Rayat Shikshan Sanstha's

Karmaveer Bhaurao Patil College Vashi, Navi Mumbai

Autonomous College

[University of Mumbai]

Syllabus for Approval

M.Sc.-II Organic Chemistry

Sr. No.	Heading	Particulars
1	Title of Course	M.Sc.-II Organic Chemistry
2	Eligibility for Admission	M.Sc.-I
3	Passing Marks	Minimum 'D' Grade or equivalent minimum marks for passing at the M.Sc.-I level.
4	Ordinances/Regulations (if any)	
5	No. of Years/Semesters	One year/Two semester
6	Level	P.G. Part-II
7	Pattern	Semester
8	Status	New
9	To be implemented from Academic year	2019-2020

AC – 02/03/2019
Item No. 2.10

Rayat Shikshan Sanstha's

KARMAVEER BHAURAO PATIL COLLEGE, VASHI.

NAVI MUMBAI

(AUTONOMOUS COLLEGE)

Sector-15- A, Vashi, Navi Mumbai - 400 703

Syllabus for M.Sc.-II Organic Chemistry

Program: M.Sc.

Course: M.Sc.-II Chemistry

(Choice Based Credit, Grading and Semester System with effect from the academic year 2019-2020)

Title of Specific Program:

M.Sc. Organic Chemistry

Program Specific Outcomes:

1. To demonstrate knowledge and understanding in their main field of Organic Chemistry, including both broad knowledge in the field and substantially deeper knowledge of certain parts of the Analytical Chemistry, together with deeper insight into current research and development work.
2. To demonstrate deeper methodological knowledge in Organic Chemistry.
3. To be able to independently pose and analyze questions of chemical relevance and, through experiments, computer calculations, and information retrieval, collect sufficient information to suggest an answer, even if full information is lacking.
4. Off assessments in their main field of study, taking into account relevant scientific, social and ethical aspects, and demonstrate an awareness of ethical aspects of research and development in Organic Chemistry.
5. To demonstrate insight into the potential and limitations of organic chemistry, its role in society and people's responsibility for how it is used.
6. To identify their need of further knowledge and to take responsibility for developing their Organic Chemistry knowledge.
7. To learn various concepts of organic, inorganic, physical chemistry, their biological aspects and their application in day-to-day life.
8. Competent to take challenging positions in industry, academics and government sectors by learning various analytical techniques such as UV, IR, NMR, Chromatography etc and their applications
9. To execute new ideas in the field of research and development using principles and techniques of science learned through seminars and the dissertation.

Course Code	Title of Course	Unit	Course Outcome
			After successful completion of each course in Chemistry a learner should be able to;
Semester-III			
PGCHO301		Organic reaction mechanisms	1. To describe, exemplify and classify the reaction intermediate [2] 2. To interpret by giving examples of the Neighbouring group participation [4] 3. To know the Banana bonding. [1] 4. To describe, exemplify, classify and investigate the product of Pericyclic reactions, [2] 5. To study Sigmatropic rearrangements, Cycloaddition reactions [2] 6. To summarize Woodward-Hoffmann Rules [2] 7. To Study Conformation analysis cyclohexane ring and their reactions [2] 8. To describe, explain and illustrate [2] 9. Photochemical behaviour of carbonyl compound, olefins [2]
		Pericyclic reactions	1. To describe Cycloaddition reaction [2] 2. To study the Supra and antra facial additions [2] 3. To explain the Diels-Alder reactions [3] 4. To study the regioselectivity, periselectivity, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions [2] 5. To study the Other Cycloaddition Reactions [2] 6. Electrocyclic reactions: Conrotatory and disrotatary motions, [2] 7. 4nπ and (4n+2)π electron and allyl systems. [2] 8. To know the Sigmatropic rearrangements 9. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A. [2]
		Stereochemistry-I	1. To describe, Conformation analysis cyclohexane ring and their reactions [2] 2. To Describe the Conformational analysis of medium rings: Eight to ten membered rings [2] 3. To know the Stereochemistry of fused ring and bridged ring compounds [1] 4. To explain the Anancomeric systems**,** [3] **5.** Effect of conformation on reactivity of cyclohexane [2] 6.To study the decalins hydrindanes, perhydroanthracenes, steroids, [2] 7. To know Bredt's rule. [1]

