M.Sc. CHEMISTRY

ANALYTICAL CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS

REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR
2016 ONWARDS
M.Sc. CHEMISTRY (ANALYTICAL CHEMISTRY SPECIALISATION)
Syllabus for III and IV Semesters
(for the batches admitted in academic year 2016 & later under CBCS pattern)
[Under Restructured CBCS Scheme]
Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits
(Approved in the P.G. BOS meeting held on 01-07-2017)

Semester - III (ANALYTICAL CHEMISTRY)
[Under CBCS Scheme]
(for the batches admitted in academic year 2016 & later under CBCS pattern)

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<th>Semester exam</th>
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Total 600 marks 24

Semester - IV (ANALYTICAL CHEMISTRY)

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Total 600 marks 24

Grand total marks and credits (all 4 semesters) 2400 marks - 96 credits
M.Sc. ANALYTICAL CHEMISTRY

Semester III

Paper I: CH (AC) 301T: CORE:
Sampling, Data handling, Classical and Atomic spectral methods of analysis
AC-1: Sampling & Data handling
AC-2: Titrimetric & Gravimetric analysis
AC-3: Thermal & Radiochemical methods of analysis
AC-4: Atomic Spectroscopy

Paper II: CH (AC) 302T: CORE:
Spectroscopic methods of Analysis-I
AC-5: Multinuclear NMR
AC-6: Advanced NMR
AC-7: Electron Spin Resonance Spectroscopy
AC-8: Mossbauer and NQR

Paper III: CH (AC) 303T: ELECTIVE IIIa:
Miscellaneous Methods of Analysis
AC-9: Surface Analysis Methods
AC-10: Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC-11: Electroanalytical Methods
AC-12: Micromeritics, Dissolution and disintegration

Paper III: CH (AC) 303T: ELECTIVE IIIb:
Bonding, Group Theory and its Applications
AC-09: Group Theory, Normal mode analysis and Spectral activity
AC-10: MOT of Metal Complexes
AC-11: Electronic Spectroscopy of Metal Complexes
AC-12: IR and Raman Spectroscopy

Paper IV: CH (AC) 304T: ELECTIVE IVa:
Applied Analysis
AC-13: Industrial Analysis
AC-14: Analysis of Air and Water Pollutants
AC-15: Clinical and Pharmaceutical analysis
AC-16: Food and Agricultural analysis

Paper IV: CH(IC) 304T: ELECTIVE IVb
Nuclear Chemistry, Zeolites, Solid State, and Surface Chemistry
AC-13: Nuclear Chemistry
AC-14: Zeolites and Molecular Sieves
AC-15: Solid State Chemistry
AC-16: Surface Chemistry & Superconductors

LABORATORY COURSE
Paper CH (AC) 351P: Titrimetry, Solvent extraction, Chromatography and Water analysis.

Paper CH (AC) 352P: Colorimetry, Spectrophotometry
Semester IV

Paper I: CH (AC) 401T: CORE : Spectroscopic Methods of Analysis-II
AC-17: U.V. visible spectroscopy,
AC-18: IR & Raman spectroscopy
AC-19: Optical Methods
AC-20: Fluorimetry, Phosphorimetry, Nephelometry and Turidimetry

Paper II: CH (AC) 402T: CORE Separation Methods
AC-21: Solvent extractions
AC-22: Chromatography
AC-23: Mass spectrometry & Hyphenated techniques
AC-24: Electrophoresis

Paper III: CH (AC) 403T: ELECTIVE IIIa: Laboratory Management
AC-25: Automation in laboratory
AC-26: LIMS & Computer aided analysis
AC-27: Laboratory Management & Standard reference materials
AC-28: Accreditation of Laboratories, Quality management

Paper IV: CH (AC) 403T: ELECTIVE IIIb: Applied analysis and Green Analytical Chemistry
AC-25: Enzyme catalysis- Analytical applications
AC-26: Forensic Chemical Analysis
AC-27: Limit tests
AC-28: Green Analytical Chemistry

Paper IV: CH (AC) 404 T: Ida Quality Assurance and Accreditation
AC-29: Quality Assurance – I
AC-30: Quality Assurance – II
AC-31: Quality Assurance – III
AC-32: Quality Accreditation

Paper IV: CH (AC) 404 T: IDb Inorganic Material Chemistry
AC-29: Composite Materials
AC-30: Liquid Crystals
AC-31: Explosives and Propellants
AC-32: Fuels and Combustion

Paper CH (AC) 451P: Electro analytical techniques:

Paper CH (AC) 452P: Spectroscopy and Evaluation of Physical Parameters Of Tablets
M.Sc. ANALYTICAL CHEMISTRY SPECIALIZATION

Syllabus for III and IV Semesters

III Semester Syllabus

Paper- I: CH (AC) 301T: CORE : Sampling, Data handling, Classical and Atomic spectral methods of analysis

AC – 01 Sampling & Data handling

AC – 02 Titrimetric & Gravimetric analysis

AC – 03 Thermal & Radiochemical methods of analysis

AC – 04 Atomic Spectroscopy

AC – 01 Sampling & Data handling

15 Hrs

Classification of Analytical Methods. Types of samples, Preparation of sample for analysis, effect of sampling uncertainties, sample treatment, moisture in sample, decomposition of organic & inorganic compounds, procedure of sampling of solids, liquids and gases.


AC – 02 Titrimetric and Gravimetric Analyses

15 Hrs

**Redox titrations:** Formal and Standard potentials in various media, standardization, Oxidizing systems: Mn(VII), Ce(IV), Cr(VI), V(V). Reducing systems: V(II), Ti(III), Sn(II), Fe(II) in H₃PO₄. Detection of end point in redox titrations – selection of suitable indicator.

**Complexometric titrations:** Introduction, stability constants of EDTA complexes, titration curves, types of EDTA titrations with examples. Standard EDTA solutions, some practical considerations during EDTA titrations. Titration of mixtures (Mg²⁺ & Ca²⁺; Pb²⁺ & Ca²⁺; Mn²⁺ & Mg²⁺), selectivity, masking and demasking agents. Metal ion indicators: General properties, theory of the use of metal ion indicators, use of Murexide, Eriochrome black- T, Calcon, Xylenol orange, Methyl thymol blue, Fast sulphon black- F.

**Gravimetric Analysis:** Theory, principles, precipitation reagents (DMG, Oxine), Determination of Nickel as dimethylglyoximate, Aluminium as 8-hydroxyquinolate & Chloride as silver chloride.

