatives and diterpenes.	[4L]

Unit 4: Green chemistry **[15L]**

4.1	Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts.	[1L]
4.2	Use of the following in green synthesis with suitable examples: a) Green reagents: dimethylcarbonate, polymer supported reagents. b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts [Aliquat 336, benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride, crown ethers], biocatalysts. c) Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide. d) Solid state reactions: solid phase synthesis, solid supported synthesis	[9L]
4.3	e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions.	[3L]
4.4	f) Ultrasound assisted reactions. Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole. Green Catayst : Nanocatalyst, Types of nanoctalysts, Advantages and Disadvantages of Nanocatalysts, Idea of Magnetically separable nanocatalysts.	[2L]

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24. Enzyme catalysis in organic synthesis, 3rd edition. Edited by Karlheinz Drauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012.
25. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.
26. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
27. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
28. Enzymes: Practical Introduction to structure, mechanism and data analysis, By Robert A. Copeland, Wiley-VCH, Inc.
29. The Organic Chemistry of Biological Pathways By John McMurry, Tadhg Begley by Robert and company publishers
30. Bioorganic Chemistry- A practical approach to Enzyme action, H. Dugas and C. Penny. Springer Verlag, 1931
31. Biochemistry: The chemical reactions in living cells, by E. Metzler. Academic Press.
32. Concepts in biotechnology by D. Balasubrarnanian & others
33. Principals of biochemistry by Horton & others.

34. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
35. Medicinal Natural Products: A Biosynthetic Approach by Paul M. Dewick. 3rd Edition, Wiley.
36. Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B. G. Torssell, Apotekarsocieteten – Swedish pharmaceutical press.
37. Natural products Chemistry and applications, Sujata V Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House.
38. Natural Products Volume- 2, By O. P. Agarwal.
39. Chemistry of Natural Products, F. F. Bentley and F. R. Dollish, 1974.
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41. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.
42. Green Chemistry: An Introductory Text, 2nd Edition, Published by Royal Society of Chemistry, Authored by Mike Lancater.
43. Organic synthesis in water. By Paul A. Grieco, Blackie.
44. Green chemistry, Theory and Practical, Paul T. Anastas and John C. Warner.
45. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2nd edition, Anamaya Publishers, New Delhi.
46. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.
47. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Course Code: PSCHOEC-II 304

~~Paper-IV~~
~~Bioorganic chemistry~~

Unit 1: Biomolecules-I **[15L]**

1.1 Amino acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α- helix, β-sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure. [2L]

1.2 Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation. [3L]

1.3 Structure: Purine & pyrimidine bases, ribose, deoxyribose, nucleosides and nucleotides (ATP, CTP, GTP, TTP, UTP) formation of polynucleotides strand with its shorthand representation**.** [3L]

1.4 RNAs (various types in prokaryotes and eukaryotes) m- RNA and r- RNA – general account , t- RNA-clover leaf model, Ribozymes**.** [2L]

1.5 DNA: Physical properties – Effect of heat on physical properties of DNA (Viscosity, buoyant density and UV absorption), Hyperchromism and Denaturation of DNA. Reactions of nucleic acids (with DPA and Orcinol). [2L]

1.6 Chemical synthesis of oligonucleotides: Phosphodiester, Phosphotriester, [3L]

Phosphoramidite and H- phosphonate methods including solid phase approach.

Unit 2: Biomolecules-II **[15L]**

2.1 Chemistry of enzymes: Introduction, nomenclature, classes and general types of reactions catalyzed by enzymes. Properties of enzymes: a) enzyme efficiency/ catalytic power b) enzyme specificity; Fischer's 'lock and key' and Koshland 'induced fit' hypothesis. Concept and identification of active site. [6L]

2.2 Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition. [4L]

2.3 Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalyzed hydrolysis of a peptide bond. [5L]

Unit 3: Biomolecules - III **[15L]**

3.1 Chemistry of coenzymes. Structure, mechanism of action and bio-modeling studies of the following coenzymes: nicotinamide adenine dinucleotide, flavin adenine dinucleotide, thiamine pyrophosphate, pyridoxal phosphate, Vitamin B12, biotin, lipoic acid, Coenzyme A. [12L]

3.2 Oxidative phosphorylation, chemiosmosis, rotary model for ATP synthesis and role of cytochrome in oxygen activation. [3L]

