Deccan Education Society's FERGUSSON COLLEGE (AUTONOMOUS), PUNE

Syllabus

for

M. Sc. (Organic Chemistry) Part II

(Semester-III and Semester-IV)

[Pattern 2019]

from Academic Year

2020-21

Program Structure of M.Sc. (Organic Chemistry) Part-II

Particulars	Paper	Paper code	Title of Paper	Type of Paper	No. of Credits
M.Sc. Semester-III	Paper- 1	CHO5301	Stereochemistry of Organic Molecules	CORE-1	4
	Paper - 2	CHO5302	Structure Determination by Analytical Methods	CORE- 2	4
	Paper - 3	CHO5303	Chemistry of Heterocycles and Medicinal Chemistry	D. elective	4
		CHO5304	Pharmaceutical Chemistry	G. Elective	
		CHO5305	MOOC Course	MOOC1	
	Paper -4	CHO5306	Organic Chemistry Practical V	PCORE-1	4
	Paper -5	CHO5307	Organic Chemistry Practical VI	PCORE-1	4
M. Sc. Semester-IV	Paper -1	CHO5401	Chemistry of Natural Products and Chiron Approach	D. elective	4
		CHO5402	Forensic Science and Toxicology	G. Elective	
		CHO5403	MOOC Course	MOOC2	
	Paper - 2	CHO5404	Advanced Synthetic Organic Chemistry	D. elective	4
		CHO5405	Analytical Spectroscopy	G. Elective	
		CHO5409	MOOC Course	MOOC3	
	Paper - 3	CHO5407	Designing of Organic Synthesis and Asymmetric Synthesis	D. elective	4
		CHO5408	Polymer Chemistry	G. Elective	
		CHO5409	MOOC Course	MOOC4	
	Paper -4	CHO5410	Organic Chemistry Practical VII	PCORE-3	4
	Paper -5	CHO5411	Organic Chemistry Practical VIII	PCORE-4	4
			OR		
	Paper -6	CHO5412	Project / Internship (Optional for practical courses CHO5410 and CHO5411)		8

MOOC courses	Course- 1	CHO-01	Environmental Chemistry	MOOCs	4
	Course- 2	CHO-02	Biophysical Chemistry	MOOCs	4
	Course-3	CHO-03	Environmental soil chemistry	MOOCs	4
	Course- 4	CHO-04	Food Analysis	MOOCs	4

CHO5301: Stereochemistry of Organic Molecules [Credits – 4]

Course Outcomes

Students will learn:

CO1 Stereochemical aspects of Six-membered and other ring systems
CO2Stereochemistry of fused and bridged rings systems
CO3Concept of racemic modification and methods to achieve it
CO4To determine the structure and stereochemistry of some naturally occurring molecules with ring structures

Unit I	Stereochemistry of Six membered rings and their reactions
Unit II	Stereochemistry of rings other than Six-membered ring
Unit III	Fused, Bridged and Caged rings, Baldwin's Rule
Unit IV	Resolution of racemic modification.
Unit V	Structure and Stereochemistry of Morphine, Quinine, Lactone Fusion in Enhydrin, Hardwickiic acid and Camptothecin

References:

1. Stereochemistry of carbon compounds - E. L. Eliel
2. Stereochemistry of carbon compounds - E. L. Eliel and S. H. Wilen
3. Chemistry of Natural Products - N. R. Krishnaswamy (University Press)
4. Stereochemistry of organic compounds - Nasipuri
5. Stereochemistry of organic compounds - Kalsi
6. Chemistry of Natural products- Kalsi
7. M. E. Wall, M. C. Wani *et al*., *J. Am Chem. Soc.*, **1966**, 88, 3888
8. M. C. Wani and M. E. Wall, *J. Org. Chem*., **1969**, 34, 1364
9. Sukh Dev *et al*., *Tetrahedron Letters*, **1964**, 5(49), 3751

CHO5302: Structure Determination by Analytical Methods [Credits – 4]

Course Outcomes
Students will learn:
CO1 Different techniques in spectroscopy
CO2Organic structure analysis
CO3Structure from spectra
CO4Spectroscopic identification of organic compounds
CO5Interpretation of different types of spectra
CO6One and two dimensional NMR spectroscopy
CO7Applications of mass spectrometry
CO8Advanced methods of spectral analysis

