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

Syllabus

for

M. Sc. (Analytical Chemistry) Part II

(Semester-III and Semester-IV)

[Pattern 2019]

from Academic Year

2020-21

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

Particulars	Paper	Paper code	Title of Paper	Type of Paper	No. of Credits
M.Sc. Semester-III	Paper- 1	CHA5301	Advance analytical techniques	CORE- 1	4
	Paper - 2	CHA5302	Extraction techniques and Metallurgy	CORE- 2	4
	Paper - 3	CHA5303	Pharmaceutical chemistry	D. Elective-1	4
		CHA5304	Structure Determination by Analytical Methods	G. Elective-1	4
		CHA5305	MOOC Course	MOOC-1	4
	Paper -4	CHA5306	Analytical Chemistry Practical V	PCORE-1	4
	Paper -5	CHA5307	Analytical Chemistry Practical VI	PCORE-2	4
M. Sc. Semester-IV	Paper -1	CHA5401	Forensic science and Toxicology	D. Elective-1	4
		CHA5402	Chemistry of Natural Products and Chiron Approach	G. Elective-1	4
		CHA5403	MOOC Course	MOOC-1	4
	Paper -2	CHA5404	Analytical spectroscopy	D. Elective-2	4
		CHA5405	Advanced Synthetic Organic Chemistry	G. Elective-2	4
		CHA5406	MOOC Course	MOOC-2	4
	Paper -3	CHA5407	Polymer Chemistry	D. Elective-3	4
		CHA5408	Designing Organic Synthesis and Asymmetric Synthesis	G. Elective-3	4
		CHA5409	MOOC Course	MOOC-3	4
	Paper -4	CHA5410	Analytical Chemistry Practical VII	PCORE-3	4
	Paper -5	CHA5411	Analytical Chemistry Practical VIII	PCORE-4	4
	OR				
	Paper -6	CHA5412	Project / Internship (Optional for practical courses CHA5410 and CHA5411)	PCORE-5	8

MOOC courses	**Note : Students offering less than 12 theory papers i.e.(48 credits) in previous semester can opt for the following MOOCs courses**				
	Course- 1	CHA-01	Research Methodology	MOOCs	4
	Course- 2	CHA-02	Solid and hazardous Waste Management	MOOCs	4
	Course- 3	CHA-03	Environmental Chemistry	MOOCs	4
	Course- 4	CHA-04	Food Microbiology and Food Safety	MOOCs	4
	Course- 5	CHA-05	Food Safety and Quality Control	MOOCs	4

Semester III

CHA5301: Advance analytical techniques [Credits – 4]

Course Outcomes

After learning this course student will be able to understand

CO1Theoretical background and develop practical skills for advanced instrumentation using modern analytical methods.

CO2 To design an analytical process for data collection and the project's research objectives.

CO3 To build an analytic skill to solve a real problem.

CO4 To interpret, communicate as well as write technical reports as per research aspect.

Unit I	**Electro-analytical technique** **a. Coulometry:** Principle and Instrumentations (Constant current and constant voltage instruments, potentiostatic, coulometry), Coulometric titrations – Apparatus, Specific Applications of Coulometry., advantages and limitations, problems. **b. Polarography:** Polarographic principles, Instrumentation, polarogram and polarographic currents, charging or capacitive current, role of supporting electrolyte, factors affecting on polarographic wave, Ilkovic Equation, advantages and disadvantages of dropping mercury electrode, Applications **c. Hydrodynamic voltametry**: Principle, instrumentation (Types of electrode - Rotating Disc Voltametry, Rotating Ring Disc voltametry, Flow through Voltametry) and applications. **d. Pulse Polarography:** Principle, Differential pulse polarography, square wave polarography, Stripping method. Voltametry with ultra-microelectrode, Applications (Cu and Zn from tap water by differential pulse polarography and by square wave polarography, Vitamin-C by differential pulse polarography, Determination of Pb in tap water by stripping method). **e. Cyclic Voltammetry and Amperometry:** Principle, instrumentation, RandlesSevcik equation, Applications (cyclic voltamogram of $K_3[Fe(CN)_6]$), amperometric titrations
Unit II	**Thermal Methods of Analysis** **a. Thermo gravimetric methods of analysis:** Instrumentation, thermogram and information from thermogram, factors affecting thermogram, applications TGA for quantitative analysis and problems based TGA. **b. Differential Thermal Analysis (DTA):** Instrumentation, general principles, differential thermogram, simultaneous TG-DTA, Applications **c. Differential Scanning Calorimetry (DSC):** Principle, Instrumentation, and Applications. **d. Thermometric titrations and evolved gas analysis(EGA):** Principle, Instrumentation, and Applications
Unit III	**Atomic Spectroscopic Techniques** **a. Introduction to Optical Atomic Spectroscopic Analysis:** Theory, atomic line width, factors affecting spectral width, effect of temperature. **b. Atomic Absorption Spectroscopy:** Flame atomizer, types of flames, flame profile, Factors affecting atomization efficiency, electro-thermal atomizers, Cold vapour technique, radiation sources-HCL, EDL and instrumentation for