AC – 03 Thermal and Radiochemical methods of Analysis

15 Hrs


**Radiochemical methods of analysis:** Radioactive tracer techniques and its applications, isotope dilution analysis, neutron activation analysis, radiometric titrations: principle, theory, applications and problems.
AC – 04 Atomic Spectroscopy


Suggested Books
10. Pharmaceutical analysis, Watson
AC – 05 Multinuclear NMR

$^{13}$C nmr spectroscopy: CW and PFT techniques. Types of $^{13}$C nmr spectra: undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. $^{13}$C chemical shifts, factors affecting the chemical shifts

Chemical equivalence and magnetic equivalence. Virtual Coupling and its importance in study of Metal Complexes [$\text{Pd}\{\text{P(CH}_3\}_3\}_2\text{I}_2$]. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-[$\text{Pt(PEt}_3\}_2\text{Cl}_2$], Sn(CH$_3$)$_4$. NMR Time Scale and its use in studying Stereo chemical Non –rigidity (PF$_5$, [$\text{Rh(PR}_3\}_3\text{Cl}_2$]). The Ring Contribution to $^{31}$P Chemical Shifts –Metal and Chelate size on $\Delta R$. Applications of $^1$H, $^{13}$C, $^{19}$F, $^{31}$P and $^{15}$N to simple inorganic and Coordination Compounds - 1) $^1$H-NMR: PtHCl(PEt$_3$)$_2$, Pt(NH$_3$)$_2$(CH$_3$)$_2$, BH$_4$, NH$_4^+$, CH$_3$CN, $^{6}$h- C$_7$H$_8$ Mo(CO)$_3$, $[^7$h-C$_7$H$_2$Mo(CO)$_3$]$, B_2H_6$; $^{29}$SiH$_3$SiH$_3$, $^{2}$F$_2$, H$_2$PF$_3$; 3) $^{31}$P: Mo(CO)$_3$(PPh$_3$)$_2$, [Rh (PPh$_3$)$_3$Cl],trans-[PtCl$_4$(PEt$_3$)$_2$], $^{31}$PF$_2$H($^{15}$NH$_2$)$_2$. 4) $^{13}$C; $^{[4}$h C$_8$H$_8$ Ru(CO)$_3$, Fe(CO)$_5$, Fe$_2$(CO)$_9$, Fe$_3$(CO)$_12$, FeICp(CO)$_2$, Cl(CH$_2$)$_2$Si(OCH$_3$)$_3$, $^{[13}C\{^{15}$N Co(DH)$_2$Pyridine$.^{13}$C{$^{1}$H} NMR spectrum of $\sigma$-bonded C$_6$H$_5$ ligand

AC – 06 Advanced NMR Spectroscopy:- Spin-Lattice ($T_1$) and Spin-Spin Relaxation ($T_2$). pin Echo Polarization Transfer – Spin Echo Measurements. $^{13}$C-NMR spectral editing techniques: Attached proton test (APT spectra) by Gated Spin Echo, Cross polarization, INEPT spectra, DEPT spectra (Distortionless enhancement by polarization transfer) (eg Cl(CH$_2$)$_2$Si(OCH$_3$)$_3$). INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment).

Two Dimensional NMR: Basic principles, Types of 2-D NMR ;i)J- resolved spectroscopy a)homo and b)Heteronuclear J- resolved spectroscopy ii) Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY) and Hetero nuclear shift correlation spectroscopy (HETCOR) iii) NOESY( Nuclear Overhauser Enhancement Spectroscopy). HOESY ( two dimensional heteronuclear NOE). Advantages of 2-D NMR

AC – 07 Electron Spin Resonance Spectroscopy

Principle- Selection Rules – Instrumentation- Microwave source( energy bands). Application of ESR to the study of simple free radicals: methyl (CH$_3$), amine (NH$_2$), diphenyl picryl hydrazyl, cyclopentadienyl (C$_5$H$_5$), hydroxy methyl(CH$_2$OH).radicals. Zero-Field Splitting (ZFS) - Effective Spin - Orbitally Non-degenerate and Degenerate States. ESR Spectra of d$^1$-d$^9$ Transition Metal Complexes with examples. Interpretation of g in cubic,axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Intensities of $^g\parallel$ and $^g\perp$ peaks . Evidence for Metal-Ligand Bond
Covalency- Cu(II)- Bis-Salicylaldimine. \([\text{(NH}_3\text{)}_5\text{O}_2\text{Co(NH}_3\text{)}_5]^ {5+}\), Cu(II)- diethylidithio phosphinate, Vanadyl dithio phosphinate, Copper(II) tetraphenyl porphyrin, Co(II)- phthalocyanine, \(\text{K}_2[\text{IrCl}_6]\). Interpretation of ‘g’ and ‘A’ values from esr spectral data in- i) \(\text{MnF}_6^{4+}\), ii) \(\text{CoF}_6^{4+}\), and \(\text{CrF}_6^{3+}\). ESR spectra of dinuclear Cu (II) complexes.

**AC – 08 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy**


Applications
Iron Compounds: Low-spin and High-spin Fe(II) and Fe(III) Complexes - \(\pi\)-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over c) Diamagnetic and Covalent Compounds - Structural aspects of Iron Carbonyls and Iron-Sulfur Proteins
Tin Compounds: Tin Halides and Organotin Compounds.
Iodine Compounds: Isomer Shifts of \(^{127}\text{I}\) and \(^{129}\text{I}\) – Applications to Alkali metal iodides and Molecular Iodine.

Nuclear Quadrupole Resonance Spectroscopy : Principle, nuclear quadrupole resonance experiment, structural information from NQR spectra, Interpretation of nuclear quadrupole coupling constants.

**SUGGESTED BOOKS**

10. Magneto Chemistry, Dutta & Shyamal
AC – 09 Surface Analysis Methods
AC – 10 Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC – 11 Electroanalytical Methods
AC – 12 Micromeritics, Dissolution and disintegration

AC-09Surface Analysis Methods
Introduction, types of surface measurements.

Photon Probe Techniques: X-Ray Photoelectron spectroscopy - Principle, Instrumentation, applications.


Ion Probe Techniques: Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation, applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle, Instrumentation (static & dynamic), applications


AC-10 : Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence

Electron Diffraction by gases: Principles, Applications to Silyl monothioacetate and Germyl monoethioacetate and HgCl₂ molecules, Advantages and Limitations


X-ray absorption method: Principle, radiographic non-dispersive x-ray Absorptiometers

X-ray fluorescence method: Instrumentation, qualitative and quantitative applications of XRF – advantages and limitations.

AC-11: Electro Analytical Methods

Electrogravimetry: Basic principles of electrogravimetry, Instrumentation, electrogravimetry determination with constant applied voltage and at constant current. Applications of electrogravimetry. Problems based on effect of concentration on electrode potentials, calculation of theoretical cathode potential at the start of deposition, effect of pH in electrolytic separations.