Unit I	**^{1}H-NMR Spectroscopy**: History of NMR, Chemical shift, factors influencing chemical shift, deshielding, chemical shift values and correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and other nuclei (alcohols, phenols, enols, acids, amides and mercaptans), chemical exchange, effect of deuteration (Driving force), spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant "J", classification of spin system like AB, AX, AX_2, ABX, AMX, ABC, A_2B_2. Spin decoupling, simplification of complex spectra, nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear Overhauser effect (NOE), resonance of other nuclei like ^{31}P, ^{19}F
Unit II	**^{13}C NMR spectroscopy**: FT NMR, Types of ^{13}C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, Homo nuclear (^{13}C-^{13}C) and Hetero nuclear (^{13}C-^{1}H)coupling constants
Unit III	**2D NMR Techniques**: General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)-Homo COSY (^{1}H-^{1}H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.
Unit IV	**Mass Spectrometry**: Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupoule mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors controlling fragmentation, HRMS.
Unit V	Problems based on joint application of UV, IR, PMR, CMR, and Mass (Including reaction sequences)

References:

1. Introduction to Spectroscopy –D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).

2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wiley and Sons.
3. Spectroscopic methods in organic chemistry -D. H. Williams and I. Flemming Mc Graw Hill
4. Absorption spectroscopy of organic molecules - V. M. Parikh
5. Nuclear Magnetic Resonance –Basic Principles-Atta-Ur-Rehman, Springer-Verlag (1986).
6. One and Two dimensional NMR Spectroscopy - Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis-Phillip Crews, Rodriguez, Jaspars,Oxford University Press (1998)
8. Organic structural Spectroscopy-Joseph B. Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).5
9. Organic structures from spectra - Field L.D., Kalman J. R. and Sternhell S. 4th Ed. John Wiley and sons Ltd.
10. Spectroscopic identification of organic compound - R M Silverstein,G C Bassler and T C Morril, John Wiley
11. Introduction to NMR spectroscopy - R. J. Abrahm, J. Fisher and P. loftus Wiley
12. Organic spectroscopy-William kemp, E L B with McMillan
13. Spectroscopy of organic molecule - P. S. Kalsi, Wiley, Esterna, New Delhi
14. Organic spectroscopy-RT Morrison and RN Boyd
15. Practical NMR spectroscopy - M. L. Martin, J. J. Delpench, and D J Martyin
16. Spectroscopic methods in organic chemistry - D H Willson, I Fleming
17. Spectroscopy in organic chemistry - C N R Rao and J R Ferraro
18. NMR –Basic principle and application - H Guntur
19. Interpretation of NMR spectra - Roy H Bible
20. Mass spectrometry organic chemical applications - J H Banyon

CHO5303: Chemistry of Heterocycles and Medicinal Chemistry [Credits-4]

Course Outcomes

Students will learn:

CO1 Five and six membered heterocycles: Synthesis, reactivity and mechanistic aspects
CO2Five and six membered fused heterocycles: Synthesis, reactivity and mechanistic aspects
CO3Heterocycles with two or more heteroatoms
CO4Medicinal chemistry:
CO5Drug targets
CO6QSAR studies
CO7Biological activities of drugs
CO8Synthetic aspects of drugs

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Unit I	Five and six membered heterocycles with one and two hetero atoms: Furan, Pyrrole, Thiophene, Pyridine, Pyrazole, Imidazole, Oxazole, Thiazole, Pyrimidines
Unit II	Condensed five and six membered heterocycles with one and two hetero atoms: Benzofuran, Indole, Benzo-[b]-thiophene, Quinoline, Isobenzofuran, Isoindole, Benzo-[c]-thiophene, Isoquinoline, Benzoxazole, Benzthiazole, Benzimidazole
Unit III	Five and six membered heterocycles with more than two hetero atoms: 1,2,3-Triazole, 1,2,4-Oxadiazole, 1,2,5-Oxadiazole, Tetrazole, Purine
Unit IV	Introduction to drugs, their action and discovery
Unit V	Drug targets
Unit VI	Relation of Drug structure and its chemical and biological properties (QSAR), Synthetic aspects
Unit VII	Antibacterial, Antiviral, Antifungal, Antiprotozoal , Anticancer, Antidiabetic, Anti-Alzheimer drugs

References:

1. Heterocyclic Chemistry - T. Gilchrist
2. An introduction to the chemistry of heterocyclic compounds - R M Acheso
   Heterocyclic Chemistry - J A Joule and K Mills
3. Principles of modern heterocyclic chemistry- A Paquette
4. Heterocyclic Chemistry - J A Joule and Smith
5. An introduction to medicinal chemistry - Graham L. Patrick 5th Ed. Oxford
6. Introduction to Medicinal Chemistry - Alex Gringauz (Wiley)
7. Foye's Medicinal Chemistry
8. Medicinal Chemistry - A. Burger
9. Medicinal Chemistry - Ashutosh Karr

