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

<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>
</tr>
</thead>
<tbody>
<tr>
<td>Paper-1 CHO5301</td>
<td>Stereochemistry of Organic Molecules</td>
<td>CORE-1</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-2 CHO5302</td>
<td>Structure Determination by Analytical Methods</td>
<td>CORE-2</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-3 CHO5303</td>
<td>Chemistry of Heterocycles and Medicinal Chemistry</td>
<td>D. elective</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5304</td>
<td>Pharmaceutical Chemistry</td>
<td>G. Elective</td>
<td>MOOC1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5305</td>
<td>MOOC Course</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-4 CHO5306</td>
<td>Organic Chemistry Practical V</td>
<td>PCORE-1</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-5 CHO5307</td>
<td>Organic Chemistry Practical VI</td>
<td>PCORE-1</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-1 CHO5401</td>
<td>Chemistry of Natural Products and Chiron Approach</td>
<td>D. elective</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5402</td>
<td>Forensic Science and Toxicology</td>
<td>G. Elective</td>
<td>MOOC2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5403</td>
<td>MOOC Course</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-2 CHO5404</td>
<td>Advanced Synthetic Organic Chemistry</td>
<td>D. elective</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5405</td>
<td>Analytical Spectroscopy</td>
<td>G. Elective</td>
<td>MOOC3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5409</td>
<td>MOOC Course</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-3 CHO5407</td>
<td>Designing of Organic Synthesis and Asymmetric Synthesis</td>
<td>D. elective</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5408</td>
<td>Polymer Chemistry</td>
<td>G. Elective</td>
<td>MOOC4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHO5409</td>
<td>MOOC Course</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-4 CHO5410</td>
<td>Organic Chemistry Practical VII</td>
<td>PCORE-3</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-5 CHO5411</td>
<td>Organic Chemistry Practical VIII</td>
<td>PCORE-4</td>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OR</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Paper-6 CHO5412</td>
<td>Project / Internship (Optional for practical courses CHO5410 and CHO5411)</td>
<td></td>
<td>8</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 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
- CO2 Stereochemistry of fused and bridged rings systems
- CO3 Concept of racemic modification and methods to achieve it
- CO4 To determine the structure and stereochemistry of some naturally occurring molecules with ring structures

<table>
<thead>
<tr>
<th>Unit</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unit I</strong></td>
<td>Stereochemistry of Six membered rings and their reactions</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Unit II</strong></td>
<td>Stereochemistry of rings other than Six-membered ring</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Unit III</strong></td>
<td>Fused, Bridged and Caged rings, Baldwin’s Rule</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Unit IV</strong></td>
<td>Resolution of racemic modification.</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Unit V</strong></td>
<td>Structure and Stereochemistry of Morphine, Quinine, Lactone Fusion in Enhydrin, Hardwickiic acid and Camptothecin</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### References:

1. Stereochemistry of carbon compounds - E. L. Elie
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
**CHO5302: Structure Determination by Analytical Methods**

**[Credits – 4]**

<table>
<thead>
<tr>
<th>Course Outcomes</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Students will learn:</td>
<td></td>
</tr>
<tr>
<td>CO1 Different techniques in spectroscopy</td>
<td></td>
</tr>
<tr>
<td>CO2 Organic structure analysis</td>
<td></td>
</tr>
<tr>
<td>CO3 Structure from spectra</td>
<td></td>
</tr>
<tr>
<td>CO4 Spectroscopic identification of organic compounds</td>
<td></td>
</tr>
<tr>
<td>CO5 Interpretation of different types of spectra</td>
<td></td>
</tr>
<tr>
<td>CO6 One and two dimensional NMR spectroscopy</td>
<td></td>
</tr>
<tr>
<td>CO7 Applications of mass spectrometry</td>
<td></td>
</tr>
<tr>
<td>CO8 Advanced methods of spectral analysis</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unit I</strong></td>
<td><strong>^1H-NMR Spectroscopy:</strong></td>
</tr>
<tr>
<td></td>
<td>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 deuteriation (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(_2)B(_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.</td>
</tr>
<tr>
<td><strong>Unit II</strong></td>
<td><strong>^13C NMR spectroscopy:</strong></td>
</tr>
<tr>
<td></td>
<td>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}\text{C}-^{13}\text{C})) and Hetero nuclear ((^{13}\text{C}-^{1}\text{H})) coupling constants.</td>
</tr>
<tr>
<td><strong>Unit III</strong></td>
<td><strong>2D NMR Techniques:</strong></td>
</tr>
<tr>
<td></td>
<td>General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)–Homo COSY ((^{1}\text{H}-^{1}\text{H})), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.</td>
</tr>
<tr>
<td><strong>Unit IV</strong></td>
<td><strong>Mass Spectrometry:</strong></td>
</tr>
<tr>
<td></td>
<td>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.</td>
</tr>
<tr>
<td><strong>Unit V</strong></td>
<td>Problems based on joint application of UV, IR, PMR, CMR, and Mass (Including reaction sequences).</td>
</tr>
</tbody>
</table>

