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

**Note:** Students offering less than 12 theory papers i.e.(48 credits) in previous semester can opt for the following MOOCs courses

<table>
<thead>
<tr>
<th>MOOC courses</th>
<th>Course-1</th>
<th>CHA-01</th>
<th>Research Methodology</th>
<th>MOOCs</th>
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<tbody>
<tr>
<td>Course-2</td>
<td>CHA-02</td>
<td>Solid and hazardous Waste Management</td>
<td>MOOCs</td>
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<td>Course-3</td>
<td>CHA-03</td>
<td>Environmental Chemistry</td>
<td>MOOCs</td>
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<td>Course-4</td>
<td>CHA-04</td>
<td>Food Microbiology and Food Safety</td>
<td>MOOCs</td>
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<tr>
<td>Course-5</td>
<td>CHA-05</td>
<td>Food Safety and Quality Control</td>
<td>MOOCs</td>
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</table>
**Semester III**

**CHA5301: Advance analytical techniques [Credits – 4]**

<table>
<thead>
<tr>
<th>Course Outcomes</th>
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<tbody>
<tr>
<td>After learning this course student will be able to understand</td>
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<tr>
<td>CO1 Theoretical background and develop practical skills for advanced instrumentation using modern analytical methods.</td>
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<tr>
<td>CO2 To design an analytical process for data collection and the project's research objectives.</td>
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<tr>
<td>CO3 To build an analytic skill to solve a real problem.</td>
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<tr>
<td>CO4 To interpret, communicate as well as write technical reports as per research aspect.</td>
</tr>
</tbody>
</table>

**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 Voltammetry, 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.
- **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.


<table>
<thead>
<tr>
<th>Reference Books:</th>
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<tbody>
<tr>
<td>5. Vogel Text Book of quantitative analysis 6th Ed.</td>
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<tr>
<td>6. J. chemical education, 60,302 to 308 (1983)</td>
</tr>
</tbody>
</table>
# 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\textsubscript{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).
4. Extraction technique in analytical science, John R. Dean, Wiley (2009)
5. Practical HPLC method Development, Snyder, Kirki and Glajch, Wiley India Pvt. Ltd.
### 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

<table>
<thead>
<tr>
<th>a. <strong>Introduction to FDA</strong></th>
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<tbody>
<tr>
<td>b. <strong>Dosage form and analysis</strong>: 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.</td>
</tr>
</tbody>
</table>

### Unit II

<table>
<thead>
<tr>
<th>a. <strong>Evaluation of solid dosage Forms-Tablets and capsule</strong></th>
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</thead>
<tbody>
<tr>
<td>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,</td>
</tr>
<tr>
<td>ii. Moisture / water content by Karl-Fischer titration- Principle, types of Karl Fischer titration, preparation and standardization of Karl Fischer reagent.</td>
</tr>
<tr>
<td>b. <strong>Sterilization</strong>: Methods for Sterilization (Physical and chemical method), Applications.</td>
</tr>
</tbody>
</table>

### 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). |

### Unit IV

<p>| a. <strong>Sources of Impurities in Pharmaceutical Raw Materials &amp; Finished Products</strong>: Raw materials, Method of manufacture, Atmospheric contaminations, Cross contamination, Microbial contamination, Container contamination, Packaging errors, Chemical instability, Temperature effect and Physical changes |
| c. <strong>Limit test</strong>: Limit tests for aluminium, arsenic, iron, lead, potassium, sulphate, chloride, heavy metals |</p>
<table>
<thead>
<tr>
<th>Unit V</th>
<th>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.</th>
</tr>
</thead>
</table>
| 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.  
4. Ansel’s Pharmaceutical Analysis.  
| Unit I | **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, 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 | **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, alkylene, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, Homo nuclear \((^{13}C,^{15}C)\) 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:

4. Absorption spectroscopy of organic molecules –V. M. Parikh
10. Spectroscopic identification of organic compound - R M Silverstein, G C Bassler and T C Morril, John Wiley
12. Organic spectroscopy-William kemp, E L B with McMillan
14. Organic spectroscopy-RT Morrison and RN Boyd
15. Practical NMR spectroscopy - ML Martin, J J Delpench, and D J Martyin
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
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 CuSO₄ 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 K₃Fe(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.
   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]**