CHO5304 Pharmaceutical Chemistry [Credits – 4]

Course Outcomes

After learning this course students will be able to understand:

CO1 Importance of FDA in pharmaceutical industries.
CO2Various dosage forms and vegetable drugs along with their analysis.
CO3 Concepts of pharmacology.
CO4Precautions needed to be taken while processing pharmaceutical product.
CO5Major source of impurities and techniques to identify it.
CO6Separation techniques and method validation.
CO7Implementation of Indian Pharmacopeia for course content..

Unit I	**Introduction to FDA:** **Dosage form and analysis:** Introduction, dosage and their types. Route of administration, factors affecting on dosage, Tablets, different types of tablets, additives used in tablet manufacture. Analysis of aspirin tablet, Capsules, types of capsules, (Rifampicin), Powders (Sodium benzoate), Solutions (saline NaCl), Suspensions (barium sulphate), (Ointments (salicylic acid) and creams Dimethicone by IR) Injections (Mannitol), Aerosols (salbutamol), Problems based on assay of these materials.
Unit II	**Evaluation of solid dosage Forms - Tablets and Capsule:** Quality: Hardness, Friability, Tablet thickness, Weight variation test, Content uniformity test, Viscosity and pH Measurement, disintegration, dissolution, stability, Disintegration and Dissolution, rate of dissolution and types dissolution apparatus, Moisture / water content by Karl-Fischer titration- Principle, types of Karl Fischer titration, preparation and standardization of Karl Fischer reagent. Sterilization**:** Methods for Sterilization (Physical and chemical method), Applications.
Unit III	**Pharmacology: Pharmacokinetics and dynamics** • **Introduction and importance** • **Pharmacokinetics**: Introduction, ADME process, pharmacokinetics models (one compartment, two compartment and multi compartment), bioavailability, Constant-rate infusion- administration rate, kinetics of elimination –clearance, first order kinetics, zero order kinetics and Half-life). • **Pharmacodynamics:** Introduction, principle of drug action, mechanism of drug action, enzymes-enzyme inhibition, Receptors- Agonists, Antagonism, Partial agonists, function of receptors, dose-response relationship, drug potency and efficiency, therapeutic efficiency, drug selectivity and specificity, Non-receptor mechanisms
Unit IV	• **Sources of Impurities in Pharmaceutical Raw Materials & Finished Products:** Raw materials, Method of manufacture, Atmospheric contaminations, Cross contamination, Microbial contamination, Container contamination, Packaging errors, Chemical instability, Temperature effect and Physical changes • **Shelf Life of Pharmaceutical Product:** shelf life of Pharmaceutical product and determination of shelf life. Water for pharmaceutical use. • **Limit test:** Limit tests for aluminium, arsenic, iron, lead, potassium, sulphate, chloride, heavy metals

Unit V	**Analysis of Vegetable Drugs:** Sampling, foreign organic matter, test for complete extraction alkaloids, ash value, acid soluble ash, acid insoluble ash, sulphated ash, Extraction of alkaloids. Loss on drying loss on ignition
Unit VI	**Separation techniques in pharmaceuticals:** • **Gas Chromatography:** Theory and Instrumentation of GC, Sample injection, Column types, Solid/Liquid Stationary phases, Column switching techniques, types of detectors, Interfacing of gas chromatography with mass spectrometry, Applications of GLC. • **High Performance Liquid Chromatography:** Theory and instrumentation of HPLC, Mobile phase delivery system, sample injection, separation column, types of column packing, detectors, normal phase chromatography, reverse phase chromatography, ion–pair chromatography, ion exchange chromatography, size exclusion chromatography, Method validation process - Precision, Accuracy, Specificity, Linearity, Range, Limit of Detection, Ruggedness, Robustness, Stability

References:

1. Indian Pharmacopeia Volume I and II.
2. Practical Pharmaceutical chemistry third edition volume 1. By A. H. Beckett & J. B. Stenlake.
3. Remington‘s Pharmaceutical sciences.
4. Ansel’s Pharmaceutical Analysis.
5. Aymanns C, Keller F, Maus S, et al. Review of pharmacokinetics and pharmaco dynamics and the aging kidney. Clin J Am SocNephrol.
6. Introduction to Instrumental Analysis, R. D. Braun, Mc Graw-Hill. Inc.1987.
7. Instrumental Methods of Chemical analysis, H. H. Willard, L. L. Merritt Jr., J. A. Dean & F. A. Settle Jr., 6th Edition, Wadsworth Publishing Company, USA,1986
8. Handbook of Instrumental Techniques for Analytical Chemistry, F. A. Settle editor, Prentice Hall Inc. A Simon and Schuster Company, New Jersey, 1997.

Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, 7th Edition, Thomson Asia Pte. Ltd, Singapore, 2004

CHO5306: Organic Chemistry Practical Course V [Credit-4]

Single stage preparations based on regio-selective and chemo selective Principles

Single stage preparations comprising of reactions involving:

- Rearrangements,
- Aromatic electrophilic substitution
- Aromatic nucleophilic substitution
- Reduction
- Ylides
- Grignard reaction
- Photochemical reaction
- Condensation reaction
- Acetyl derivatives
- Heterocylic synthesis
- Self-redox
- Wittig reaction

References:

1. A Textbook of Practical Organic Chemistry - A. I. Vogel - ELBS with Longman, 5th Ed., (1989)
2. Laboratory Manual of Organic Chemistry - R. K. Bansal - Wiley Eastern 3rd Ed., (1994)
3. Advanced Practical Organic Chemistry - N. K. Vishnoi - Vikas 2nd Ed., (1996)

CHO5307: Organic Chemistry Practical Course VI [Credit-4]

Two stage preparations involving:

- Aldol reaction
- Epoxidation
- Oxidation
- Reduction
- Condensation
- Acetylation
- Schiff base formation
- Cyclization
- Alkylation
- Rearrangement
- Nitration
- Hydrolysis
- Enamine
- Halogenation
- Oxime

References:

1. A Textbook of Practical Organic Chemistry - A. I. Vogel - ELBS with Longman, 5th Ed., (1989)
2. Laboratory Manual of Organic Chemistry - R. K. Bansal - Wiley Eastern 3rd Ed., (1994)
3. Advanced Practical Organic Chemistry - N. K. Vishnoi - Vikas 2nd Ed., (1996)

CHO5401: Chemistry of Natural Products and Chiron Approach

[Credits – 4]

Course Outcomes

Students will learn:

CO1 The retro synthetic analysis of important natural products

CO2The synthesis of important natural products

CO3Various building blocks in synthesis natural products

CO4Biogenesis of various oxygen and nitrogen containing natural products

CO5Chiral nature of sugars and their use as chiron in syntheses of various chiral molecules

CO6Importance of chiral drugs and syntheses of few chiral drug molecules

CO7Various drug targets and structure activity relationship between drug molecules and their targets.

Unit I	**Total Synthesis of some important Natural products:** • Taxol • Estrone • Mifepristone • Juvabione (Mori and Matsui synthesis and Pawson and Cheung Synthesis) • Fredericamycin A • Reserpine
Unit II	**Biogenesis**: The building blocks and construction mechanism of • Terpenoids – Mono, Sesqui, Di and Triterpenoids and cholesterol • Alkaloids derived from ornithine, lysine, nicotinic acid, tyrosine and tryptophan. • The shikimate pathway - cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavanoids and terpenoid quinones
Unit III	**Chiron Approach:** • Introduction • The concept of chiral templates and chirons wherein the carbon skeleton is the chiral precursor, Utilization of the basic concepts for retrosynthetic strategy and synthesis of the (*S*) Propanediol, (*R*) and (*S*) - Epichlorohydrin, *L*-(+)-Alanine, 9(-) Multistratin, (-) Pentenomycin, (-) Shikimic acid **Chiral Drugs:** Introduction of chiral drugs, Eutomer, Distomer and eudesmic ratio. a) with no side effects b) with undesirable side effects Synthesis and pharmacological activity of *S*-Ibuprofen, *S*-Metaprolol, Indinavir sulfate, Dextropropoxyphen, (+)-Ephedrine, Griseofulvin, *R*-Indacrinnone, hydrochloride, *S*-Captopril

References:

1. Chemistry of Natural products - Kalsi
2. Principles of organic synthesis by R. O. C. Norman and J. M. Coxon; Chapman and Hall
3. Classics in organic synthesis – K. C. Nicolaou & E. J. Sorensen
4. J. Indian Inst. Sci., 81, 287 (2001)
5. Medicinal Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd Ed.(Wiley)
6. Secondary metabolism - J. Mann, 2nd edition.
7. Chemical aspects of Biosynthesis - J. Mann (1994).
8. i) J.C.S. Perkin Transactions II, **1973**, 288-292

ii) J. Am. Chem. Soc., **1955**, 77, 432-437
9. Advanced Organic Chemistry- Carey and Sundberg Part B 5th Ed.
10. Organic Chemistry - R. P. Morrison and R. N. Boyd
11. Organic Chemistry - I. L. Finar, volume II
12. Chiron Approach in organic synthesis - S. Hanessianh
13. Pharmaceutical Chemistry and drug synthesis - Rot and Kleeman
14. Drug Design - E. J. Arienes

CHO5402: Forensic Science and Toxicology [Credits – 4]

Course Outcomes

Students will learn:

CO1 History and role of Forensic science in crime investigations.

CO2Importance of toxicology and its role.

CO3Different Forensic Laboratory Units and their roles.

CO4Different methods of isolations of poisons from body fluid

CO5Analysis of crime scene evidences using different techniques.

Unit I	**Forensic Science:** • **Introduction:** History, role of forensic science in crime investigation, collection and preservation of biological materials. • **Physical Evidence**: Common Types of Physical Evidences and its Significance. **Trace evidence:** Introduction, principle, Hair and fibre analysis
Unit II	• **Bloodstain Pattern Analysis**: Blood and blood grouping, type of bloodstain pattern and application. • **DNA Profiling:** Introduction, principle, DNA and its polymorphism, DNA typing procedures-RFLP, PCR, MVR-PCR, Dot-blot, AMP-FLP, STR, other methods, paternity testing, applications, interpretation and practical use**.** • **Fingerprint Analysis:** Latent fingerprints; optical, physical, physico-chemical & chemical detection methods; fingerprints in blood, fingerprint detection sequences.
Unit III	**Explosives and firearms:** Types, analytical methods for identification of low and high explosives in post-blast debris
Unit IV	• **Hairs, Fibers, and Paint:** Identification, Comparison Collection and Preservation of Hair Fiber and Paint evidences. • **Glass and Soil analysis:** Identification, Comparison, Collection and Preservation of samples • **Document Analysis:** Principle and application
Unit V	**Forensic Toxicology:** • **Introduction**: Introduction to toxicology, role of forensic toxicology. • **Poisons:** Type of poisons, detection of poison in biological fluid- physical and chemical method, the role of the clinical toxicology laboratory, diagnosis of acute poisoning and their treatment. • **Drugs:** Classification of drugs, isolation, identification and determination of following, Narcotics- heroin and cocaine, Stimulants- caffeine, amphetamines, Depressants- Barbiturates, Benzodiazepines. • **Alcohol in body fluids:** Legal background, Sampling and sample preservation, analysis-GC, IR, enzymatic and other methods

References:

1 Basic Analytical Toxicology Published by WHO, By R. J. Flanagan, R. A. Braithwaite, S. S. Brown Available Online

2 http://www.forensicsciencesimplified.org/

3 Textbook of Medicinal Jurisprudence, Forensic Medicine and Toxicology, 6th edition By Dr. C. K Parikh.

4 Forensic Chemistry, 1st edition, By Suzanne Bell, Person Education Ltd.

5 Shreves' Chemical Process Industries fifth edition by George Austin Mg Graw Hill Practical Pharmceutical Chemistry by Becket

6	Biochemical Methods, Third Edition, By S. Sadashivan, A. Manickam; NEW AGE International (P) limited, Publication, Pearson's chemical analysis of food.
7	Practical Biochemistry in Clinical Medicine, R. L Nath, Academic Publishers 2nd edition (1990)

CHO5404: Advanced Synthetic Organic Chemistry [Credits – 4]

Course Outcomes

Students will learn:

CO1 Applications of transition metals in metal mediated coupling reactions
CO2Various reactions involving C=C formation
CO3Multicomponent reactions (MCR)
CO4Ring formation reactions
CO5Click chemistry
CO6Metathesis reactions
CO7Reactions involving Boron and Silicon
CO8 Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction.