Unit 4: Biomolecules – IV **[15L]**

4.1 Role of main enzymes involved in the synthesis and breakdown of glycogen. [2L]

4.2 Enzyme catalyzed organic reactions: Hydrolysis, hydroxylation, oxidation and reduction. [6L]

4.3 Enzymes in organic synthesis. Fermentation: Production of drugs/drug intermediates by fermentation. Production of chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics. Synthesis of chemicals via microbial transformation, synthesis of L-ephedrine. Chemical processes with isolated enzymes in free form (hydrocyanation of m-phenoxybenzaldehyde)and immobilized form (production of 6-aminopenicillanic acid). [7L]

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3.Voet, D. and J. G. Voet (2004) Biochemistry, 3rd Edition, John Wiley & sons, Inc. USA.

4. Zubay, Goffrey L; Biochemistry; Wm C. Brown publishers.
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10. D. Astruc, Nanomaterials and Catalysis, Wiley-VCH Verlag GmbH & Co. KGaA, 2008, 1-48;
11. C. N. R. Roa, A. Muller and A. K. Cheetham, The chemistry of Nanomaterials, Wiley-VCH Verlag GmbH & Co. KGaA, 2005, 1-11;
12. The organic chemistry of drug design and drug action, Richard B. Silverman, 2nd edition, Academic Press
13. Medicinal chemistry, D.Sriram and P. Yogeeswari, 2nd edition, Pearson
14. An introduction to drug design-S. S. Pandeya and J. R. Dimmock (New age international)
15. Burger's medicinal chemistry and drug discovery. by Manfred E. Wolf
16. Introduction to Medicinal chemistry. by Graham Patrick
17. Medicinal chemistry-William O. Foye
18. T. B. of Organic medicinal and pharmaceutical chemistry-Wilson and Gisvold's (Ed. Robert F. Dorge)
19. An introduction to medicinal chemistry-Graham L. Patrick, OUP Oxford, 2009.
20. Principles of medicinal chemistry (Vol. I and II)-S. S. Kadam, K. R. Mahadik and K.G. Bothara , Nirali prakashan.
21. Medicinal chemistry (Vol. I and II)-Burger
22. Strategies for organic drug synthesis and design - D. Lednicer Wiley
23. Pharmacological basis of therapeutics-Goodmanand Gilman's (McGraw Hill)
24. Enzyme catalysis in organic synthesis, 3rd edition. Edited by Karlheinz Drauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012.
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27. The Organic Chemistry of Enzyme-Catalysed Reactions, Academic Press, By Richard B. Silverman
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41. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co.
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43. Organic synthesis in water. By Paul A. Grieco, Blackie.
44. Green chemistry, Theory and Practical, Paul T. Anastas and John C. Warner.
45. New trends in green chemistry By V. K. Ahulwalia and M. Kidwai, 2nd edition, Anamaya Publishers, New Delhi.
46. An introduction to green chemistry, V. Kumar, Vishal Publishing Co.
47. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Semester III: Practicals

Course code: PSCHO3P1

Separation of a ternary mixture of organic compounds and identification including derivative preparations using micro-scale technique

1. Separation of a ternary mixture (S-S-S, S-S-L, S-L-L and L-L-L) (for solid mixture: water insoluble/ soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components.
2. Identification of the two components (indicated by the examiner) using micro-scale technique.
3. Preparation of derivatives (any one of separated compound).

(**Minimum 8 experiments**)

Course code: PSCHO3P2

Single step organic preparation(1.0 g scale) involving purification by Steam distillation / Vacuum distillation or Column chromatography.

1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography)
2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation)
3. .Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography)

4. .Preparation of 3-nitroaniline from 1,3-dinitrobenzene. (Purification by column chromatography)
5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation).
6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation).
7. .Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation).
8. .Preparation of phenyl acetate from phenol. (Purification by vacuum distillation)
9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation)
10. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography)
11. Preparation of fluorenone from fluorene. (Purification by column chromatography)
12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation)

(Minimum 8 experiments)

Note:

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

References for Practicals

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
5. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
10. Vogel's Textbook of Practical Organic Chemistry, Fifth edition,2008,

B.S.Furniss, A. J.Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education.
11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
12. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

Semester – IV
Course Code: PSCHO401
Paper - I (**Theoretical organic chemistry-II**)

Unit 1: Physical organic chemistry **[15L]**

1.1 **[7L]**
Structural effects and reactivity**:** Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of σ-values, reaction constants ρ, Yukawa-Tsuno equation**.**

1.2 **[8L]**
Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, σI and σR scales, steric parameters Es and β. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's ET parameter, Solvatochromism Z- scale, Spectroscopic Correlations, Thermodynamic Implications.