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

<table>
<thead>
<tr>
<th>Unit I</th>
<th>Forensic Science:</th>
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</thead>
<tbody>
<tr>
<td>a. <strong>Introduction</strong>: History, role of forensic science in crime investigation, collection and preservation of biological materials.</td>
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<tr>
<td>b. <strong>Physical Evidence</strong>: Common Types of Physical Evidences and its Significance.</td>
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<td>c. <strong>Trace evidence</strong>: Introduction, principle, Hair, fibre and paints analysis.</td>
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<thead>
<tr>
<th>Unit II</th>
<th>a. <strong>Bloodstain Pattern Analysis</strong>: Blood and blood grouping, type of bloodstain pattern and application.</th>
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</thead>
<tbody>
<tr>
<td>b. <strong>DNA Profiling</strong>: 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.</td>
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<tr>
<td>c. <strong>Fingerprint Analysis</strong>: Latent fingerprints; optical, physical, physico-chemical &amp; chemical detection methods; fingerprints in blood, fingerprint detection sequences.</td>
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<tr>
<th>Unit III</th>
<th>Explosives and firearms:</th>
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<tbody>
<tr>
<td>Types, analytical methods for identification of low and high explosives in post-blast debris.</td>
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<thead>
<tr>
<th>Unit IV</th>
<th>a. <strong>Glass and Soil analysis</strong>: Identification, Comparison, Collection and Preservation of samples</th>
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<tbody>
<tr>
<td>b. <strong>Document and Voice Analysis</strong>: Principle and application.</td>
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<tr>
<td>c. <strong>Internet and Forensic</strong></td>
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<tr>
<th>Unit V</th>
<th>Forensic Toxicology:</th>
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<tbody>
<tr>
<td>a. <strong>Introduction</strong>, clinical and practical aspects of analytical toxicology.</td>
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<tr>
<td>b. <strong>Poisons</strong>: Type of poisons, detection of poison in biological fluid - physical and chemical method.</td>
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<tr>
<td>c. <strong>Drugs</strong>: Classification of drugs, isolation, identification and determination of Narcotics - heroin and cocaine, Stimulants - caffeine, amphetamines, Depressants - Barbiturates, Benzodiazepines.</td>
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<tr>
<td>d. <strong>Alcohol in body fluids</strong>: Legal background, Sampling and sample preservation, analysis-GC, IR, enzymatic and other methods.</td>
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</table>

<table>
<thead>
<tr>
<th>Reference Books:</th>
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<tbody>
<tr>
<td>1 Basic Analytical Toxicology Published by WHO, By R. J. Flanagan, R. A. Braithwaite, S. S. Brown Available Online</td>
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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 Various 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, isoflavonoids 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) Propandiol, (R) and (S) - Epichlorohydrin, L (+)-Alanine, 9(-) Multistatin, (-) 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-Indacrinone, hydrochloride, S-Captopril

Reference Books:
1. Chemistry of Natural products- Kalsi
5. Medicinal Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd Ed.(Wiley)
<p>| | |</p>
<table>
<thead>
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</table>
# 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

<table>
<thead>
<tr>
<th>Unit</th>
<th>Subject</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unit I</strong></td>
<td><strong>Electron Microscopy</strong></td>
</tr>
<tr>
<td></td>
<td>a. <strong>Electron spectroscopy</strong>: 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.</td>
</tr>
<tr>
<td><strong>Unit II</strong></td>
<td><strong>X-ray Methods of Analysis</strong>:</td>
</tr>
<tr>
<td></td>
<td>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.</td>
</tr>
<tr>
<td><strong>Unit III</strong></td>
<td><strong>Chemiluminescence, Fluorescence and phosphorescence</strong>: 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.</td>
</tr>
<tr>
<td><strong>Unit IV</strong></td>
<td><strong>Nuclear magnetic resonance spectroscopy</strong>:</td>
</tr>
<tr>
<td></td>
<td>$^1$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.</td>
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<tr>
<td></td>
<td>$^{13}$C NMR: Introduction, interpretation, chemical shifts, spin coupling, quantitative analysis, problems.</td>
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<tr>
<td></td>
<td>$^2$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.</td>
</tr>
<tr>
<td><strong>Unit V</strong></td>
<td><strong>Electron Paramagnetic Resonance Spectroscopy (EPR)</strong></td>
</tr>
<tr>
<td></td>
<td>Theory and Instrumentation, Spin Hamiltonian, Isotropic and anisotropic EPR spectra, Magic Pentagon rule. Applications of EPR spectroscopy.</td>
</tr>
</tbody>
</table>
**Reference Books:**

2. Instrumental methods of chemical analysis by Willard, Dean and Merittee- Sixth edition.
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)
5. Organic synthesis – Michael B. Smith
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
Course Outcomes

After learning this course student will be able to understand
CO1 Concept and classification of polymer.
CO2 Polymerisation 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).
Polymerisation 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.

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.
 d. Optical properties: transmittance, colour, gloss, haze and transparency.
 e. Electrical properties: dielectric constant and loss factor, resistivity, dielectric strength, electronic properties.

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:**
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.

<table>
<thead>
<tr>
<th>Unit I</th>
<th>Designing Organic Synthesis:</th>
</tr>
</thead>
<tbody>
<tr>
<td>a.</td>
<td>Retrosynthesis</td>
</tr>
<tr>
<td>b.</td>
<td>Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions</td>
</tr>
<tr>
<td>c.</td>
<td>Umpolung in organic synthesis</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit II</th>
<th>symmetric Synthesis:</th>
</tr>
</thead>
<tbody>
<tr>
<td>a.</td>
<td>Chirality transfer, Asymmetric inductions; Chiral pools, Chiral auxiliaries and chiral reagents</td>
</tr>
<tr>
<td>b.</td>
<td>Organocatalysis</td>
</tr>
<tr>
<td>c.</td>
<td>Asymmetric Reactions:</td>
</tr>
<tr>
<td>d.</td>
<td>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 aldo), Baylis-Hillman-Morita reactions.</td>
</tr>
<tr>
<td>e.</td>
<td>Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram’s rule, Felkin Anh rule, Cram’s chelate model, etc.</td>
</tr>
<tr>
<td>f.</td>
<td>Enzyme catalyzed reactions binding mechanism of enzymes</td>
</tr>
</tbody>
</table>

Reference Books:
1. Designing of organic synthesis - S. Warren (Wiley)
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
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

VIII. Forensic Science
   1. Comparison of two presumptive tests for blood.
   2. Identification of drugs and poisons by chemical method (Ba, aniline, antimony, CCl₄ 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

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.
   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.