		Photochemistry	1. To describe Principles of photochemistry [2] 2. To study the Jablonski diagram [2] 3. To explain the electronic energy transfer: photosensitization and quenching [2] 4. To Study Norrish- I and Norrish-II cleavages [1] 5. To know the Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of α, β-unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction [2] 6. To explain the Photochemistry of olefins: cis-trans isomerizations [2] 7. To study the Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes. [2] 8. To explain the Photochemistry of arenes**:** 1, 2- , 1, 3- and 1, 4- additions [2] 9. To know the Photocycloadditions of aromatic Rings [2] 10. To explain the Singlet oxygen and photo-oxygenation reactions [2] 11. To Study the Chemiluminescence. [2]
PGCHO302		Name reactions with mechanism and application	1. To describe, exemplify, investigate the product of reaction and construct the mechanism of various rearrangement reactions, [2] 2. Multicomponent reactions and click reactions, reactions involving free radicals. [1] **3.** To enlist, exemplify and **4.** Discuss the use of various organometallic compounds, ylides in organic synthesis. [3] 5. To make the use of the basic knowledge of various reactions, reagents and [3] 6. Organometallic compound to Plan for the research project [3] 7. To know the **Domino reactions**: Characteristics; Nazerov cyclization [2] 8. To Study the **Multicomponent reactions**: Strecker Synthesis, Ugi [2] 9. To Explain the Characteristics; Huisgen 1,3-Dipolar Cycloaddition [2] 10. To Apply for various reactions [3]
		Radicals in organic synthesis	1. To Study Generation, stability, reactivity and structural [2] 2. To Know the stereochemical properties of free radicals, [2] 3. To study the Persistent and charged radicals [2] 4. To Explain the Electrophilic and nucleophilic radicals [2] 5. To know the azobisisobutyronitrile (AIBN) and dibenzoyl peroxide [2] 6. To know the Free radical substitution, addition to multiple [2] 7. To know the radical cyclizations, autoxidations:

			synthesis of cumene hydroperoxide from cumene. [2] 8. To explain the Ulmann coupling,Gomberg coupling Applications [2] 9. To apply the Hunsdiecker reaction, McMurry coupling [3] 10. To study the Acyloin condensation. , Glaser coupling, Corey-House synthesis [2]
		Enamines, Ylides and α-C-H functionalization	1. To Study Generation & application in organic synthesis with mechanistic [2] 2. To know the Stork enamine reaction. [2] 3. To study the eactivity, comparison between [2] 4. To know the Synthetic reactions of enamines [2] 5. To explain the including asymmetric reactions of chiral enamines derived from chiral secondary amines. [3] 6. To study Phosphorus, Sulfur and Nitrogen Ylides [2] 7. To know the Preparation and their synthetic [1] 8. To study the Wittig reaction, [2] 9. To Explain the Horner-Wadsworth-Emmons Reaction, [2] 10. To know the Barton-Kellogg olefination. [2] 11. To explain the **α-C-H functionalization:** By nitro, sulfoxide [2] 12. To know the generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. [2] 13. To explify the Bamford-Stevens reaction, Julia olefination and its modification, [2] 14. To know the Seyferth-Gilbert homologation, Steven's rearrangement [1]
		Metals / Non-metals in organic synthesis	1. To Study Mercury in organic synthesis [2] 2. To explain the oxymercuration and demercuration of alkenes, [2] 3. mercuration of aromatics, transformation of aryl mercurials to aryl halides. [2] 4. To know the Organomercurials as carbene transfer reagents. [1] 5. To study the **Organoboron compounds:** Mechanism [2] 6. To study the asymmetric hydroboration using chiral boron reagents, 9-BBN hydroboration [2] 7. To know the functional group reduction by diborane [1] 8. To explain the functional group reduction by diborane [3] 9. To know the preparation and important bond-forming reactions of alkyl silanes, [1] 10. alkenyl silanes, aryl silanes and allyl silanes. β-silyl cations as intermediates. Iodotrimethylsilane in organic synthesis [2] 11. To explain the Silyl enol ethers: Application [3]

			12. To know the Organotin compounds: Preparation of alkenyl [1] 13. To study Selenium in organic synthesis: Preparation of selenols/selenoxide [2]
PGCHO303		Natural products-I	1. To describe, exemplify, classify and draw structures [2] 2. To study Synthesis of the Carbohydrates, [2] 3. To know Natural pigments, Insect pheromones, [1] 4. To Study alkaloids. Lipids, prostaglandins [2] 5. To study Structure elucidation of β- carotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5- trimethoxyacetophenone. [2] 6. To know the **Insect pheromones:** General structural features and importance [1] 7. To study the **Alkaloids:** Occurrence and physiological importance of morphine [2] 8. To study the Structure elucidation, spectral data and synthesis of coniine [2]
		Natural products-II	1. To describe, Multi-step synthesis of natural products [2] 2. To Know natural products with special reference to reagents used, stereochemistry and functional group transformations [1] 3. To Study Woodward synthesis of Reserpine from benzoquinone [2] 4. To Explain Synthesis of cefalosphorine [3] 5. To explain the Gilbert-Stork synthesis of Griseofulvin from phloroglucinol [3] 6. To know the Synthesis of Fedricamycine) [1] 7. To explain the Synthesis of Juvabione from Limonene [3] 8. To study the Synthesis of Taxol. [2] 9. To study the **Prostaglandins:** Classification, general structure [2] 10. To know the **Lipids:** Classification, role of lipids, Fatty acids and glycerol [1] 11. To study the **Insect growth regulators:** General idea, structures of JH2 and JH3 [2] 12. To write Multi-step synthesis of natural products [2]
		Advanced Spectroscopic Techniques-I	1. To describe, **Proton NMR spectroscopy:** Recapitulation structures [2] 2. To study equivalence of protons, First order, second order, [2] 3. To know Spin system notations (A2, AB, AX, AB2, AX2, AMX and A2B2-A2X2 spin systems with suitable examples). [1] 4. To know Long range coupling (Allylic coupling, 'W' coupling and Coupling in aromatic and heteroaromatic systems), [1] 5. To study Temperature effects, Simplification of complex spectra, [2] 6. To explain nuclear magnetic double resonance, [3]