Unit 2 Supramolecular chemistry **[15L]**

2.1 **[3L]**
Principles of molecular associations and organizations as exemplified in

2.2 **[3L]**
biological macromolecules like nucleic acids, proteins and enzymes.

2.3 **[5L]**
Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.
Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.

2.4 **[4L]**
Molecular recognition and catalysis, molecular self-assembly.Supramolecular Polymers, Gelsand Fibres.

Unit 3 Stereochemistry- II **[15L]**

3.1 Racemisation and resolution of racemates including conglomerates: **[3L]** Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds. Determination of enantiomer and diastereomer composition:
3.2 enzymatic **[3L]** method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR). Correlative method for configurational assignment: chemical, optical **[4L]** rotation, and NMR
3.3 spectroscopy. Molecular dissymmetry and chiroptical properties: Linearly and circularly **[5L]**
3.4 polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial α–haloketone rule with applications.

Asymmetric synthesis

Unit 4: **[15L]**

4.1 Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, **[3L]** methods of asymmetric induction – substrate, reagent and catalyst controlled reactions.

4.2 Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactions **[9L]** with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantioselective epoxidation, hydroxylation, aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.

4.3 Use of chiral auxiliaries in diastereoselective reductions, asymmetric **[3L]** amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.

REFERENCES:

1 March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons.

2 **th**A guide to mechanism in Organic Chemistry, 6 edition, 2009, Peter Sykes, Pearson education, New Delhi.

3 Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).

4 Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.

5 thOrganic Reaction Mechanism, 4 edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.

6 Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.

7 Organic Chemistry, Part A and B, Fifth edition,2007, Francis A. Carey and Richard J. Sundberg, Springer.

8 Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th. Nelson and Sons Ltd., London 1969.

9 Organic reactive intermediates, Samuel P. MacManus, Academic Press.

10 Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).
11 Organic Chemistry, Seventh Edition, R.T. Morrison, R. N. Boyd & S. K. Bhattacharjee, Pearson.Advanced Organic Chemistry: Reactions & Mechanisms, second edition, B. Miller and R. Prasad, Pearson.
12 Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
13 Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012
14 Organic Chemistry, W. G. Solomons, C. B. Fryhle, , 9th Edition, Wiley India Pvt. Ltd.,2009.
15 Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
16 Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
17 Pericyclic reactions, Ian Fleming, Oxford university press, 1999.
18 Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979.
19 8thOrganic chemistry, edition, John McMurry
20 thModern methods of Organic Synthesis, 4 Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004
21 Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books,2006
22 Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
23 Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.
24 Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit
25 thStereochemistry, P. S. Kalsi, 4 edition, New Age International Ltd
26 Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
27 Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
28 Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
29 Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
30 Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
31 Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley-Eastern
32 Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.
33 Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34 Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
35 Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
36 Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.

37 Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A john Wiley and Sons, Ltd., Publication)

Course Code: PSCHO402
Paper - II (Synthetic organic chemistry-II)

Unit 1: Designing Organic Synthesis-I **[15L]**

1.1 **Protecting groups in Organic Synthesis:** Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications. [3L]

1.2 **Concept of umpolung (Reversal of polarity):** Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers. [3L]

1.3 **Introduction to Retrosynthetic analysis and synthetic planning:** Linear and convergent synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR) importance of order of events in organic synthesis, one and two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds), selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity. [9L]

Unit 2: Designing Organic Synthesis-II **[15L]**

2.1 **General strategy:** choosing a disconnection-simplification, symmetry, high yielding steps, and recognisable starting material. [3L]

2.2 **One group C-C Disconnections:** Alcohols (including stereoslectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. [6L]

2.3 **Two group C-C Disconnections:** 1,2- 1,3- 1,4- 1,5- and 1,6- difunctionalized compounds, Diels-Alder reactions, α, β-unsaturated compounds, control in carbonyl condensations, Michael addition and Robinson annelation. [6L]

Unit 3: Electro-organic chemistry and Selected methods of Organic synthesis **[15L]**

3.1 **Electro-organic chemistry:** [7L]

3.1.1 Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.

3.1.2 Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization.