**References:**

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 - M. L. 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
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
CO2 Five and six membered fused heterocycles: Synthesis, reactivity and mechanistic aspects
CO3 Heterocycles with two or more heteroatoms
CO4 Medicinal chemistry:
    CO5 Drug targets
    CO6 QSAR studies
CO7 Biological activities of drugs
CO8 Synthetic aspects of drugs

<table>
<thead>
<tr>
<th>Unit I</th>
<th>Five and six membered heterocycles with one and two hetero atoms:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Furan, Pyrrole, Thiophene, Pyridine, Pyrazole, Imidazole, Oxazole, Thiazole, Pyrimidines</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit II</th>
<th>Condensed five and six membered heterocycles with one and two hetero atoms:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Benzofuran, Indole, Benzo-[b]-thiophene, Quinoline, Isobenzofuran, Isoindole, Benzo-[c]-thiophene, Isoquinoline, Benzoxazole, Benzothiazole, Benzimidazole</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit III</th>
<th>Five and six membered heterocycles with more than two hetero atoms:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1,2,3-Triazole, 1,2,4-Oxadiazole, 1,2,5-Oxadiazole, Tetrazole, Purine</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit IV</th>
<th>Introduction to drugs, their action and discovery</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Drug targets</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit VI</th>
<th>Relation of Drug structure and its chemical and biological properties (QSAR), Synthetic aspects</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Unit VII</th>
<th>Antibacterial, Antiviral, Antifungal, Antiprotozoal, Anticancer, Antidiabetic, Anti-Alzheimer drugs</th>
</tr>
</thead>
</table>

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
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]

<table>
<thead>
<tr>
<th>Course Outcomes</th>
</tr>
</thead>
<tbody>
<tr>
<td>After learning this course students will be able to understand:</td>
</tr>
<tr>
<td>CO1 Importance of FDA in pharmaceutical industries.</td>
</tr>
<tr>
<td>CO2 Various dosage forms and vegetable drugs along with their analysis.</td>
</tr>
<tr>
<td>CO3 Concepts of pharmacology.</td>
</tr>
<tr>
<td>CO4 Precautions needed to be taken while processing pharmaceutical product.</td>
</tr>
<tr>
<td>CO5 Major source of impurities and techniques to identify it.</td>
</tr>
<tr>
<td>CO6 Separation techniques and method validation.</td>
</tr>
<tr>
<td>CO7 Implementation of Indian Pharmacopeia for course content.</td>
</tr>
</tbody>
</table>

#### 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:**
- 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.
4. Ansel’s Pharmaceutical Analysis.
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
- Heterocyclic synthesis
- Self-redox
- Wittig reaction

References:

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:
CHO5401: Chemistry of Natural Products and Chiron Approach

[Credits – 4]

Course Outcomes
Students will learn:
CO1 The retro synthetic analysis of important natural products
CO2 The 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:
- 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, isoflavonoids 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(-) 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

References:
1. Chemistry of Natural products - Kalsi
5. Medicinal Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd Ed.(Wiley)

11 | Department of Chemistry, Fergusson College (Autonomous), Pune
12. Chiron Approach in organic synthesis - S. Hanessianh
13. Pharmaceutical Chemistry and drug synthesis - Rot and Kleeman

CHO5402: Forensic Science and Toxicology [Credits – 4]
Course Outcomes
Students will learn:
CO1 History and role of Forensic science in crime investigations.
CO2 Importance of toxicology and its role.
CO3 Different Forensic Laboratory Units and their roles.
CO4 Different methods of isolations of poisons from body fluid
CO5 Analysis of crime scene evidences using different techniques.

<table>
<thead>
<tr>
<th>Unit I</th>
<th>Forensic Science:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Introduction:</strong> History, role of forensic science in crime investigation, collection and preservation of biological materials.</td>
</tr>
<tr>
<td></td>
<td><strong>Physical Evidence:</strong> Common Types of Physical Evidences and its Significance.</td>
</tr>
<tr>
<td></td>
<td><strong>Trace evidence:</strong> Introduction, principle, Hair and fibre analysis</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit II</th>
<th>Explosives and firearms: Types, analytical methods for identification of low and high explosives in post-blast debris</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Bloodstain Pattern Analysis:</strong> Blood and blood grouping, type of bloodstain pattern and application.</td>
</tr>
<tr>
<td></td>
<td><strong>DNA Profiling:</strong> 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.</td>
</tr>
<tr>
<td></td>
<td><strong>Fingerprint Analysis:</strong> Latent fingerprints; optical, physical, physico-chemical &amp; chemical detection methods; fingerprints in blood, fingerprint detection sequences.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit III</th>
<th>Explosives and firearms: Types, analytical methods for identification of low and high explosives in post-blast debris</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Hairs, Fibers, and Paint:</strong> Identification, Comparison Collection and Preservation of Hair Fiber and Paint evidences.</td>
</tr>
<tr>
<td></td>
<td><strong>Glass and Soil analysis:</strong> Identification, Comparison, Collection and Preservation of samples</td>
</tr>
<tr>
<td></td>
<td><strong>Document Analysis:</strong> Principle and application</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Unit IV</th>
<th>Forensic Toxicology:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Introduction:</strong> Introduction to toxicology, role of forensic toxicology.</td>
</tr>
<tr>
<td></td>
<td><strong>Poisons:</strong> 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.</td>
</tr>
<tr>
<td></td>
<td><strong>Drugs:</strong> Classification of drugs, isolation, identification and determination of following, Narcotics- heroin and cocaine, Stimulants- caffeine, amphetamines, Depressants- Barbiturates, Benzodiazepines.</td>
</tr>
<tr>
<td></td>
<td><strong>Alcohol in body fluids:</strong> Legal background, Sampling and sample preservation, analysis-GC, IR, enzymatic and other methods</td>
</tr>
</tbody>
</table>