			7. To study chemical shift reagents. [2] 8. To study the **13C -NMR spectroscopy:** Recapitulation, equivalent and non-equivalent [2] 9. To study the 13C- chemical shifts of aromatic carbons, heteronuclear [2] 10. To know Spectral problems based on UV, IR, 1HNMR [4]
		Advanced Spectroscopic Techniques-II	1. To know the **Advanced NMR techniques:** DEPT experiment, determining number attached hydrogens (Methyl/methylene/methine and quaternary carbons), [1] 2. To study two dimensional spectroscopic techniques, [2] 3. To explain the COSY and HETCOR spectra, NOE and NOESY techniques. [3] 4. Spectral problems based on UV, IR, 1HNMR, 13CNMR (Including 2D technique) and Mass spectroscopy [4]
PGCHO EC-II 304	**Course Code: PSCHOEC-I 304 Paper-IV Medicinal, Biogenesis and green chemistry**	**Drug discovery, design and development**	1. To know about medicinal chemistry, [1] 2. to explain, describe and illustrate [3] 3. To know basic pharmacokinetics as well as different procedures [1] 4. To know modifications in drug designing [1] 5. Procedures in drug design: Drug discovery without a lead: Penicillin, [2] 6. To study the Librium. Lead discovery: random screening, non-random (or targeted) screening. Lead modification: [2] 7. To explain the Identification of the pharmacophore, Functional group modification. Structure-activity relationship, [2] 8. To know the Structure modification to increase potency and therapeutic index: Homologation, chain branching, ring-chain [2] 9. To study transformation, bioisosterism, combinatiorial synthesis (basic idea). [2]
		Polymer chemistry	1. To know and describe chain growth and free radical polymerization, [2] 2. To illustrate its mechanism, to interpret stereochemistry [4] 3. kinetics of polymerization and to determine the molecular weights of different polymers [2] 4. To Study mechanistic details, kinetics, energetics of polyreactions. [2] 5. To know recent developments and important examples. [1] 6. To study Macromolecules: Number-average [2] 7. To study Chain-growth polymerizations: [2] 8. To know Radical, anionic, cationic, Ziegler/Natta, ring [2]
		Biogenesis and biosynthesis of natural products	1. To know and describe the primary and secondary metabolites, [1] 2. To explain the Primary and secondary metabolites

			and the building blocks, general pathway of amino acid biosynthesis. [2] 3. To know Shikimic Acid pathway: Biosynthesis of shikimic acid, [2] 4. To study aromatic amino acids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isofalvonoid [2] 5. To know Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes - [2] 6. To explain the geranyl cation and its derivatives, sesquiterpenes - [2] 7. To know the farnesyl cation and its derivatives and diterpenes. sesterpenes, triterpenes, steriods. [2]
		Green chemistry	1. To take review of green principles, to exemplify and explain various green reagents, [5] 2. To know green catalysts ,and green solvents , [1] 3. to compare and illustrate the use of green method of synthesis over traditional method of synthesis, [5] 4. to plan and design new synthesis by using green technologies. [3] 5. To know the Green Cataysts : Nanocatalyst, Types of nanoctalysts, Advantages and [2] 6. To study the Disadvantages of Nanocatalysts, Idea of Magnetically separable nanocatalysts [2] 7. To know the Solid state reactions: solid phase synthesis, solid supported synthesis [2] 8. To explain the Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions [2] 9. To know Comparison of traditional processes versus green processes in the syntheses [2] 10. To explain the Green Cataysts : Nanocatalyst, Types of nanoctalysts, [2]
PGCHOP301			1.To know Separation of a ternary mixture of organic compounds and identification [2] 2.To study Separation of a ternary mixture (S-S-S, S-S-L, S-L-L and L-L-L) [2] 3.To know Identification of the two components using micro-scale technique. [2] 4.To know the derivative preparations using micro-scale technique [2]
PGCHOP302			1. To know the planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS [2] 2. To know the possible mechanism, expected spectral data [2] 3. 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. [2]

			4. Single step organic preparation (1.0 g scale) involving purification by Steam distillation / Vacuum distillation or Column chromatography. [2]

***Note: [1]: Remembering, [2]: Understanding, [3]: Applying, [4]: Analysing, [5]: Evaluating, [6]: Creating**

Scheme of Examination for Each Semester:

Continuous Internal Evaluation: 40 Marks (Common Written Test-20 Marks & 20 Marks For- Seminar, Assignment, Projects, Group discussion, Open book test, online test, Industrial visits, etc.)