3.1.3 Anodic oxidation: Oxidation of alkylbezene, Kolbe reaction, Non-Kolbe oxidation, Shono oxidation.

3.2 **Selected Methods of Organic synthesis** [8L]

Applications of the following in organic synthesis:

3.2.1 Crown ethers, cryptands, micelles, cyclodextrins, catenanes.

3.2.2 Organocatalysts: Proline, Imidazolidinone.

3.2.3 Pd catalysed cycloaddition reactions: Stille reaction, Saeguse-Ito oxidation

to enones, Negishi coupling.

3.2.4 Use of Sc(OTf), and Yb(OTf) as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction.

Unit 4: Transition and rare earth metals in organic synthesis [15L]

4.1 **Introduction to basic concepts:** 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion. [3L]

4.2 **Palladium in organic synthesis:** π-bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerisation, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miayura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N, S, or P atoms. [5L]

4.3 **Olefin metathesis** using Grubb's catalyst. [1L]

4.4 **Application of Ni, Co, Fe, Rh, and Cr carbonyls** in organic synthesis. [4L]

4.5 **Application of samarium iodide** including reduction of organic halides, aldehydes and ketones, α-functionalised carbonyl and nitro compounds. [1L]

4.6 **Application of Ce(IV)** in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent**.** [1L]

REFERENCES:

- **Advanced Organic Chemistry,** Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag
- **Modern Methods of Organic Synthesis,** 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
- **Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis,** S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam.
- **Organic Chemistry,** Clayden Greeves Warren and Wothers, Oxford Press (2001).
- **Moder Organic Synthesis: An Introduction,** G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
- **Advanced Organic Chemistry: Reaction Mechanism,** R. Bruckner, Academic Press (2002).
- **Principles of Organic Synthesis,** R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes.
- **Organic Chemistry,** 7th Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson
- **Strategic Applications of Name Reactions in Organic Synthesis**, L. Kurti & B. Czako (2005), Elsevier Academic Press

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- **Organic reactions and their mechanisms,** 3rd revisededition, P.S. Kalsi, New Age International Publishers
- **Organic Synthesis: The Disconnection Approach,** Stuart Warren, John Wiley & Sons, 2004
- **Name Reactions and Reagents in Organic Synthesis,** 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
- **Name Reactions,** Jie Jack Lie, 3rd Edn., Springer
- **Organic Electrochemistry,** H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Course Code: PSCHO403
Paper - III (Natural products and heterocyclic chemistry)

Unit 1: **Natural products-III** **[15L]**

1.1 **Steroids:** General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acids. [5L]

1.2 1.3 Synthesis of 16-DPA from cholesterol and plant sapogenin. [2L]
Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone. [5L]

1.4 Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone. [3L]

Unit 2:

2.1 **Natural products-IV** **[15L]**

Vitamins: Classification, sources and biological importance of vitamin B1, B2, B6, folic acid, B12, C, D1, E (α-tocopherol), K1, K2, H (β- biotin). [5L]
Synthesis of the following:
Vitamin A from β-ionone and bromoester moiety.
Vitamin B1 including synthesis of pyrimidine and thiazole moieties
Vitamin B2 from 3, 4-dimethylaniline and D(-)ribose
Vitamin B6 from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethyl ester of N-formyl-DL-alanine (Harris synthesis)
Vitamin E (α-tocopherol) from trimethylquinol and phytyl bromide
Vitamin K1 from 2-methyl-1, 4-naphthaquinone and phytol.

2.2 **Antibiotics:** Classification on the basis of activity. Structure elucidation, spectral data of penicillin-G, cephalosporin-C and chloramphenicol. [6L]
Synthesis of chloramphenicol (from benzaldehyde and β-nitroethanol) penicillin-G and phenoxymethylpenicillin from D-penicillamine and t-butyl phthalimide malonaldehyde (synthesis of D-penicillamine and t-butyl phthalimide malonaldehyde expected).

2.3 **Naturally occurring insecticides:** Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I. [2L]

2.4 **3.4 Terpenoids**: Occurrence, classification, structure elucidation, [2L]

stereochemistry, spectral data and synthesis of zingiberene .

Unit 3: **Heterocyclic compounds-I** **[15L]**

Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch-Widman) and replacement nomenclature) Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazines, pyrimidine, pyrazines and oxazines.

Unit 4: **Heterocyclic compounds-II** **[15L]**

Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6 Membered) fused heterocycles (up to three hetero atoms)**.** (Common, systematic (Hantzsch-Widman) and replacement nomenclature) Nucleophilic ring opening reactions of oxiranes, aziridines, oxetanes and azetidines. Structure, reactivity, synthesis and reactions of coumarins, quinoxalines, cinnolines, indole, benzimidazoles, benzoxazoles, benzothiazoles, Purines and alkaloids.