	AAS, chemical and spectral interferences, standard addition, internal standard method of analysis, Applications of AAS. **c. Atomic Emission Spectrometry (AES):** Sources, inductively coupled plasma and direct current plasma, Instrumentation of ICP-AES, AES with electric arc discharges, electrodes in AES, DC Arc, AC Arc and Spark sources, Stallwood jet apparatus, comparison of atomic absorption and emission methods, Applications of AES. **d. Atomic Fluorescence Spectroscopy (AFS):** Principle and working of AFS, applications of AFS. **e. Atomic Mass Spectroscopy:** Atomic weight in mass spectroscopy, mass to charge ratio, Types of atomic mass spectroscopy, transducer for mass spectroscopy, quadrupole mass analyzer, time of flight mass analyzer, double focusing mass analyzer, inductively coupled mass spectroscopy (ICPMS), Applications of ICPMS. **f. Laser Based Techniques:** Concept of LASERS, types of lasers, solid state laser: Ruby laser, Nd:YAG laser, comparison of 3L and 4L laser system, dye laser, gaseous laser: He:Ne laser, CO_2 laser, Resonant Ionization Spectroscopy, Laser-enhanced ionization spectroscopy.

Reference Books:

1. Introduction to instrumental analysis by R. D. Broun, Mc Graw Hill (1987)
2. Instrumental methods of chemical analysis by H. Willard, L. Merrit, J.A. Dean and F.A. settle. Sixth edition CBS (1986)
3. Fundamentals of analytical chemistry by D. A. Skoog, D. M. West and H. J. Holler sixth edition (1992)
4. Principles of Instrumental Analysis Skoog, West, Niemann.
5. Vogel Text Book of quantitative analysis 6th Ed.
6. J. chemical education, 60,302 to 308 (1983)
7. Thermal analysis by W.W. Wendlandt, John Wiley, (1986)
8. Cyclic Voltammetry and frontiers of electrochemistry by N.Noel and K.I. Vasu IBH, New Delhi (1990)
9. Electrochemical Methods: Fundamentals and Applications by Allen J. Bard and Larry R. Faulkner.

CHA5302: Extraction techniques and Metallurgy [Credits – 4]

Course Outcomes

After learning this course student will be able to understand
CO1 Basic principle, various methods and applications of liquid phase and solid phase extraction.
CO2 Advance automation of SPME.
CO3 Methods of microwave and supercritical extractions.
CO4 Chemical methods for analysis of ores, alloys and soil samples.
CO5 Metallurgy of different metals and their refining techniques.