Semester End Examination: 60 Marks will be as follows -

I.	**Theory:**	
	Each theory paper shall be of two- and half-hour duration.	
	All questions are compulsory and will have internal options.	
	Q – I	From Unit – I (having internal options.) 12 M
	Q – II	From Unit – II (having internal options.) 12 M
	Q – III	From Unit – III (having internal options.) 12 M
	Q – IV	From Unit – III (having internal options.) 12 M
	Q – V	Questions from all the FOUR Units with equal weightage of marks allotted to each unit 12M
II.	**Practical**	following scheme.

Sr. No.	**Particulars of External Practical Examination**	**Marks%**
1	Laboratory Work	80
2	Journal	10
3	Viva	10
	TOTAL	**100**

Choice Based Credit, Grading and Semester System with effect from the academic year 2019-2020

M.Sc.-II Organic Chemistry

Semester - III

Course Code	Unit	Topics	Credits	L/Week
PGCHO301	I	ORGANIC REACTION MECHANISMS	4	1
	II	PERICYCLIC REACTIONS		1
	III	STEREOCHEMISTRY-I		1
	IV	PHOTOCHEMISTRY		1
PGCHO302	I	NAME REACTIONS WITH MECHANISM AND APPLICATION	4	1
	II	RADICALS IN ORGANIC SYNTHESIS		1
	III	ENAMINES, YLIDES AND A-C-H FUNCTIONALIZATION		1
	IV	METALS / NON-METALS IN ORGANIC SYNTHESIS		1
PGCHO303	I	NATURAL PRODUCTS-I	4	1
	II	NATURAL PRODUCTS-II		1
	III	ADVANCED SPECTROSCOPIC TECHNIQUES-I		1
	IV	ADVANCED SPECTROSCOPIC TECHNIQUES-II		1
PGCHO304	I	DRUG DISCOVERY, DESIGN AND DEVELOPMENT	4	1
	II	Polymer Chemistry		1
	III	BIOGENESIS AND BIOSYNTHESIS OF NATURAL PRODUCTS		1
	IV	GREEN CHEMISTRY		1
PGCHOP301 PGCHOP302	-	Practical Course	8	16

Note: 1. Blue Highlighted Topic / Course has focus on employability/ entrepreneurship/skill development

2. Yellow Highlighted Topic / Course is related to professional ethics, gender, human values, Environment & sustainability

M.Sc. Organic Chemistry

Semester - III
Course Code: PGCHO301
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 an chimeric 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 NGP by cyclopropyl ring,Pinacol rearrangement reaction, \Concept of Banana bonding

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 -

i. The Woodward-Hoffmann Rules-Class by Class

ii. The generalized Woodward-Hoffmann Rule

Explanations for Woodward-Hoffmann Rules

i. The Aromatic Transition structures [Huckel and Mobius]

ii. Frontier Orbitals

iii. 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 **Pericyclic reactions** **[15L]**

2.1 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, Ketene 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 oxyCope 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	Conformation analysis cyclohexane ring and their reactions	
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 $LiAlH_4$, 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: $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of α, β-unsaturated ketones and 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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2 A guide to mechanism in Organic Chemistry, 6th 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 Organic Reaction Mechanism, 4th 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.

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17 Pericyclic reactions, Ian Fleming, Oxford university press, 1999.
18 Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979.
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20 Modern methods of Organic Synthesis, 4th 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 Stereochemistry, P. S. Kalsi, 4th 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: PGCHO302

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
Ulmann coupling,Gomberg coupling Applications [4L]

2.5 Hunsdiecker reaction, McMurry coupling, [3L]
Acyloin condensation. , Glaser coupling, Corey-House synthesis

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 of 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]

References

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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) Synthesis of cefalosphorine.
c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol
d) Synthesis of Fedricamycine)
e) Synthesis of Juvabione from Limonene

f) Synthesis of Taxol.

2.2 **Prostaglandins:** Classification, general structure and biological importance. Structure elucidation of **PGE_1**. [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 JH_2 and JH_3 . [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 (A_2, AB, AX, AB_2, AX_2, AMX and A_2B_2-A_2X_2 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. [7] [8L]

1.2 Procedures in drug design: Drug discovery without a lead: Penicillin, 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, combinatiorial synthesis (basic idea).

Unit 2: **Polymer chemistry** [5L]

2.1 Chain-growth polymerizations: Radical, anionic, cationic, Ziegler/Natta, ring opening. 'living' methods (group transfer polymerization, nitroxide [5L]

2.2 Mediated free radical polymerization, atom transfer radical polymerization), mechanistic details, kinetics, energetics of polyreactions. recent developments and important examples.Macromolecules : Number-average and weight-average molecular weights. Determination of molecular weights. [5L]

2.3 Kinetics of polymerisation. Stereochemistry and mechanism of polymerisation.

Unit 3: **Biogenesis and biosynthesis of natural products**

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

[3L]

3.2 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 isofalvonoids. [5L]

3.3 Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes - geranyl cation and its derivatives, sesquiterpenes - farnesyl cation and its derivatives and diterpenes. sesterpenes, triterpenes, steriods. [7L]

Unit 4: Green chemistry

4.1 Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts. **[15L]** [1L]

4.2 Use of the following in green synthesis with suitable examples: [7L]

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

e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions.

f) Ultrasound assisted reactions.