Coulometry: Basic principles, Types of coulometers, constant current coulometric analysis, coulometric titrations – principle, circuit and cell for coulometry, Application to neutralization, Redox, precipitation, complexometric titrations, Advantages of coulometric
titrations and errors. Controlled potential coulometry – Technique & applications of inorganic & organic compounds.

**High Frequency Titrations**  
Introduction, Theory, Instrumentation, Applications, Advantages and disadvantages

**AC-12: Micromeritics, Dissolution and disintegration**  
15 Hrs
Particle size analysis- concepts of particle size, size distribution, mean size of particulate system, methods of particle size analysis (sieving, microscopic method, sedimentation methods, electrical sensing zone method, optical sensing zone and light diffraction method). Dissolution: Drug absorption, theories of drug dissolution – Diffusion layer model, Danckwert’s model & interfacial barrier model. Dissolution tests for tablets and capsules (basket apparatus, paddle apparatus, flow through cell apparatus). Disintegration tests for tablets, capsules and enteric coated tablets.

**Suggested Books**
AC-09: Group Theory, Normal mode analysis and Spectral Activity  
AC-10: MOT of Metal Complexes  
AC-11: Electronic Spectroscopy of Metal Complexes  
AC-12: IR and Raman Spectroscopy  

AC-09: Group Theory, Normal Mode Analysis and Spectral Activity  
Properties of a Group: Closure rule, Identity rule, associative rule, inverse rule, Abelian and Non-abelian groups. Classes of Symmetry Elements of a Group: Similarity transformation, properties of conjugate elements, rules of Classes, Classes of $C_{2v}$, $C_{2h}$ and $C_{3v}$. Matrix Representation of Symmetry Elements: Simple Matrices, Matrix addition, subtraction and multiplication, Block-Factorization. Matrix Representation of $E$, $C_n$, $S_n$, $i$ and $\sigma$ Elements and $C_{2v}$, $C_{3v}$, $C_{2h}$, $C_{4v}$ & $D_{2h}$. Great Orthogonality Theorem: Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for $C_{2v}$, $C_{2h}$ and $C_{3v}$. Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula – Direct Products. Use of Character tables for IR & Raman spectroscopy, symmetry based selection rules for IR and Raman activity. Standard reduction formula. Type and Symmetry of Normal Modes and IR and Raman activity of molecules: Cartesian coordinate method of analysis for $C_{2v}$ (e.g. H$_2$O/SO$_2$, SF$_4$, ClIF$_3$, Cis-N$_2$F$_2$), $C_{3v}$ (NH$_3$/SO$_3^2-$/PCl$_3$, POCl$_3$), $C_{2h}$ (trans-N$_2$F$_2$), $D_{3h}$ (CO$_3^{2-}$/BF$_3$), $T_d$(SO$_4^{2-}$/PO$_4^{3-}$/CIO$_4^-$/NH$_4^+$), $O_h$ (SF$_6$). Internal coordinate method of analysis for $C_{2v}$(H$_2$O), $C_{3v}$ (NH$_3$), $T_d$ (SO$_4^{2-}$). Internal Coordinates and Redundancy (Qualitative concept).

AC-10: Molecular Orbital Theory of Metal Complexes  
Symmetry Classification of Metal and Ligand Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, Trigonal Bipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams for Octahedral, Tetrahedral and Square Planar Metal Complexes with Sigma ($\sigma$) and Pi ($\pi$) Bonding Contribution from the Ligands.

AC-11: Electronic Spectroscopy of Metal Complexes  

AC-12: Infrared and Raman Spectroscopy  
Conditions for Infrared and Raman Spectroscopies – Structure Fitting. Determination of Coordination Sites and Linkage Isomers(NO$_2^-$, SCN$^-$), Assigning Denticity of Ligands (SO$_4^{2-}$, CO$_3^{2-}$), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Sulfur, Nitrogen, Phosphorous, Carbon and Halogen Donors (NH$_3$, H$_2$O, Glycine, PPh$_3$, 2,2,-Bipy, 1,10-Phen, Carbonyl and halides). Raman effect and molecular structure- CO, HCN, CO$_2$, N$_2$O, H$_2$O.

SUGGESTED BOOKS
7. *Molecular Symmetry*, Schoenland
9. *Introduction to Ligand fields*, B. N. Figgis
10. *Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds*, K. Nakamoto
11. *Infrared spectroscopy of Inorganic Compound*, Bellamy.
Paper - IV CH(AC) 304T: ELECTIVE IVa: Applied Analysis

AC – 13 Industrial Analysis
AC – 14 Analysis of Air and Water Pollutants
AC – 15 Clinical and Pharmaceutical analysis
AC – 16 Food and Agricultural analysis

AC – 13 Industrial Analysis
15 Hrs
Analysis of Ferroalloys: Analysis of steel - Molybdenum, Phosphorous. Analysis of Ferromanganese, Ferrovanadium. Analysis of non-Ferrous alloys: Analysis of Tin, Zinc and Copper in Brass, Bronze. Analysis of Tin and lead in Solder. Analysis of Air Pollutants: Air quality standards, sampling, analysis of air pollutants - SO₂ (UV_Vis, IR), H₂S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO₂ (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O₃ (Chemiluminescence & Spectrophotometry), particulate matter analysis.

Analysis of Water Pollutants: Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total dissolved solids (turbidimetry). Chemical analysis of anions – CN-, Cl-, F-, NO₂⁻, NO₃⁻ (spectrophotometry), SO₄²⁻, PO₄³⁻. Determination of BOD, COD, TOC & DO. Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

AC – 15 Clinical and Pharmaceutical Analysis
15 Hrs
Clinical Analysis: Determination of (1) Serum Calcium (2) Serum/Plasma Bicarbonate (Titrimetry). (3) Serum sodium and potassium (Flamephotometry). Determination of Serum Chloride (Coulometry) - Determination of (1) Cholesterol (2) Total Protein (3) Blood Urea in Serum (4) Amylase (5) Aspartate Amino Transferase (AST) and Alanine Amino Transferase (ALT) (by Spectrophotometry). Determination of (1) Thyroxin and (2) Thyroid-Stimulating Hormone (TSH) (by RIA Method)

Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium in Vitamin D and Calcium formulations (Complexometry), Sulphanilamide (potentiometry), Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin, paracetamol and codein in APC tablets (NMR), Phenobarbitone in tablets (IR), pivolic acid in dipivefrin eye drops (GC),
Assay of hydrocortisone cream. (HPLC). Impurity profiling of Propranolol (GC-MS), famotidine (LC-MS).