Unit I	**Liquid-Liquid extraction (LLE):** Introduction, selection of solvents, types of solvent extractions, problems and remedies of LLE process, purge and trap for volatile organics in aqueous samples. **Solid Phase Extraction (SPE):** Introduction, Types of SPE media, SPE apparatus, method for SPE operation, solvent selection, factors affecting SPE, Automation and On-Line SPE. Introduction to Solid phase micro-extraction, Automation of SPME, New development in micro extraction (liquid micro extraction, membrane micro extraction).
Unit II	**Microwave Assisted and Supercritical Fluid Extraction** Microwave assisted Extraction: Introduction, concept of magnetron, atmospheric MAE process, pressurised MAE process, Applications. Supercritical fluid extraction: concept of critical state of matter and super critical state, properties of CO_2 SFE, instrumentation and applications.
Unit III	**Analysis of Ores and Alloys:** Ores and minerals, Dolomite (For silicate, Mg and Ca), Ilmenite (for silicate, Ti and Fe), Monazite (for rare earth metals), Hematite (silicate and Fe), Pyrolusite (for silicate and Mn) and bauxite (for Al and Silicate). Alloy: Types, composition and analysis of Copper based alloy like cupronickel (Cu, Ni), bronze (Cu, Sn) and brass (Cu, Zn), Aluminum based alloy Duralumin and Magnalium, stainless steel (Fe, Cr, Ni, Co, Cu, Mn), and Solder (Pb and Sn).
Unit IV	**Metallurgy:** Sources of raw material, Concentration of ores, methods of metal dressing (hand picking, magnetic separation, centrifuge, froth flotation etc.), pollution due to metallurgical process (Metal dressing, calcinations, smelting). Principles of pyrometallurgy-roasting, agglomeration, smelting, refining & secondary refining, extraction of Fe from Hematite ore. Principles of hydrometallurgy, extraction of Al from bauxite. Principles of Electrometallurgy, extraction of Cu from Copper pyrites.
Unit V	**Analysis of Soil:** Chemical and mineralogical composition of soil, classification of soil, macro and micronutrients (functions and deficiency) for plant growth, Sampling, determination of Moisture Content, Water Holding Capacity. Analysis of Carbonate, Organic carbon, and organic matter, Total nitrogen, ammonia and nitrates, Total determination of major soil constituents by fusion analysis, silica and total combined oxides of iron, aluminium, and titanium, Determination Ca, Mg, Na, K, phosphate, Exchangeable cations, Cation exchange capacity.

Reference Books:

1. Vogel's Textbook of Quantitative analysis 6th Ed.

2. Modern analytical techniques in the pharmaceutical and bio analysis by Dr. Istvan Bak (Book Available Online).
3. Preparative chromatography Chrome Ed. book series, Raymond P. W. Scott (free e-book available on internet)
4. Extraction technique in analytical science, John R. Dean, Wiley (2009)
5. Practical HPLC method Development, Snyder, Kirki and Glajch, Wiley India Pvt. Ltd.

CHA5303: Pharmaceutical Chemistry [Credits-4]

Course Outcomes

After learning the course student will be able to understand
CO1 Importance of FDA in pharmaceutical industries.
CO2 Various dosage forms and vegetable drugs along with their analysis.
CO3 Concepts of pharmacology.
CO4 Precautions needed to be taken while processing pharmaceutical product.
CO5 Major source of impurities and techniques to identify it.
CO6 Separation techniques and method validation.
CO7 Implementation of Indian Pharmacopeia for course content.

Unit I	**a. Introduction to FDA** **b. 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	**a. Evaluation of solid dosage Forms-Tablets and capsule** **i.** 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, **ii.** Moisture / water content by Karl-Fischer titration- Principle, types of Karl Fischer titration, preparation and standardization of Karl Fischer reagent. **b. Sterilization:** Methods for Sterilization (Physical and chemical method), Applications.
Unit III	**Pharmacology: Pharmacokinetics and dynamics** **a. Introduction and importance** **b. 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). **c. 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	**a. 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 **b. Shelf Life of Pharmaceutical Product:** shelf life of Pharmaceutical product and determination of shelf life. Water for pharmaceutical use. **c. Limit test:**Limit tests for aluminium, arsenic, iron, lead, potassium, sulphate, chloride, heavy metals

Unit V	**Analysis of plant derived 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** **a. 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. **b. 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.

Reference Books:

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.