4.3 Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole. [3L]

4.4 Green Catayst : Nanocatalyst, Types of nanoctalysts, Advantages and Disadvantages of Nanocatalysts, Idea of Magnetically separable nanocatalysts. [3] [2L]

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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), Hypochromism, 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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47. Organic synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.

Semester III: Practicals
Course code: PGCHO3P1

Part A Separation of a ternary mixture of organic compounds and identification

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.

Part B derivative preparations using micro-scale technique

3. Preparation of derivatives (any one of separated compound).

(**Minimum 8 experiments**)

Course code: PGCHO3P2

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.

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 Vaniline alchohol from vaniline using sodium borohydride.
3. Preparation of Benzoic acid and benzyl achohol using Cannizarro reaction.

4.Preparation of Preparation oof Coumarin using Peachman condensation.

5. Preparation of Benzaminde using Beckmann rearrangement.
6. .Preparation of Schiff base from aromatic aldehyde.
7. Preparation of Dibezilidine acetone using Aldol condensation
8. Triphenyl or diphenyl methyl carbinol (Grignard reaction)
9. Benzotriazole
10. 1-Phenyl-3-methyl pyrazol-5-one
11. Glucose pentaacetate
12. 2,4-diethoxycarbonyl-3,4-dimethyl pyrrole from ethyl acetoacetate
13. Quinoline from aniline Skraup synthesis)
14. Benzimidazole from benzyl 21. Cyclohexanol from cyclohexanone (LAH reduction)
15. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation)
16. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography)
17. Preparation of fluorenone from fluorene. (Purification by column chromatography)
18. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation)

Note: (Minimum 8 experiments)

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,

11. Practical organic chemistry by F.G.Mann and B.S. Saunders, Orient Longman, fourth edition, 2004.
12. 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.

Note:

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.

Course Code	Title of Course	Unit	Course Outcome
			After successful completion of each course in Chemistry a learner should be able to;
SEMESTER-IV			
PGCHO401		PHYSICAL ORGANIC CHEMISTRY	1.To know Physical organic chemistry [2] 2.To know Structural effects and reactivity [2] 3.To paraphrase Uses of Hammett equation [2] 4.To know Problems based on Hammett Equation and sigma and rho [2] 5.To know the Uses of Hammett equation, deviations from Hammett equation [2] 6.To Explain the parameter correlations, Inductive substituent constants. The Taft model, [2] 7.To study parameters Es and β. [2] 8.To know Solvent effects, Okamoto-Brown equation, Swain-Scott equation.[2] Problems based on hammet equation and sigma and rho [4]
		Supramolecular chemistry	1. To know Principles of molecular associations and organizations as exemplified in [2] 2. To study biological macromolecules like nucleic acids, proteins and enzymes [2] 3. To know Synthetic molecular receptors: [2] 4. To explain receptors with molecular cleft, molecular [2] 5. To explain the tweezers, receptors with multiple hydrogen sites [2] 6. To study Structures and properties of crown ethers, cryptands, cyclophanes [2] 7. To explify the calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers [2] 8. To study cryptands and calixarenes.applications in synthetic chemistry [2]

		Stereochemistry- II	1. To study the Racemisation and resolution of racemates including conglomerates [2] 2. To know Mechanism of racemisation, methods of resolution: [2] 3. To study mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds. [2] 4. To study chromatographic methods. Methods based on NMR spectroscopy: [2] 5. To know use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR). Coupling constant [2] 6. To study Correlative method for configurational assignment [2] 7. To know Molecular dissymmetry and chiroptical properties: [2] 8. To study the Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. [2] 9. To know The octant rule [2] 10. α- haloketone rule wit applications.Problems based on ORD and CD [2]
		Asymmetric synthesis	**1.** To know Principles of asymmetric synthesis: Introduction, the chiral pool in Nature [2] **2.** To study the substrate, reagent and catalyst controlled reactions. [2] **3.** To study Synthesis of L-DOPA [Knowles's Mosanto process]. [2] **4.** To explain the Aldol and related reactions, Cram's rule, Felkin-Anh model, [2] **5.** To study Sharpless enantioselective epoxidation, [2] **6.** To know hydroxylation, amino hydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins. [2] **7.** To know Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations [2]
PGCHO402		Designing Organic Synthesis-I	1.To know Protecting groups in Organic Synthesis [2] 2.To study Concept of umpolung (Reversal of polarity) [2] 3.To know the hydroxyl, carbonyl, [2] 4.To study amino and carboxyl functional groups and its applications [2] 5.To explain the **Concept of umpolung (Reversal of polarity):** Generation of acyl anion [2] 6.To explain the 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers. [2] 7. To know two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds), selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity,