Unit I	Transition metal complexes in organic synthesis ; only Pd, Ni, Co, Fe (Metal mediated C-C and C-X bond formation reactions: Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada, Hiyama, Negishi, Buchwald-Hartwig, Noyori, Reppe, Oxo process
Unit II	C=C formation reactions: Wittig, Horner-Wordworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions, Titanium-carbene mediated olefination: Tebbe, Petasis and Nysted reagent
Unit III	Multi-component reactions: Ugi, Passerini, Biginelli and Mannich reactions
Unit IV	Ring formation reactions: Pausan-Khand, Bergman and Nazerov cyclization
Unit V	Click chemistry: criterion for click reaction, Sharpless azides cycloadditions
Unit VI	Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, applications
Unit VII	Use of Boron and Silicon in organic synthesis
Unit VIII	Other important reactions: Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction

References:

1. Organic synthesis using transition metals - Roderick Bates (Wiley)
2. Organic chemistry - J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
3. Designing of organic synthesis - S. Warren (Wiley)
4. Some modern methods of organic synthesis - W. Carruthers (Cambridge)
5. Organic synthesis - Michael B. Smith
6. Organometallics in organic synthesis - J. M. Swan and D. C. Black (Chapman and Hall)
7. Advanced organic chemistry, Part B - F. A Carey and R. J. Sundberg, 5^{th} edition (2007)
8. Guidebook to organic synthesis – R. K. Meckie, D. M. Smith and R. A. Atken
9. Organic synthesis - Robert E. Ireland
10. Strategic Applications of named reactions in organic synthesis - Laszlo Kurti and Barba

CHO5405: Analytical Spectroscopy [Credits – 4]

Course Outcomes

Students will learn:

CO1 Concepts of different spectroscopic techniques.

CO2Principle and instrumentation of electron spectroscopy, chemiluminescence, fluorescence and phosphorescence, surface characterization techniques and XRD.

CO3Applications of spectroscopic techniques..

Unit I	**Electron Microscopy** • **Electron spectroscopy:** Introduction, principle of ESCA, electron spectroscopy for chemical analysis, ESCA satellite peaks, spectral splitting, ESCA chemical shifts, Instrumentation of ESCA, Chemical analysis using ESCA, Applications, Auger electron microscopy, Ultraviolet photoelectron spectroscopy. • **Surface Characterization by spectroscopy and microscopy:** Introduction to study of surface, Electron stimulated microanalysis methods- (electron microprobe, Transmission Electron Microscope, Scanning Electron Microscope, Scanning Transmission Electron Microscope, Analytical Electron Microscopy, Scanning-Probe Microscopes) – principle, instrumentation and application
Unit II	**X- ray Methods of Analysis:** Principle, Theory- X-ray spectral lines, X-ray tube, X-ray emission, Absorptive apparatus, X-ray Sources, Collimation, sample handling, wavelength dispersive devices, Energy dispersive devices, detectors, readout device, Powder XRD and Single crystal XRD, Chemical analysis using X-ray absorption, X-ray Fluorescence- instrumentation and chemical analysis, X-ray Diffraction, Chemical analysis with X-ray diffraction, numerical problems.
Unit III	**Chemiluminescence, Fluorescence and phosphorescence:** Introduction, principle, types, measurement of chemiluminescence, instrumentation, quantitative chemiluminescence, gas phase chemiluminescence analysis, chemiluminescence titrations, electro-chemiluminescence**,** Photo luminescent theory, Electron transitions during photoluminescence, factors affecting photoluminescence, Luminescent apparatus, Optical extractive sources, wavelength selectors, detectors ad readout devices, photo luminescent spectra, photo luminescent analysis, analysis of non-photoluminating compounds specific examples of analysis using photoluminescence, application of Fluorescence-Polarization Assays in Small Molecule Screening
Unit IV	**Nuclear magnetic resonance spectroscopy:** **^{1}H NMR :**Introduction, theory, Instrumentation, Chemical Shifts, Spin-Spin splitting, protons on hetero atoms, coupling protons with other nuclei, solvents, qualitative and quantitative analysis, problems. **^{13}C NMR:** Introduction, interpretation, chemical shifts, spin coupling, quantitative analysis, problems. **2D NMR:** Introduction, ^{1}H-^{1}H connectivity, ^{1}H-^{13}C connectivity, ^{13}C-^{13}C connectivity, Through space ^{1}H-^{1}H proximity, option and how to use them, problems.
Unit V	**Electron Paramagnetic Resonance Spectroscopy (EPR)** Theory and Instrumentation, Spin Hamiltonian, Isotropic and anisotropic EPR spectra, Magic Pentagon rule. Applications of EPR spectroscopy

References:

1. Introduction to instrumental analysis by R. D. Braun, Mc Graw Hill- International edition.
2. Instrumental methods of chemical analysis by Willard, Dean and Merittee - Sixth edition.
3. Analytical chemistry principles by John H. Kenedey- Second edition, Saunders college publishing.
4. Spectroscopic identification of organic compounds Fifth Ed., Silvestrine, Bassler, Morrill, John Wiley and sons.
5. Analytical Chemistry, Ed. by Kellner, Mermet, otto, Valcarcel, Widmer, Second Ed. Wiley –VCH.
6. Vogel's Textbook of quantitative Chemical Analysis, sixth Ed., Mendham, Denney, Barnes, Thomas, Pub: Pearson Education.
7. Electron microscopy in the study of material, P. J. Grundy and G. A. Jones, Edward Arnold.
8. Solid state chemistry by D. K. Chakrabarty.
9. Instrumental analysis By Skoog and Holler

CHO5407: Designing Organic Synthesis and Asymmetric Synthesis [Credits – 4]

Course Outcomes

Students will learn:

CO1 Use of retro synthetic analysis to work out and compare alternative syntheses of complex organic molecules.

CO2To outline important classical and modern reactions used in organic synthesis.

CO3Designing synthetic routes by using choice of reagents and conditions taking into account cost, safety and environmental factors

CO4To develop problem solving ability

CO5Problems involved in process development and the scale up of synthesis of commercially important compounds

CO6The importance of the use of protection and de-protection in organic synthesis

CO7The concept and principles of asymmetric synthesis

CO8The applications of asymmetric syntheses in various synthetic methodologies

Unit I	**Designing Organic Synthesis:** • Retrosynthesis: one-group disconnection, two-group disconnection, Illogical two-group disconnection, Special methods for small rings, Strategy • Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions • Umpolung in organic synthesis
Unit II	**Asymmetric Synthesis:** • Chirality transfer, Asymmetric inductions; Chiral pools, Chiral auxiliaries and chiral reagents • Organocatalysis • Asymmetric Reactions: Asymmetric oxidations: Epoxidation (Sharpless, Shi, Jorgensen and etc.), Asymmetric Dihydroxylation, Aminohydroxylation, Asymmetric Reduction: Asymmetric Reduction of Ketones, Imines and Olefins, Asymmetric C-C bond forming reaction: Simmon-Smith reaction, Aldol reaction and alkylation based on Evans method, Mukayama Aldol Reaction; Michael Reaction, Henry Reaction (Nitro aldol), Baylis-Hillman-Morita reactions. • Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, Felkin Anh rule, Cram's chelate model, etc. • Enzyme catalyzed reactions binding mechanism of enzymes

References:

1. Designing of organic synthesis - S. Warren (Wiley)
2. Organic chemistry - J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
3. Advanced organic chemistry, Part B - F. A Carey and R. J. Sundberg, 5th edition (2007)
4. Asymmetric Reactions and Processes in Chemistry - Ernest L. Eliel
5. Catalytic Asymmetric Synthesis: 2nd Ed., Iwao Ojima
6. Asymmetric Organocatalysis: From Biomimetic Concept to Applications in Asymmetric Synthesis - David MacMillan
7. Asymmetric synthesis Vol.1-5 - J. D. Morrison
8. Principles and Applications of Asymmetric Synthesis - Guo-Qiang Lin, Yue-Ming Li and Albert S. C. Chan, Wiley
9. Advanced Asymmetric Synthesis - Stephenson and George Richard, Springer

CHO5408: Polymer Chemistry [Credits – 4]

Course Outcomes

Students will learn:

CO1 Concept and classification of polymer.

CO2Polymerization techniques.

CO3Physic-chemical properties and analysis of polymers.

CO4Concept of calculating average molecular weight by different methods.