AC -16: Food and Agricultural Analysis  

Food Analysis: Analysis of Chemical Additives in foods: Division of colour additives, Chromatographic identification of colours, and quantitative estimation of added dyes in foods (Titanium Trichloride Method) - chemical preservatives and synthetic sweetening agents (Organic-ether extractable and Non-ether extractable) - Analysis of SO₂ & Sodium Benzoate (Chemical Methods), Sorbic Acid (Chromatography) - Types of Antioxidants used in Foods, Analysis of Butylated Hydroxy Toluene (BHT) (Spectrophotometry).

Agricultural Analysis: Analysis of soils for available Major Nutrients - Estimation of available Nitrogen (Kjeldahl Method), Phosphorus (Olsen’s Method and Bray and Kurtz Method), and Exchangeable Calcium & Magnesium (by EDTA). Soil analysis for Micronutrients - Estimation of Available Zinc, Copper, Manganese and Iron (AAS) - Analysis of Pesticide Residues - Determination of Methyl Parathion Residues in food grains & vegetables (Solvent Extraction and Titrimetry) - Determination of Organochlorine pesticides by Gas Chromatography (Cypermethrin) - Determination of Malathion and DDT Residues in food grains (Spectrophotometry).

SUGGESTED BOOKS
2. Fundamentals of Analytical Chemistry, Skoog & West
3. Pharmaceutical Drug Analysis, Ashtoshkar
4. Vogel’s Text Book of Quantitative Chemical Analysis, 6th Ed, Pearson Education Ltd
5. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd 1995
9. Introduction to chemical analysis of foods, S Suzanna & Nielsen, CBS Publishers & Distributors
12. Handbook of analysis of drugs, Nagavi
AC-13: Nuclear Chemistry
Introduction: The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy.
Nuclear structure: Shell model-salient features, forms of the nuclear potential, magic numbers, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model.
Nuclear reactors: General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials, reactor moderators and reflects, coolants, control materials, shield, regeneration and breeding of fissile matter, types of research reactors.
Nuclear reactions, fission and fusion, radio-analytical
Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of α, β-, β+ and γ-decay, internal conversion, Auger effect. Radio isotopes & its applications.

AC-14: Zeolites and Molecular Sieves
Introduction to porous materials:
Classification into micro-, meso- and macro porous materials, the origin of pores and its significance, distinction from condensed materials.
Zeolites:
Definition, natural and synthetic zeolite or aluminosilicates, the primary and secondary building blocks, final framework structures, Lowensteins rule, sodalite and other structures, Nomenclature: Atlas of zeolite; structural distinctions, Novel zeolites, examples of small, medium, large and extra large pore zeolites; general properties and application of molecular sieves.
Characterization of zeolite:
XRD, SEM and other techniques; spectral techniques: FT-IR and solid-state NMR; sorption capacity, surface area by BET method, pore volume and pore structure, the origin of Brönsted and lewis acidity in zeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

AC-15: Solid State Chemistry
Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.
Structure of ionic Crystals & Compounds: Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX2, spinel structure, perovskite structure. AB [nickel arsenide (NiAs)], AB2 [fluorite (CaF2) and anti-fluorite structures, rutile (TiO2) structure and layer structure [cadmium chloride and iodide (CdCl2, CdI2)].
Crystal Defects and non-stoichiometry:
Classification of Defects: subatomic, atomic and lattice defects in solids; Thermodynamics of vacancy in metals; Thermodynamics of Schottky defects in ionic solids ; Thermodynamics of Frenkel defects in silver halides; Calculation of number of defects and average energy
required for defect. Other examples of defect structure; Non-stoichiometry and its classifications.

Preparative method of solids:

Crystal Growth: law governing nucleation; Growth of nuclei; Reaction between two solids; Improving the reactivity of solids; Zone refining method; Crystal growth.

**AC-16: Surface Chemistry & Superconductors**

Surface Chemistry:
Mechanism of catalytic reactions on the surfaces – diffusion of reactants to the surfaces, adsorption of reactants, reaction within the adsorbed layer, desorption of the products, diffusion of the products away from the surface; The mechanism of chemisorption on metals – The formation of chemisorptions layer, the character and nature of the chemisorption bond, the mechanism of chemisorptions for some gases; Nature of adsorbates on surfaces.

Superconductors:
Discovery of super conductors, Meissner effect, Type I and II conductors, Leavitation, BCS theory and Cooper pairs, High Tc Super Conductors, applications of super conductors.

**SUGGESTED BOOKS**
2. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9.
10. Superconductivity, Joi, Khachan & Stephen Bio Science, ----- 
LABORATORY COURSE
Paper CH (AC) 351P: Titrimetry, Solvent extraction, Chromatography and Water analysis.

I. Titrimetry:
   1. Determination of Ca\(^{2+}\), Mg\(^{2+}\), CO\(_3^{2-}\) & HCO\(_3^-\) in soil sample.
   2. Determination of Calcium in Vitamin-D and Calcium tablets
   3. Determination of Fe & Ca in Cement
   4. Determination of Saponification value and Iodine value of an oil sample

II. Solvent extraction:
   1. Determination of Pb using Dithiazone

III. Chromatography (Demonstration):
   1. Separation of Co & Ni in Cellulose column
   2. Separation of amino acids in a mixture by TLC using Ninhydrin
   3. Separation of additives in Ink by GC.
   4. Separation of synthetic corticosteroids in by HPLC.

IV. Water analysis:
   1. Determination of residual Chlorine in water by Iodometry
   3. Determination of COD.
   4. Determination of BOD.
   5. Determination of residual Chlorine in water by Iodometry

Paper CH (AC) 352P: Colorimetry, Spectrophotometry

I. COLORIMETRY:
   1. Determination of blood sugar
   2. Determination of blood cholesterol
   3. Determination of Paracetamol
   4. Determination of Ampicillin
   5. Estimation of Ascorbic acid

II. SPECTROPHOTOMETRY:
   1. Determination of Manganese in steel
   2. Determination of Phosphorous in human serum
   3. Determination of Creatinine in a sample
   4. Determination of pKa of an organic Indicator (Methyl Orange)
   5. Simultaneous determination of Cr and Mn in an admixture
   6. Spectrophotometric Titration of Fe(II) with o-Phen
   7. Determination of composition of Complex by Job’s Method and Mole ratio Method of Cu(II)-EDTA complex

SUGGESTED BOOKS
1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William
5. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition
IV SEMESTER

Paper-I: CH (AC) 401T CORE: Spectroscopic methods of Analysis-II

AC – 17: U.V. visible spectroscopy,
AC –18 :IR & Raman spectroscopy
AC – 19:Optical Methods
AC – 20: Fluorimetry, Phosphorimetry,Nephelometry and Turidimetry

AC – 17: UV and visible spectroscopy 15 Hrs

AC – 18 : IR & Raman spectroscopy


AC – 19:Optical Methods 15 Hrs
Refractometry: Theory, instrumentation, specific and molecular refraction, Abbe, Pulfrich and immersion types, applications
Polarimetry: Theoretical considerations – Plane polarized light, optical activity, specific and molecular rotations. Instrumentation, applications.