			enantioselectivity [2]
		Designing Organic Synthesis-II	1. To know Introduction to Retrosynthetic analysis and synthetic planning [1] 2. To prepare a General strategy of synthesis [3] 3. To study One group C-C Disconnections: [2] 4. To know Two group C-C Disconnections [2] 5. To study Two group C-C Disconnections: 1,2- 1,3- 1,4- 1,5- and 1,6 [2] 6. To know difunctionalized compounds, Diels-Alder reactions, α, β-unsaturated compounds, control in carbonyl condensations, Michael addition and [2] 7. To explain Robinson annelation [2]
		Electro-organic chemistry and Selected methods of Organic synthesis	1. To know Electrode potential [2] 2. To know Selected Methods of Organic synthesis [2] 3. To study Use of Sc(OTf), and Yb(OTf) [2] 4. To prepare a Transition and rare earth metals in organic synthesis [2] 5. To study Use of Sc(OTf), and Yb(OTf) as water tolerant Lewis acid catalyst in aldol [2] 6. To carry condensation, Michael reaction, Diels-Alder reaction, Friedel - Crafts reaction. [3] 7. To analyse Pd catalysed cycloaddition reactions: [3] 8. To study Stille reaction, Saeguse-Ito oxidation [2] 9. To know to enones, Negishi coupling [2] To explain Organocatalysts: Proline, Imidazolidinone. applications in synthetic chemistry [2]
		Transition and rare earth metals in organic synthesis	1. To know Palladium in organic synthesis [1] 2. To study Palladium in organic synthesis [2] 3. To study Application of Ni, Co, Fe, Rh, and Cr carbonyls [2] 4. To study Application of samarium iodide [2] 5. To study Application of samarium iodide [2] 6. Application of Ce(IV) in synthesis of heterocyclic quinoxaline derivatives [3] 7. Its role as a de-protecting agent [2]
PGCHO403	**Paper - III (Natural products and heterocyclic chemistry)**	Natural products-III	1.To study Natural products [2] 2.To know Steroids [1] 3.To study Synthesis of 16-DPA from cholesterol and plant sapogenin [2] 4.To study Synthesis of cinerolone, [2] 5.To study jasmolone, allethrolone, exaltone and muscone [2] 6.To carry Synthesis of the: androsterone, testosterone, [2] 7.To study oestrone, oestriol, oestradiol and progesterone [2]
		Drug design, development and synthesis	1. To study Introduction to quantitative structure activity relationship studies [2] 2. To study QSAR [2] 3. To know Introduction to modern methods of drug

			design and synthesis [2] 4. To study Concept of prodrugs and soft drugTo know Synthesis and application of the following drugs: [2] 5. To study Fluoxetine, cetrizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate [2]
		Heterocyclic compounds-I	1. To study Heterocyclic compounds, pyrazole, imidazole, [2] 2. To know oxazole, isoxazole, [2] 3. To study thiazole, isothiazole, pyridazines, [2] 4. To Study pyrimidine, [2] To apply pyrazines and oxazines [3]
		Heterocyclic compounds-II	1. To study coumarins, [2] 2. To know Quinoxalines [2] 3. To study cinnolines, [2] 4. To understand indole,benzimidazoles, [2] 5. benzoxazoles, [2] 6. To Study Purines and acridines, benzothiazoles, stereochemistry, spectral data and synthesis of zingiberene. [2]
PGCHO404	Research methodology	**Print:**	1.To know Primary, Secondary and Tertiary sources [2] 2.To study Journal abbreviation and journals [2] 3.To know Web sources, E-journals, Journal acces [2] 4.To study ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus [2] 5.To describe Information Technology and Library Resources [2] 6.To describe the Internet and World wide web, Internet resources for Chemistry, finding and citing published information. [2]
		METHODS OF SCIENTIFIC RESEARCH AND WRITING	1. To describe SCIENTIFIC PAPERS [2] 2. To study Justification for scientific contributions, bibliography, description of methods, conclusions, [2] 3. To know the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism [2]
		Intellectual Property Right:	1. To know Historical Perspective [2] 2. To know Importance of protecting IP [2] 3. To study Industrial Designs: Definition, How to obtain, features, International design registration. [2] 4. To study Copyrights [2] 5. To know differences from Patents. Trade Marks: Introduction [2] 6. To study Geographical Indications: Definition, rules for registration, prevention of illegal exploitation, importance to India. [2]

		Chemical Safety and Ethical Handling of Chemicals	1. To describe Safe working procedure in laboratories, safe storage and use of hazardous chemicals. [2] 2. To work safely with substances that pose hazards, flammable or explosive hazards. [2] 3. To demonstrate disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals [2] 4. To identify, verify and segregate laboratory waste and perform proper disposal of chemicals [2]
PGCHOP401			1.To study two step synthesis [2] 2.Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS [2] 3.(ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product. [2] 4.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. [2]
PGCHOP402			1. A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information to any book/reference material. [2] 2. The complete structure of the compound may then be elucidated by referring to any standard text-book/reference material [2]