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3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
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42. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., .3122
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46. Alkaloids,V.K. Ahuluwalia,Ane Books Pvt.Ltd.
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Course Code: PSCHOOC-I 404

Paper – IV (INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS)

Unit 1: **[15L]**

Introduction to Intellectual Property: [2L]

Historical Perspective, Different types of IP, Importance of protecting IP.

Patents: [5L]

Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.

Industrial Designs: [2L]

Definition, How to obtain, features, International design registration.

Copyrights: [2L]

Introduction, How to obtain, Differences from Patents.

Trade Marks: [2L]

Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.

Geographical Indications: [2L]

Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit 2: [15L]

Trade Secrets: [2L]

Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.

IP Infringement issue and enforcement: [2L]

Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.

Economic Value of Intellectual Property: [2L]

Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.

Different International agreements:

(a) World Trade Organization (WTO): [5L]

(i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement

(ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.

(iii) Berne Convention

(iv) Budapest Treaty

(b) Paris Convention [6L]

WIPO and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.

Unit III: Introduction to Cheminformatics: History and evolution of [15L]

cheminformatics, Use of Cheminformatics, [5L]
Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions:

Nomenclature, Different types of notations, SMILES coding, Matrix [5L]
representations, Structure of Molfiles and Sdfiles, Libraries and toolkits,
Different electronic effects, Reaction classification.

Searching Chemical Structures:

Full structure search, sub-structure search, basic ideas, similarity [5L]
search,
three dimensional search methods, basics of computation of physical and
chemical data and structure descriptors, data visualization.

Unit IV: [15L]

Applications:

Prediction of Properties of Compound, Linear Free Energy Relations,

Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design.

REFERENCES:

1. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley–VCH
3. Gupta, S. P. *QSAR and Molecular Modeling.* Springer-Anamaya Pub.: New Delhi.

Course Code: PSCHOOC-II 404

PAPER – IV: RESEARCH METHODOLOGY

[15L]

Unit 1:

[5L]

Print:

Primary, Secondary and Tertiary sources.

Journals:

Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: [5L]

Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.

Information Technology and Library Resources: [5L]

The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.

[15L]

Unit II: DATA ANALYSIS

The Investigative Approach:

Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.

Analysis and Presentation of Data:

Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.

[15L]

Unit III: METHODS OF SCIENTIFIC RESEARCH AND WRITING

SCIENTIFIC PAPERS

Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.

Writing Scientific Papers:

Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.

Unit IV: CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS [15L]

Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressur, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

REFERENCES:

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4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6th Ed., Freeman Chapters 3-5
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Semester IV: Practicals
Course code: PSCHO4P1

Two steps preparations

1. Acetophenone → Acetophenone phenyl hydrazine → 2-phenyl

indole.

2. 2-naphthol → 1-phenyl azo-2-naphthol → 1-amino-2-naphthol.
3. Cyclohexanone → cyclohexanone oxime → Caprolactum.
4. Hydroquinone → hydroquinone diacetate → 2,5-dihydroxyacetophenone.
5. 4-nitrotoluene → 4-nitrobenzoic acid → 4-aminobenzoic acid.
6. *o*-nitroaniline → *o*-phenylene diamine → Benzimidazole.
7. Benzophenone → benzophenone oxime → benzanilide.
8. *o*-chlorobenzoic acid → N-phenyl anthranilic acid → acridone.
9. Benzoin → benzil → benzilic acid.
10. Phthalic acid → phthalimide → anthranilic acid.
11. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-methyl-7-acetoxy coumarin.
12. Anthracene → anthraquinone → anthrone.

(Minimum 8 experiments)

Note:

1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS** (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.
2. Students are expected to purify the product by recryllization, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

Course code: PSCHO4P2

Session-I: Combined spectral identification: Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra).

A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete structure of the compound may then be elucidated by referring to any standard text-book/reference material etc (**Minimum 8 spectral analysis).**

Session-II: Project evaluation

References for Practicals

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.
K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
5. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall

7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath. 8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold. 9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold. 10. Vogel's Textbook of Practical Organic Chemistry, Fifth edition,2008, B.S.Furniss, A. J.Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education. 11. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers. 12. Organic structures from spectra, L. D. Field, S. Sternhell, John R.

Kalman, Wiley, 4th ed., 2011.

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.