AC –20: Fluorimetry, Phosphorimetry,Nephelometry and Turbidimetry 15 Hrs
Fluorimetry and Phosphorimetry: Theory of Fluorescence and Phosphorescence- Excited states producing Fluorescence and Phosphorescence. Rates of absorption and emission. Deactivation processes, Variables affecting Fluorescence and Phosphorescence. Types of Photoluminescence spectra for Phenanthrene. Instrumentation – Components of Fluorimeter,

**Nephelometry and Turbidimetry:** Principles and instrumentation for Nephelometry and Turbidimetry, Applications

**Suggested Books**


**Paper-II: CH (AC) 402T: CORE: Separation Methods**

AC – 21: Solvent extractions
AC – 22: Chromatography
AC – 23: Mass spectrometry & Hyphenated techniques
AC – 24: Electrophoresis

**AC-21: Solvent extractions**

15 Hrs

The distribution coefficient, distribution ratio, relation between KD & D, the percent extracted.

Solvent extraction of metals – ion association complexes, metal chelates, effect of pH and reagent concentration, extraction process, separation efficiency of metal chelates, analytical separations – multiple counter current distribution, solid phase extraction, solvent extraction of flow injection analysis. Super critical fluid extraction.

Organic reagents in Inorganic analysis :- Theoretical basis for the use of organic reagents in inorganic analysis. Extraction of metal ions by the use of organic reagents – acetylacetone,
thionyl-trifluoroacetone, tri-n-octyl phosphine oxide. Applications to extractions of metal ions by chelating agent (Dithiazone, 8-hydroxy quinoline and cupferron) Determination of salts of organic acids and bases, determination of alkaloids in crude drugs.

**AC –22: Chromatography**  
15 Hrs  
HPTLC: Principle, Technique, advantages over TLC  
Gas Chromatography (GC) – Theory, Data acquisition and processing Applications - Derivatization techniques. Monitoring of ethylene dibromide (EDB) residue in Indian Black pepper by GC using electron capture detector. Analysis of petroleum products. Headspace analysis of tobacco. Preparative gas chromatography  
High Performance Liquid Chromatography (HPLC) – Theory, and separation modes, Applications with respect to separation of enantiomers, Organic and inorganic systems.  
Supercritical fluid chromatography (SFC) – Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and applications of SFC.  
Ultra Performance Liquid Chromatography: Principle, Instrumentation

**AC-23: Mass Spectrometry & Hyphenated techniques**  
15 Hrs  
Advanced Mass spectrometry  
Quadruple analysers, Ion traps. Time of flight mass spectrometry.  
Mass Spectrometry / Mass Spectrometry Tandem Mass Spectrometry. Ion cyclotron resonance spectrometers and Ion traps for MS/MS.  
Quantitative mass spectrometry: Introduction, principle, calibration and internal standards.  
Hyphenated techniques:  
GC-MS: Principle, instrumentation, Interfaces, Mass analyzer, Mass chromatogram, Applications. Analysis of metabolite of drug Imipramine  
GC-FT-IR: Principle, Instrumentation and Applications  
LC-MS: Principle, Instrumentation, Interfaces and Applications.  
ICP-MS: Instrumentation, principles, Quantitative analysis and applications.

**AC-24: Electrophoresis**  
Introduction, Definition  
Paper Electrophoresis: Principle, Experimental Requirements, Technique, Factors governing the migration of ions, Applications  
Capillary Electrophoresis: Electro osmotic flow, migration in CE, instrumentation, control of separation, applications  
Gel Electrophoresis: Principle, technique, applications  
Immunoelectrophoresis: Principle, technique, applications

**Suggested Books**  


Paper-III CH (AC) 403T: ELECTIVE IIIa: Laboratory Management
AC – 25 Automation in laboratory
AC – 26 LIMS & Computer aided analysis
AC – 27 Laboratory Management & Standard reference materials
AC – 28 Accreditation of Laboratories, Quality management

AC- 25 Automation in Laboratory. 15 Hrs

Good laboratory practices: Instrumental standardization, optimization of procedures.

AC-26 LIMS and Computer aided Analysis 15 Hrs
Laboratory Information Management System: Laboratories as information producers, properties of good information, Laboratory information management system, conclusions. Computer aided analysis: Computer-instrument interaction, computer organization-Hardware -Basic Digital circuit components, Microprocessors and Microcomputers, Computer Software -Software control of the computer-instrument interfaces. Automated laboratory – Automated instruments (AAS), Applications of computers, Computer Networks.

AC- 27 Laboratory Management & Standard reference materials 15 Hrs
Introduction – Administration, Geographical location of the laboratory, relationship with the industrial exploratory and regulatory work and the analytical laboratory. Disciplines represented in the Laboratory. Educational requirements of the laboratory personnel. Workload statistics of the laboratory coordination between routine work and research cell. Regular academic research work, opportunities for training. Internal organization of the laboratory. Architectural issues, laboratory infrastructure of equipment and instrumentation.

Standard reference materials

AC- 28 Accreditation of Laboratories, Quality Management 15 hrs
Quality systems, the operational aspects required to deliver a quality system (Traceability, quality control, quality assurance, quality management and quality manual) calibration and testmethods.
Total Quality Management (TQM) – Essentials of TQM: Quality Planning, Quality control, Quality Audit, Quality surveillance, Quality assurance, Quality circles.
Analytical methods of validation: Characteristics of Analytical procedures – Accuracy, precision, linearity, Range specificity, Detection limit, Quantitation limit, robustness process validation. Types of process validation – prospective, concurrent and retrospective process validation.

Suggested Books
2. Model for Quality assurance in design/development production, installation and servicing, ISO 9001.
AC-25: Enzyme catalysis- Analytical applications

AC-26: Forensic Chemical Analysis
Contact traces – Analysis of soil, fiber and paint evidence in forensic work.
Analysis of narcotic drugs and psychotropic substances (opiates, cannabinoids, barbiturates, benzodiazepines, amphetamines with one example each and LSD) by colour/micro crystal tests, chromatographic methods (TLC, GC, and LC) and spectroscopic methods (UV-Vis, IR, MS and GC-MS). Analysis of explosives and explosion residues (Low explosive residues – cations and anions; High explosive residues – RDX) by spot tests, chromatographic methods (TLC, GC AND GCMS) and spectroscopic methods (UV-Vis, IR, MS and GC-MS).
Analytical toxicology – extraction techniques for drugs and pesticides – analytical techniques in forensic toxicology for alcohols, drugs and pesticides involving spot tests (TLC, GC & LCMS). Interpretation of analytical data – court testimony.