CHA5304 Structure Determination by Analytical Methods [Credits – 4]

Course Outcomes

After learning this course student will be able to understand
CO1 Different techniques in spectroscopy
CO2 Organic structure analysis
CO3 Structure from spectra
CO4 Spectroscopic identification of organic compounds
CO5 Interpretation of different types of spectra
CO6 One and two dimensional nmr spectroscopy
CO7 Applications of mass spectrometry
CO8 Advanced 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-spincoupling, (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, 4Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear over-hauser 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)

Reference Books:

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 - ML 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

CHA5306: Analytical Chemistry Practical V [Credit-4]

Any 15 Practical

Title of Experiment

I. Ore and alloy analysis
1. Dolomite
2. Magnalium

II. Analysis of industrial material
1. Cement
2. Fertilizer (N)
3. Fertilizer (P)
4. Assay of Detergent
5. Fe from detergent
6. Estimation of Urea
7. Loss on Drying of $CuSO_4$ and LOI of ZnO

III. Analysis of pharmaceutical product
1. Nicotine
2. Limit tests for acid and basic radicals
3. Milk of Magnesia

IV. Analysis of Blood
1. Ketone bodies
2. Cholesterol

V. Isolation and Analysis of plant materials
1. Lycopene
2. Citric acid
3. Resin (Ginger sample)
4. Volatile Oils (Bitter Almond or Thujone oil)
5. Determination of equivalent weight of carboxylic acid by titration with Std. alkali solution.
6. Determination of water soluble ash in Ginger

Note: Any other equivalent practical

CHA5307: Analytical Chemistry Practical VI

[Credit-4]

Any 15 Practical

Title of Experiment

I. Conductometry
1. Estimation of aspirin from tablet
2. Determination of concentration of acid mixture and copper sulphate
3. Compare relative strengths of different acids

II. pH metry
1. Determination of strength of acid in a mixture
2. Determination of strength of ammonia solution.

III. Flame photometer
1. Estimation of sodium
2. Estimation of potassium
3. Estimation of calcium
4. Estimation Na and K from mixture

IV. Nephelometry
1. Determination of sulphate ion
2. Determination chloride from water sample

V. Cyclic voltamogram
1. Diffusion current of $K_3Fe(CN)_6$
2. Estimation of commercial samples.

VI. Spectrophotometer
1. Estimation of Amino acid.
2. Estimation of protein.
3. Estimation of reducing sugar.
4. Determination of Iron from pharmaceutical dosage form
5. Estimation of Aspirin.
6. Estimation of chlorophylls in leaf pigments.
7. Determination of phosphorous content from fruit juice
8. Ferric thiocyanate complex by Ostwald method

VII. Polarography
1. Determination of Cu and Zn
2. Amperometric titration of Pb(II) with potassium dichromate solution.

VIII. Atomic absorption spectroscopy
1. Analysis of metal ions

IX. Pharmacology
1. Pharmacokinetic study of drug action

Note: Any other equivalent practical

Semester IV

CHA5401: Forensic science and Toxicology [Credits – 4]

Course Outcomes

After learning this course student will be able to understand
CO1 History and role of Forensic science in crime investigations.
CO2 Importance of toxicology and its role.
CO3 Roles of different Forensic Laboratory Units.
CO4 Principles of different techniques used in crime scene investigation.
CO5 Identification of different drugs and isolations of poisons from body fluid.

Unit I	**Forensic Science:** **a. Introduction:** History, role of forensic science in crime investigation, collection and preservation of biological materials. **b. Physical Evidence**: Common Types of Physical Evidences and its Significance. **c. Trace evidence:** Introduction, principle, Hair, fibre and paints analysis.
Unit II	**a. Bloodstain Pattern Analysis**: Blood and blood grouping, type of bloodstain pattern and application. **b. DNA Profiling:** Introduction, principle, DNA and its polymorphism, DNA typing procedures-RFLP, PCR, AFLP, STR, other methods, paternity testing, applications, interpretation and practical use**,** southern blotting technique. **c. 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	**a. Glass and Soil analysis:** Identification, Comparison, Collection and Preservation of samples **b. Document and Voice Analysis:** Principle and application. **c. Internet and Forensic**
Unit V	**Forensic Toxicology:** **a.** Introduction, clinical and practical aspects of analytical toxicology. **b. Poisons:** Type of poisons, detection of poison in biological fluid- physical and chemical method. **c. Drugs:** Classification of drugs, isolation, identification and determination of Narcotics- heroin and cocaine, Stimulants- caffeine, amphetamines, Depressants- Barbiturates, Benzodiazepines. **d. Alcohol in body fluids:** Legal background, Sampling and sample preservation, analysis-GC, IR, enzymatic and other methods.