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 Pharmaceutical Chemistry by Becket
<table>
<thead>
<tr>
<th>No.</th>
<th>Reference</th>
</tr>
</thead>
</table>
CHO5404: Advanced Synthetic Organic Chemistry [Credits – 4]

Course Outcomes
Students will learn:

CO1 Applications of transition metals in metal mediated coupling reactions
CO2 Various reactions involving C=C formation
CO3 Multicomponent reactions (MCR)
CO4 Ring formation reactions
CO5 Click chemistry
CO6 Metathesis reactions
CO7 Reactions 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)
3. Designing of organic synthesis - S. Warren (Wiley)
5. Organic synthesis - Michael B. Smith
6. Organometallics in organic synthesis - J. M. Swan and D. C. Black (Chapman and Hall)
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.
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>Analytical Method</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unit I</strong></td>
<td><strong>Electron Microscopy</strong></td>
</tr>
<tr>
<td></td>
<td>- <strong>Electron spectroscopy</strong>: 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.</td>
</tr>
<tr>
<td><strong>Unit II</strong></td>
<td><strong>X-ray Methods of Analysis:</strong></td>
</tr>
<tr>
<td><strong>Unit III</strong></td>
<td><strong>Chemiluminescence, Fluorescence and phosphorescence:</strong></td>
</tr>
<tr>
<td></td>
<td>Introduction, principle, types, measurement of chemiluminescence, instrumentaion, quantitative 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>- <strong>1H NMR</strong>: Introduction, theory, Instrumentation, Chemical Shifts, Spin-Spin splitting, protons on hetero atoms, coupling protons with other nuclei, solvents, qualitative and quantitative analysis, problems.</td>
</tr>
<tr>
<td></td>
<td>- <strong>13C NMR</strong>: Introduction, interpretation, chemical shifts, spin coupling, quantitative analysis, problems.</td>
</tr>
<tr>
<td></td>
<td>- <strong>2D NMR</strong>: Introduction, <strong>1H-1H connectivity</strong>, <strong>1H-13C connectivity</strong>, <strong>13C-13C connectivity</strong>, Through space <strong>1H-1H proximity</strong>, 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>
### References:

2. Instrumental methods of chemical analysis by Willard, Dean and Merittee - Sixth edition.
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.
CO2 To outline important classical and modern reactions used in organic synthesis.
CO3 Designing synthetic routes by using choice of reagents and conditions taking into account cost, safety and environmental factors.
CO4 To develop problem solving ability.
CO5 Problems involved in process development and the scale up of synthesis of commercially important compounds.
CO6 The importance of the use of protection and de-protection in organic synthesis.
CO7 The concept and principles of asymmetric synthesis.
CO8 The 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:
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

<table>
<thead>
<tr>
<th>Unit I</th>
<th><strong>Introduction of Polymers:</strong> Basic concepts, History of polymers, Classification of polymers, classification of polymers based on: Origin, structure, stereochemistry, synthesis, type of chain and mechanical properties</th>
</tr>
</thead>
</table>
| 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. |
<table>
<thead>
<tr>
<th>Unit VI</th>
<th>Polymer additives:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical Test: Immersion test, vapor permeability, staining resistance, solvent stress cracking resistance, environmental stress cracking</td>
<td></td>
</tr>
<tr>
<td>Fillers, plasticizers, UV stabilizers and absorbers, antioxidants, flame retardants, colourants.</td>
<td></td>
</tr>
<tr>
<td>Application of polymers:</td>
<td></td>
</tr>
<tr>
<td>Plastics, Natural and synthetic fibers, acrylic fibers, elastomers, adhesives</td>
<td></td>
</tr>
</tbody>
</table>

**References:**

7. Principle of polymer science, Bahadhrur 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:

Experiments in applied chemistry:
- Isolation of Natural products
- Synthesis of Schiff bases for dyes
- Pharmaceutical scaffold synthesis
- Industrially useful Monomers
- Synthesis of agrochemicals

References:
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.