AC-27: Limit tests

AC-28: Green Analytical Chemistry
Green Analytical Chemistry: Concepts and trends
“Greening” Sample Treatment: Reduced and solvent-free sample preparation methodologies, alternative solvents, energy saving procedures.

Suggested Books
PAPER – IV: CH (AC) 404T: IDa: Quality Assurance and Accreditation

AC-29 Quality Assurance – I
AC-30 Quality Assurance – II
AC-31 Quality Assurance – III
AC-32 Quality Accreditation

AC -29: Quality Assurance – I  
Introduction to Quality Control and quality assurance: Concepts and significance.
Quality control and statistical techniques: Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, use of blindsamples in quality control, use of proficiency evaluations in quality control.
Calibration and maintenance of Instruments / Equipment: Instrument calibration – linear calibration curves, equipment calibration, frequency of calibration, calibration of common laboratory instrument and equipment (Analytical balances, volumetric glassware, ovens, furnaces, UV / Visible spectrophotometer, pH meter, conductivity meter, IR spectrophotometers, AAS, GC, HPLC etc.,). Maintenance of instruments and equipment.

AC-30: Quality Assurance – II  
Good laboratory practices and personnel, Quality Programme, Instrument and Organisation calibration, Customer Satisfaction.

AC -31: Quality Assurance – III  

AC -32: Quality Accreditation:  

Suggested Books:
3. How to practice GLP, PP Sharma, Vandana Publications, 2000, New Delhi

PAPER – IV: CH (AC) 404T: IDb: Inorganic Material Chemistry
AC-29: Composite Materials
AC-30: Liquid Crystals
AC-31: Explosives and Propellants
AC-32: Fuels and Combustion

AC-29: Composite Materials
Ceramics: Plasticity of Clays, Whitewares or White-Pottery, Manufacture of White-Pottery, Glazing, Methods of glazing, Earthenwares and Stonewares.

AC-30: Liquid crystals

AC-31: Explosives and Propellants
Explosives: Introduction, Classification of Explosives, Primary Explosives, Low Explosives, High Explosives, Precautions During Storage of Explosives, Blasting Fuses, Manufacture of Important Explosives-Lead azide, Diazonitrophenol (DDNP), Trinitrotoluene (TNT), Nitroglycerine (NG) or Glycerol trinitrate (GTN), Pentaerythritol tetranitrate (PETN) and RDX; Recent uses of Explosives
Propellants: Rocket Propellants - Introduction, Principle of Rocket Propulsion, Classifications of Propellants-Solid propellants, Composite propellants, Liquid Propellants, Mono-propellants, Bi-propellants; Differences between Solid propellants and Liquid Propellants

AC-32: Fuels and Combustion

SUGGESTED BOOKS
LABORATORY COURSE
Paper CH (AC) 451P: Electro analytical techniques:

I. POTENTIOMETRY:
1. Determination of Ferrous using $K_2Cr_2O_7$
2. Determination of iron in iron wire using $KMnO_4$
3. Determination of a mixture of Ferrous and Vanadyl using Ceric ammonium nitrate
4. Determination of silver in silver metal
5. Assay of sulphanilamide in samples
Use of ion selective electrodes:
6. Determination of mixture of halides using Ag ion electrode

II. pH METRY:
1. Strong acid Vs strong base titration
2. Mixture of acids Vs strong base
3. Determination of mixture of carbonates and bicarbonates
4. Determination of Dissociation constants of Histidine monohydrochloride
5. Determination of binary stability constants of Cu(II) – Histidine complexes

III. POLAROGRAPHY:
1. Polarographic determination of Cu & Zn in brass

IV. CONDUCTOMETRY:
1. Mixture of acids Vs strong base titration
2. Mixture of bases Vs strong acid titration
3. $K_2SO_4$ Vs $BaCl_2$ titration.
4. Determination of the composition of Cu(II) oxine complex
5. Determination of Quinine dihydrochloride with NaOH
6. Determination of Aspirin with KOH

Paper CH (AC) 452P: Spectroscopic Techniques, Spectral problems and Evaluation of Physical Parameters Of Tablets

I. FLAME PHOTOMETRY:
1. Determination of i)Na, ii)K, iii)Ca, iv)Li

II. FLUORIMETRY
1. Determination of Vitamin – B₁ (Thiamine)
2. Determination of Vitamin – B₂ (Riboflavin)
3. Determination of Quinine sulphate.

III. ATOMIC ABSOPPTION SPECTROSCOPY

IV. Structural elucidation based on spectral data from UV – Vis, IR, NMR and Mass Spectrometry

V. EVALUATION OF SOME PHYSICAL PARAMETERS OF TABLETS:
1. Dissolution profile of Ampicillin.
2. Disintegration test for Ibuprofen (coated tablet).
3. Determination of friability of Paracetamol tablet.
SUGGESTED BOOKS
M.Sc. CHEMISTRY

INORGANIC CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR
2016 ONWARDS
Osmania University  
M.Sc. Chemistry (Inorganic Chemistry) III and IV Semesters Programme  
(For the batch admitted during the academic year 2016-2017 under the CBCS pattern)  
[Under Restructured CBCS Scheme]