***Note: [1]: Remembering, [2]: Understanding, [3]: Applying, [4]: Analysing, [5]: Evaluating, [6]: Creating**

Choice Based Credit, Grading and Semester System with effect from the academic year 2019-2020

M.Sc.-II Organic Chemistry
Semester - IV
Course Code: PGCHO401

Course Code	Unit	TOPICS	Credits	L/Week
PGCHO401	I	**PHYSICAL ORGANIC CHEMISTRY**	4	1
	II	**SUPRAMOLECULAR CHEMISTRY**		1
	III	**STEREOCHEMISTRY- II**		1
	IV	**ASYMMETRIC SYNTHESIS**		1
PGCHO402	I	**DESIGNING ORGANIC SYNTHESIS-I**	4	1
	II	**DESIGNING ORGANIC SYNTHESIS-II**		1
	III	**ELECTRO-ORGANIC CHEMISTRY AND SELECTED METHODS OF ORGANIC SYNTHESIS**		1
	IV	**TRANSITION AND RARE EARTH METALS IN ORGANIC SYNTHESIS**		1
PGCHO403	I	**NATURAL PRODUCTS-III**	4	1
	II	DRUG DESIGN, DEVELOPMENT AND SYNTHESIS		1
	III	HETERO CYCLIC COMPOUNDS-I		1
	IV	HETERO CYCLIC COMPOUNDS-II		1
PGCHOE-I404	I	**INTRODUCTION TO INTELLECTUAL PROPERTY**	4	1
	II	TRADE SECRETE		1
	III	INTRODUCTION TO CHEMINFORMATICS		1
	IV	APPLICATIONS		1
PGCHOE-II404	I	PRINT	4	1
	II	DRUG DESIGN, DEVELOPMENT AND SYNTHESIS		1
	III	**METHODS OF SCIENTIFIC RESEARCH**		1

		AND WRITING		
	IV	INTELLECTUAL PROPERTY RIGHT		1
PGCHOP401 PGCHOP402	-	PRACTICAL COURSE	8	16

Note: 1. Blue Highlighted Topic / Course has focus on employability/ entrepreneurship/skill development

3. Yellow Highlighted Topic / Course is related to professional ethics, gender, human values, Environment & sustainability

Paper - I (Theoretical Organic Chemistry-II)

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

1.1 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**.** **[7L]**

1.2 Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, σ_I and σ_R scales, steric parameters Es and β. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Problems based on Hammet Equation and sigma and rho **[8L]**

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

2.1 Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes. **[3L]**

2.2 Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites. **[3L]**

2.3 Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes applications in synthetic chemistry **[5L]**

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

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

3.1 Racemisation and resolution of racemates including conglomerates: Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds. **[3L]**

3.2 Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR). Coupling constant **[3L]**

3.3 Correlative method for configurational assignment: chemical, optical rotation, and NMR spectroscopy. **[4L]**

3.4 Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial α- **[5L]**

haloketone rule with applications.Problems based on ORD and CD

Unit 4: Asymmetric synthesis **[15L]**

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

4.2 Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactions 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. **[9L]**

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

REFERENCES:

1. March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons.
2. A guide to mechanism in Organic Chemistry, 6th 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. Organic Reaction Mechanism, 4th 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 Organic chemistry, 8th edition, John McMurry
20 Modern methods of Organic Synthesis, 4th 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 Stereochemistry, P. S. Kalsi, 4th 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. Kalsiand 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.6 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 [6L]

and aliphatic nitro compounds in organic synthesis.

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 Organocatalysts: Proline, Imidazolidinone applications in synthetic chemistry

3.2.2 Pd catalysed cycloaddition reactions: Stille reaction, Saeguse-Ito oxidation to enones, Negishi coupling.

3.2.3 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:

1. **Advanced Organic Chemistry,** Part A and Part B: Reaction and Synthesis, Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer Verlag
2. **Modern Methods of Organic Synthesis,** 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
3. **Chem.Rev. 2002, 102, 2227-2302, Rare Earth Metal Triflates in Organic Synthesis,** S. Kobayashi, M. Sugiura, H. Kitagawa, and W.W.L. Lam ·
4. **Organic Chemistry,** Clayden Greeves Warren and Wothers, Oxford Press (2001).
5. **Moder Organic Synthesis: An Introduction,** G.S. Zweifel and M.H. Nantz, W.H. Freeman and Company, (2007).
6. **Advanced Organic Chemistry: Reaction Mechanism,** R. Bruckner, Academic Press (2002).
7. **Principles of Organic Synthesis,** R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes
8. **Organic Chemistry,** 7th Edn, R. T .Morrison, R. N. Boyd, & S. K. Bhattacharjee, Pearson
9. **Strategic Applications of Name Reactions in Organic Synthesis**, L. Kurti & B. Czako (2005), Elsevier Academic Press.
10. **Advanced Organic Chemistry: Reactions & Mechanisms,** 2nd Edn., B. Miller & R. Prasad, Pearson
11. **Organic reactions and their mechanisms,** 3rd revisededition, P.S. Kalsi, New Age International Publishers
12. **Organic Synthesis: The Disconnection Approach,** Stuart Warren, John Wiley & Sons, 2004
13. **Name Reactions and Reagents in Organic Synthesis,** 2nd Edn., Bradford P. Mundy, Michael G. Ellard, and Frank Favoloro, Jr., Wiley-Interscience
14. **Name Reactions,** Jie Jack Lie, 3rd Edn., Springer
15. **Organic Electrochemistry,** H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Course Code: PGCHO403
Paper - III (Natural products and heterocyclic chemistry)