Reference Books:

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 ByDr. 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 2ndEdn (1990)

CHA5402: Chemistry of Natural Products and Chiron Approach

[Credits – 4]

Course Outcomes

After learning this course student will be able to understand
CO1 Retro synthetic analysis of important natural products
CO2 Synthesis of important natural products
CO3 Sarious building blocks in synthesis natural products
CO4 Biogenesis of various oxygen and nitrogen containing natural products
CO5 Chiral nature of sugars and their use as chiron in syntheses of various chiral molecules
CO6 Importance of chiral drugs and syntheses of few chiral drug molecules
CO7 Various drug targets and structure activity relationship between drug molecules and their targets

Unit I	**Total Synthesis of some important Natural products:** **a.** Taxol **b.** Estrone and Mifepristone **c.** Juvabione (Mori and Matsui synthesis and Pawson and Cheung Synthesis) **d.** Fredericamycin A
Unit II	**Biogenesis**: The building blocks and construction mechanism of **a.** Terpenoids – Mono, Sesqui, Di and Triterpenoids and cholesterol **b.** Alkaloids derived from ornithine, lysine, nicotinic acid, tyrosine and tryptophan. **c.** The shikimate pathway – cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavanoids and terpenoid quinones.
Unit III	**Chiron Approach:** **a.** Introduction **b.** 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

Reference Books:

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, 288-292, (1973).
   ii) J.Am.Chem.Soc. Vol.77.432-437,(1955).

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. Hanessianh4.Pharmaceutical Chemistry and drug synthesis –Rot and Kleeman
13. Drug Design –E.J. Arienes

CHA 5404: Analytical Spectroscopy [Credits-4]

Course Outcomes

After learning the course student will be able to understand

CO1 Concept of different spectroscopic techniques.

CO2 Principle and instrumentation of electron spectroscopy, chemiluminescence, fluorescence and phosphorescence, surface characterization techniques and XRD.

CO3 Applications of spectroscopic techniques

Unit I	**Electron Microscopy** **a. Electron spectroscopy:** Introduction, principle of Ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS), types of peaks, chemical shifts, Instrumentation, Applications, Auger electron microscopy-principle, instrumentation and applications, similarities and differences in ESCA and AES, advantages and disadvantages. **b. 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 applications.
Unit II	**X- ray Methods of Analysis:** Principle, Theory- X-ray spectral lines, instrumentation, 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. **2-D 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.

Reference Books:

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.

CHA5405 Advanced Synthetic Organic Chemistry [Credits – 4]

Course Outcomes

After learning this course student will be able to understand
CO1 applications of transition metals in metal mediated coupling reactions
CO2 various reactions involving C=C formation
CO3 multicomponent reactions (MCR)
CO4 study ring formation reactions, Click chemistry
CO5 metathesis reactions
CO6 reactions involving Boron and Silicon
CO7 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

Reference Books:

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, 5th 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

CHA 5407: Polymer Chemistry [Credits – 4]

Course Outcomes

After learning this course student will be able to understand
CO1 Concept and classification of polymer.
CO2 Polymerization techniques.
CO3 Physic-chemical properties and analysis of polymers.
CO4 Concept of calculating average molecular weight by different methods.
CO5 Application 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, dispersity, 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, 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, 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, The Flory-Huggins theory, nature of polymer molecules in solution.
Unit V	**Analysis and Testing of Polymers:** **a.** Thermal analysis (TGA, DTA and DSC) of polymers **b.** Physical testing of polymers: Mechanical properties, Fatigue testing, impact testing, tear resistance, hardness, abrasion resistance. **c.** Thermal Testing: flammability, Heat deflection temperature, Vicat softening temperature, torsion pendulum test, thermal conductivity, thermal expansion. **d.** Optical properties: transmittance, colour, gloss, haze and transparency. **e.** Electrical properties: dielectric constant and loss factor, resistively, dielectric strength, electronic properties.

	f. 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, colorants. **Application of polymers:** Plastics, Natural and synthetic fibers, acrylic fibers, elastomers, adhesives

Reference Books:

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. Vishvanathane, 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.