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<th>III Semester</th>
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</table>
| **CORE**     | Paper-I: CH(IC) 301T: Bonding, Group Theory and its Applications  
IC-09: Group Theory, Normal mode analysis and Spectral Activity  
IC-10: MOT of Metal Complexes  
IC-11: Electronic Spectroscopy of Metal Complexes  
IC-12: IR and Raman Spectroscopy | 4     | 4      | 100   |
| **CORE**     | Paper-II: CH(IC) 302T: Organo Metallic Chemistry of Transition Metal Complexes  
IC-13: Mono, Di and Trihapto Complexes  
IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes  
IC-15: Catalytic Role of OTMC-I  
IC-16: Catalytic Role of OTMC-II | 4     | 4      | 100   |
| **ELECTIVE IIIa** | Paper-III: CH(IC) 303T: Analytical Techniques-I  
IC-17: Data Handling  
IC-18: AAS, AES, ICP-AES  
IC-19: Diffraction Methods  
IC-20: Advanced Mass spectrometry | 4     | 4      | 100   |
| **ELECTIVE IIIb** | Paper-III: CH(IC) 303T: Supramolecular Chemistry, Photochemistry, Green Chemistry and Nanotechnology  
IC-21: Supramolecular Chemistry  
IC-22: Photochemistry of Metal Complexes  
IC-23: Green Chemistry  
IC-24: Nanotechnology | 4     | 4      | 100   |
| **ELECTIVE IVa** | Paper-IV: CH(IC) 304T: Analytical Techniques-II  
IC-25: Thermal Methods  
IC-26: Surface Analysis Methods/ Microscopic analysis  
IC-27: Advanced Separation Techniques  
IC-28: Optical Methods | 4     | 4      | 100   |
| **ELECTIVE IVb** | Paper-IV: CH(IC) 304T: Nuclear Chemistry, Zeolites, Solid State, and Surface Chemistry  
IC-29: Nuclear Chemistry  
IC-30: Zeolites and Molecular Sieves  
IC-31: Solid State Chemistry  
IC-32: Surface Chemistry & Superconductors | 4     | 4      | 100   |
<p>| <strong>LABORATORY COURSE -I</strong> | CH (IC) 351P: Synthesis and Characterization of Metal Complexes | 9     | 4      | 100   |
| <strong>LABORATORY COURSE –II</strong> | CH (IC) 352P: Electro-Analytical techniques | 9     | 4      | 100   |</p>
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<td>Paper-I: CH(IC)401T: Molecular Spectroscopy of Inorganic Compounds</td>
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<td>IC-34: Advanced NMR techniques</td>
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<td>IC-35:Applications of ESR to Metal Complexes</td>
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<td>IC-36:Mossbauer Spectroscopy and Nuclear Quadrupole Resonance Spectroscopy</td>
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<td>IC-40:Metallo-Enzymes of Cobalt, Copper Molybdenumand Manganese</td>
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<td>Paper-III: CH(IC)403T: Medicinal Inorganic Chemistry, Spectroscopic Analysis of Drug/Metal Complexes and Applications of Nanomaterials</td>
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<td>IC-42: Metal complexes as Drugs and Anticancer agents</td>
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<td>IC-43:Spectroscopic analysis of drug/metal complexes binding to DNA</td>
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<td>IC-44: Applications of Nanomaterials</td>
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<td>Paper-III:CH(IC)403T:Analytical Techniques-III</td>
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<td>IC-46: Radiochemical Methods</td>
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<td>IC-48: Industrial Analysis</td>
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<td>IC-50: Food and Agricultural analysis</td>
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<td>IC-51: Analysis of Air and Water Pollutants</td>
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<td>IC-52: Drinking Water and Sewage Water Treatment</td>
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<td>CH (IC) 452P: Spectroscopic Techniques</td>
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## CH(IC)301T: Bonding Group Theory and its Applications

### IC-09: Group Theory, Normal mode analysis and Spectral Activity
- Properties of a Group-Closure rule, Identity rule, associative rule, inverse rule, Abelian and Non-abelian groups.
- Classes of Symmetry Elements of a Group: Similarity transformation, properties of conjugate elements, salient features about Classes, Classes of \( C_{2V} \), \( C_{2h} \) and \( C_{3V} \). Matrix Representation of Symmetry Elements: Simple Matrices, Matrix addition, subtraction and multiplication, Block-Factorization. Matrix Representation of \( E, C_n, S_n, i \) and \( \sigma \) Elements. Great Orthogonality Theorem: Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for \( C_{2V}, C_{2h} \) and \( C_{3V} \). Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula.
- Use of Character tables for IR & Raman spectroscopy, symmetry based selection rules for IR and Raman activity. Type and Symmetry of Normal Modes and IR and Raman activity of molecules: Cartesian coordinate method of analysis for \( C_{2V} \) (eg. \( H_2O \), \( SF_4 \)), \( C_{3V} \) (\( NH_3 \), \( POCl_3 \)), \( C_{2h} \) (trans-\( N_2F_2 \)), \( D_{3h} \) (\( BF_3 \)), \( Td(SO_4^{2-}) \), \( Oh(\text{SF}_6) \). Internal coordinate method of analysis for \( C_{2V} \) (\( H_2O \)), \( C_{3V} \) (\( NH_3 \)), \( Td \) (\( SO_4^{2-} \)).

### IC-10: Molecular Orbital Theory of Metal Complexes
- Limitations of Crystal Field Theory, Adjustments to the Crystal Field Theory to allow for covalence. -Experimental evidences for Metal - Ligand orbital overlap. The Adjusted Crystal Field Theory. Introduction to Molecular Orbital Theory. Symmetry Classification of Metal and Ligand Group Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, TrigonalBipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams - Octahedral Metal Complexes with (i) Sigma (\( \sigma \)), (ii) sigma(\( \sigma \)) &Pi (\( \pi \)) and (iii) sigma (\( \sigma \)), Pi (\( \pi \)) and Pi* (\( \pi^* \)) bonding contribution from the Ligands - Tetrahedral Metal Complexes with (i) Sigma (\( \sigma \)) and (ii) sigma(\( \sigma \)) &Pi (\( \pi \)), and Square Planar Metal Complexes with (i) Sigma (\( \sigma \)) and (ii) sigma(\( \sigma \)) &Pi (\( \pi \)) bonding contribution from the ligands - Molecular orbital electron configurations and calculation of Magnetic Moments.

### IC-11: Electronic Spectroscopy of Metal Complexes

### IC-12: Infrared and Raman Spectroscopy
- Conditions for Infrared and Raman Spectroscopies, Direct product – symmetry requirements for overtones, binary and ternary combination bands. Partial Normal mode analysis-Structure Fitting, Determination of Coordination Sites and Linkage Isomers(\( NO_2^- \), \( SCN^- \)), Assigning Denticity of
Ligands (SO$_4^{2-}$, CO$_3^{2-}$), Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. Effect of Coordination on Ligand Vibrations: Examples involving Mono, Bi and/or Polydentate Ligands of Oxygen, Nitrogen, Carbon and Halogen Donors (NH$_3$, H$_2$O, Glycine, Carbonyl and halides). Raman effect and molecular structure- CO, HCN, CO$_2$, N$_2$O, H$_2$O. Principles of Resonance Raman Spectroscopy. Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers

**SUGGESTED BOOKS**
7. Molecular Symmetry, Schoenland
8. Electronic Spectroscopy, A. B. P. Lever
9. Introduction to Ligand fields, B. N. Figgis
10. Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto
11. Infrared spectroscopy of Inorganic Compound, Bellamy.