Unit 1: Natural products [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 Synthesis of 16-DPA from cholesterol and plant sapogenin. [2L]

1.3 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: Drug design, development and synthesis [15L]

2.1 Introduction to quantitative structure activity relationship studies.

2.2 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. [5L]

2.3 Introduction to modern methods of drug design and synthesis- computer aided molecular graphics based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design. [3L]

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

2.5 Synthesis and application of the following drugs: Fluoxetine, cetrizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate [4]

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, Purines and acridines, benzothiazoles, stereochemistry, spectral data and synthesis of zingiberene.

REFERENCES:

1. Natural product chemistry, A mechanistic, biosynthetic and ecological approach, Kurt B.G. Torssell, Apotekarsocieteten - Swedish Pharmaceutical Press.
2. Natural products chemistry and applications, Sujata V. Bhat, B.A. Nagasampagi and S. Meenakshi, Narosa Publishing House, 2011.
3. Organic Chemistry Natural Products Volume-II, O. P. Agarwal, Krishna Prakashan, 2011.
4. Chemistry of natural products, F. F. Bentley and F. R. Dollish, 1974
5. Natural Product Chemistry Vol.1 and 2, K. Nakanishi J. Goto. S.Ito Majori and S. Nozoo, Academic Press, 1974.
6. Chemistry of natural products, V.K. Ahluwalia, Vishal Publishing Co. 2008.
7. Heterocyclic chemistry, 3rd edition, Thomas L. Gilchrist, Pearson Education, 2007.
8. Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, R. K. Bansal, Wiley Eastern Ltd., 1990.
9. Heterocyclic Chemistry, J. A. Joule and G. F. Smith, ELBS, 2nd edition, 1982.
10. The Conformational Analysis of Heterocyclic Compounds, F.G. Riddell, Academic Press,1980.
11. Principles of Modern Heterocyclic Chemistry, L.A. Paquette, W.B. Benjamin, Inc., 1978.
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Course Code: PGCHO 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.

<u>Unit II:</u> [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: [15L]

Introduction to Cheminformatics: [5L]

History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.

Representation of molecules and chemical reactions: [5L]

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

Searching Chemical Structures: [5L]

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

Unit IV:

Applications of computers in research : [15L]

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:

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2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook*. Wiley-VCH
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Course Code: PGCHO-II 404

PAPER - IV: RESEARCH METHODOLOGY

Unit 1: [15L]

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:

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:

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

Unit II: METHODS OF SCIENTIFIC RESEARCH AND WRITING [15]

3.1 SCIENTIFIC PAPERS

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

3.2 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 III Intellectual Property Right: [15L]

Historical Perspective, Different types of IP, Importance of protecting IP Patents: 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: Definition, How to obtain, features, International design registration.

Copyrights: Introduction, How to obtain, Differences from Patents. Trade Marks: Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc. Geographical Indications: Definition, rules for registration, prevention of illegal exploitation, importance to India.

Unit IV: Chemical Safety and 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 pressure, 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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2. Hibbert, D. B. & Gooding, J. J. (2006) *Data Analysis for Chemistry* Oxford University Press.
3. Topping, J., (1984) *Errors of Observation and their Treatment* 4th Ed., Chapman Hill, London.
4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6th Ed., Freeman Chapters 3-5
5. Levie, R. De. (2001) *How to use Excel in Analytical Chemistryand in general scientific data analysis* Cambridge Universty Press.
6. Chemical Safety matters - IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

Semester IV: Practicals
Course code: PGCHO4P1

Two steps preparations:

1. Acetophenone → Acetophenone phenyl hydrazine → 2-phenylindole.
.1 Benzaldehyde →b.Benzyl Acetophenone→Epoxide
2. Cyclohexanone →Phenyl hydrozone →1,2,3,4-tetracarbazole.
3. Pthalamide →N-Benzyl Pthalamide →Benzyl amine
4. *o*-nitroaniline → *o*-phenylene diamine → Benzimidazole.

5. Benzophenone → benzophenone oxime → benzanilide.
6. *o*-chlorobenzoic acid → N-phenyl anthranilic acid → acridone.
7. Benzoin → benzil → benzilic acid.
8. Phthalic acid → phthalimide → anthranilic acid.
9. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-methyl-7-acetoxy coumarin.
10 Anthracene → anthraquinone → anthrone.
11 Benzyl cyanide→ p-Nitrobenzyl cyanide→p-Nitro phenyl acetic acid
12 Acetanilide → p-Acetamidobenzene sulphonyl chloride → P. Acetamidobenzene sulphonamide

(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.

Session-II:

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.