CHA5408: Designing Organic Synthesis and Asymmetric Synthesis [Credits – 4]

Course Outcomes

After learning this course student will be able to understand

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

CO2 Outline important classical and modern reactions used in organic synthesis.

CO3 To design of synthetic routes by using choice of reagents and conditions taking into account cost, safety and environmental factors

CO4 Problem solving ability, involved in process development and the scale up of synthesis of commercially important compounds

CO5 The importance of the use of protection and de-protection in organic synthesis

CO6 The concept and principles of asymmetric synthesis

CO7 The applications of asymmetric syntheses in various synthetic methodologies

Unit I	**Designing Organic Synthesis:** **a.** Retrosynthesis **b.** Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions **c.** Umpolung in organic synthesis
Unit II	**symmetric Synthesis:** **a.** Chirality transfer, Asymmetric inductions; Chiral pools, Chiral auxiliaries and chiral reagents **b.** Organocatalysis **c.** Asymmetric Reactions: **d.** 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. **e.** Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, Felkin Anh rule, Cram's chelate model, etc. **f.** Enzyme catalyzed reactions binding mechanism of enzymes

Reference Books:

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 by 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, George Richard, Springer

CHA 5410: Analytical Chemistry Practical VII

[Credit-4]

Any 15 Practical

Title of Experiment

I. Ore and alloy analysis
1. Bronze
2. Brass

II. Analysis of industrial material
1. Plaster of Paris
2. Talcum powder
3. Pigment (Ti)
4. Pigment (zinchrome)
5. End group analysis of polymer (acid number /hydroxyl values/ Iodine value)

III. Analysis of food sample
1. Caffeine
2. HMF
3. Casein
4. Fat
5. Vit-C
6. Acid value from oil
7. Saponification value from oil
8. Rancidity of oil

IV. Analysis of Blood
1. Creatinine
2. Glucose

V. Isolation and Analysis of plant materials
1. Tannin
2. Flavanoide (Hespridine-orange peel)

VI. Assay by non-aqueous titration method
1. Sulpha drug

VII. Nanomaterial
1. Synthesis of nanoparticles and its analysis.

VIII. Forensic Science
1. Comparison of two presumptive tests for blood.
2. Identification of drugs and poisons by chemical method (Ba, aniline, antimony, CCl_4 etc.)

Note: Any other equivalent practical

CH5411: Analytical Chemistry Practical VIII

[Credit-4]

Any 15 Practical

Title of Experiment

I. Conductometry
1. Determination of strength of commercial vinegar
2. Determination of strength of borax
3. Determination of the basicity

II. pH metry
1. Analysis of mixture of carbonate and bicarbonate present in water sample using pH metry.

III. Spectrophotometer
1. Determination of the amount of carbohydrate in potato by Anthrone method.
2. Estimation of fluoride in commercial sample
3. Determination of ionisation constant of indicator
4. Determination of dissociation constant of indicator
5. Determination of isobestic point of indicator
6. Drug action of salicylic acid by spectrophotometry
7. Determination of p-nitrophenol from the given mixture
8. Estimation of Cu and Fe
9. Removal of toxic dyes /metals.

IV. Spectroflurometry
1. Analysis of Thaimine
2. Analysis of Quinine sulphate
3. Analysis of Riboflavin

V. Chromatographic techniques (HPLC/GC)
1. Estimation of alcohol content
2. Pesticide residue

VI. TGA
1. Thermal Thermo gravimetric analysis.

VII. Polymer
1. Determination of molecular weight by viscosity measurement.
2. Determination of polymer chain linkage
3. Determination of moisture content of resins or polymer solutions.
4. Determination of swelling of network polymer.
5. Determination of K value of polymer.

VIII. Karl-Fischer titrator
1. Determination of moisture content using Karl-Fischer titrator

IX. Data Analysis
1. A Statistical Evaluation of Data including Linear Regression Analysis.

Note: Any other equivalent practical

CH5412: Project / Internship [Credit-8]

Student 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