CO5Application in various fields

Unit I	**Introduction of Polymers:** Basic concepts, History of polymers, Classification of polymers, classification of polymers based on: Origin, structure, stereochemistry, synthesis, type of chain and mechanical properties
Unit II	**Polymer synthesis mechanisms:** Chain polymerization (Free radical polymerisation, cationic polymerisation, anionic polymerisation, co-ordination polymerisation) and step polymerization (Polycondensation, polyaddition and ring opening polymerisation). **Polymerization techniques:** bulk, solution, suspension, emulsion, melt polycondensation, interfacial condensation, solid and gas phase polymerization
Unit III	**Molecular Weight and Size of Polymers**: Concept of average molecular weight, determination of average molecular weight, Number average and weight average molecular weight, size of polymers, degree of polymerisation, polydispersity, molecular weight distribution-fractionation methods (fractionation precipitation, fractional elution, gel permeation chromatography,), determination of molecular weight by- End group analysis, colligative properties measurements, dilution solution viscosity method (Huggins and Kraemer viscosity plot), molecular weight distribution curve (simple representation of MWD), problem solving
Unit IV	**Properties of polymer** : **Glass Transition Temperature (Tg):** State of aggregation, state of phase, transition and associated properties, factors affecting on Tg, relation of Tg with molecular weight, Tg and copolymers. **Crystallinity of Polymers:** Degree of crystallinity, polymer crystallization, structural regularity, crystallites, Helix structures, spherulites, effect of crystallinity on polymer properties. **Polymer degradation:** Thermal degradation, photodegradation, degradation by ultrasonic waves, degradation by high energy radiation, oxidative degradation. **Polymer Solution**: Process of polymer dissolution, effect of molecular weight, solubility of amorphous and crystalline system, The Flory-Huggins theory, nature of polymer molecules in solution
Unit V	**Analysis and Testing of Polymers:** • Thermal analysis (TGA, DTA and DSC) of polymers • Physical testing of polymers: Mechanical properties, Fatigue testing, impact testing, tear resistance, hardness, abrasion resistance. • Thermal Testing: flammability, Heat deflection temperature, Vicat softening temperature, torsion pendulum test, thermal conductivity, thermal expansion. • Optical properties: transmittance, color, gloss, haze and transparency. • Electrical properties: dielectric constant and loss factor, resistively, dielectric strength, electronic properties.

	Chemical Test: Immersion test, vapor permeability, staining resistance, solvent stress cracking resistance, environmental stress cracking
Unit VI	**Polymer additives:** Fillers, plasticizers, UV stabilizers and absorbers, antioxidants, flame retardants, colourants. **Application of polymers :** Plastics, Natural and synthetic fibers, acrylic fibers, elastomers, adhesives

References:

1. Textbook of polymer science 3rd edition by F. W. Billmeyer (1994).
2. Principles of polymer systems by F. Rodrigue, Tata McGraw Hill, New Delhi.
3. Principles of polymer systems by P. J. Flory, Cornell University press, New York.
4. Polymer chemistry-an introduction Seymour-Carraher-Marcel Dekker. Inc. New York.
5. Polymer Science by V.R. Gowarikar, N. B. Vishvanathan, New Age International Ltd. Publisher (1998).
6. Polymer Science by Vasant Gowarikar, Wiley Easteren New York (1998).
7. Principle of polymer science, Bahadhur and Sastri, Narosa publishing house.
8. Textbook of Polymer Chemistry by M. S. Bhatnagar, S. Chand publication

CHO5410: Organic Chemistry Practical Course VII [Credits – 4]

Green Chemistry and Chemical Biology Experiments

- Solvent free reactions
- Room temperature reactions
- Use of environment friendly and non-hazardous reagents
- Use of environment friendly catalysts
- Atom economic reactions
- Rearrangements
- Condensation reactions
- Aldol reaction
- Fermentation reaction

References:

1. Practical Approach to Green Chemistry, Int. J. Pharm. Sci., Vol 9, Issue 4, 10-26 DOI: http://dx.doi.org/10.22159/ijpps.2017v9i4.15640
2. A Textbook of Practical Organic Chemistry - A. I. Vogel - ELBS with Longman, 5th Ed., (1989)
3. Laboratory Manual of Organic Chemistry - R. K. Bansal - Wiley Eastern 3rd Ed., (1994)
4. Advanced Practical Organic Chemistry - N. K. Vishnoi - Vikas 2nd Ed., (1996)

CHO5411: Organic Chemistry Practical Course VIII [Credits – 4]

Experiments in applied chemistry:

- Isolation of Natural products
- Synthesis of Schiff bases for dyes
- Pharmaceutical scaffold synthesis
- Industrially useful Monomers
- Synthesis of agrochemicals

References:

1. A Textbook of Practical Organic Chemistry - A. I. Vogel - ELBS with Longman, 5th Ed., (1989)
2. Laboratory Manual of Organic Chemistry - R. K. Bansal - Wiley Eastern 3rd Ed., (1994)
3. Advanced Practical Organic Chemistry - N. K. Vishnoi - Vikas 2nd Ed., (1996)

CHO5412: Project / Internship [Credits – 8]

Students need to select **project or internship** in industry/ R and D Institutes.

1. It is expected to spend minimum 120 hours for project or internship for 8 credits.
2. Monthly reporting of the progress of work should be done to the Faculty Mentor of the department.