**PAPER II**

**CH(IC)302T: Organo Metallic Chemistry of Transition Metal Complexes**

**IC-13: Mono, Di and Trihapto Complexes**
**IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes**
**IC-15: Catalytic Role of OTMC-I**
**IC-16: Catalytic Role of OTMC-II**

**IC-13: Mono, Di and Trihapto Complexes**

**IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes**
$\eta^4$ Complexes: Structure and Bonding in $\eta^4$ Complexes – Butadiene and Cyclobutadiene Complexes. $\eta^5$ Complexes: General methods of Preparation – Bis ($\eta^5$-cyclopentadienyl) metal complexes (Metalloccenes) – Ferrocene: Structure and Bonding – Reactions of Ferrocene – Mechanism of Electrophilic substitution – Friedel Crafts acylation, alkylation, nitrilation, halogenation and Metallation Reactions.
$\eta^6$ Complexes: Metal – Arene Complexes – Dibenzenechromium – Preparation, Structure and Bonding in Bis(arene)-Metal Complexes – Reactions. $\eta^7$ Complexes: Preparation, Structure and Reactions of $\eta^7$ –
C$_7$H$_7$ Complexes. $\eta^8$Complexes : C$_8$H$_8$ as a Ligand – Cyclooctatetraene Complexes – Preparation, Structure and Bonding in Uranocene.

**IC-15: Catalytic Role of OTMC-I**


**IC-16: Catalytic Role of OTMC- II**


**SUGGESTED BOOKS**

1. Organometallics-A Concise Introduction, Ch.Eischeinbroich and Salzer-VCH
3. Homogeneous Catalysis by Metal Complexes, M M Taqui Khan and A E Martel
5. Organometallic Compounds, G E Coates, M C H Green, K Wade vol II
6. Advanced Inorganic Chemistry, Cotton and Wilkinson, V & VI Ed
7. Symmetry and spectroscopy, K Veera Reddy

**PAPER III**

CH(IC) 303T (Elective IIIa): Analytical Techniques - I

**IC-17: Data Handling**

**IC-18: AAS, AES, ICP-AES**

**IC-19: Diffraction Methods**

**IC-20: Advanced Mass spectrometry**

**IC-17: Data Handling**

Accuracy, Precision, Types of errors – determinate and indeterminate errors, minimization of determinate errors, statistical validation- statistical treatment of finite data (mean, median, average deviation, standard deviation, coefficient of variation and variance), significant figures – computation rules, comparison of results – student’s t-test, F-test, statistical Q test for rejection of a result, confidence limit, regression analysis – method of least squares, correlation coefficient, detection limits. Calculations.
IC-18: AAS, AES, ICP-AES


Flame Photometry: Principle, Theory, Instrumentation and Applications

IC-19: Diffraction Methods

X-ray Diffraction: X-rays and their generation – choice of radiation; Miller indices, Bragg's equation, Experimental methods – Powder and single crystal methods, Indexing the reflections, Systematic absences, Electron density studies by X-rays – Platinum phthalocyanine complex, Silyl acetate, Tetraalkylbiphosphate; Advantages and limitations of X-ray Diffraction.

Electron Diffraction by gases: Principles, Radial distribution curves- Interpretation of results for PBrF$_3$, PF$_3$, PF$_3$HS, HClO$_4$, Silylmethionioacetate and Germylvmonothioacetate and HgCl$_2$ molecules, Advantages and Limitations


IC-20: Advanced Mass spectrometry

Mass Analyzers: Quadruple, Ion traps, Time of flight (TOF) mass analyzers


Matrix-assisted laser desorption/ionization-Time of flight Mass spectrometry (MALDI-TOF-MS): Principle, Matrix, Sample Preparation for MALDI-MS - Dried droplet Crystallization, Thin layer method, Sandwich Crystallization, Instrumentation, Applications

SUGGESTED BOOKS

2. Instrumental Methods of Chemical Analysis, H. Kaur.
5. Instrumental Techniques for Analytical Chemistry, Frank Settle.
8. Introduction to Solids, Azaroff.
IC-21: Supramolecular Chemistry

Host – Guest chemistry: Definition and different types of host and guests with examples – types of non-
covalent interactions – binding constants of host guest complex and thermo dynamics involved in it –
designing principles of host.

Cation guest binding – binding between metal cations and macro cycles – chelate and cryptate effects –
relationship between cavity size of host and cation radius and stability of resultant complexes – binding of
macro cycles having secondary binding sites.

Anion guest binding – different hosts for anionic guests capable of binding through electro static
interactions, hydrogen bonds, lewis acidic hosts – enhancement of binding strength using more than non-
covalent interactions.

Neutral guest binding – binding of neutral guest using hydrogen bonding, π - π stacking, hydrophobic
effect and charge transfer interactions – simultaneous binding of cation and anion guests – cascade
approach, individual binding sites and zwitter ions approach – present and future applications – phase
transfer agents – separation of mixtures – molecular sensors – switches and molecular machinery.

IC-22: Photochemistry of Metal Complexes

Energy, Structure, Electron Distribution and Chemical reactivity of Electronically Excited states of
Coordination Compounds. Photochemistry of Cr(III) and Co(III) metal complexes. Photochemistry of
Cr(CO)6 , Mn2(CO)10 and Fe(CO)5.

Structuredphosphorescence of Ruthenium Bipyridyl and Ortho-phenanthroline Complexes. Energy
transfer Spin Correlation energy levels in the energy Transfer Systems:[Ru(bipy)3]2+ [Cr(CN)6]3+. Metal
Sensitizers and Quenchers - Electron Relay. Photochemical Hydrogen production by oxidative quenching
of [Ru(bipy)3]2+ by Methyl Viologen.

IC-23: Green Chemistry

Principles and concepts of green chemistry

Introduction, sustainable development and green chemistry, atom economy, atom economic reactions,
rearrangement reactions, addition reactions, atom uneconomic reactions- substitution reactions,
elimination reactions, Wittig reactions. Reducing toxicity, measuring toxicity.

Organic solvents: Environmentally benign solutions: Organic solvents and volatile organic compounds,
solvent free systems, super critical fluids- supercritical carbon dioxide and supercritical water. Water as a
reagent solvent, water based coatings.

Industrial case studies: A brighter shade of green – greening of acetic acid, Vitamin C synthesis –enzyme
routes. Polythene manufacture-metalloocene catalysis.
**IC-24: Nanotechnology**

**Metal Nanoclusters** – Introduction, Magic numbers, theoretical modeling of nanoparticles, geometric structure, electronic structure, reactivity, fluctuations, magnetic clusters, bulk to nanotransition.

**Methods of synthesis:** RF plasma, thermolysis, pulsed laser, chemical methods.

**Carbon nanostructures** - Introduction, carbon molecules, new carbon structures,

**Carbon clusters** - small carbon clusters, discovery of C_{60}, structure of C_{60} and its crystal, alkali doped C_{60}, superconductivity in C_{60}.

**Carbon nanotubes:** Fabrication, structure, electrical properties, vibrational properties, mechanical properties.

**Nanophase and nanostructured materials:** Micells and Microemulsions - Formation mechanisms of micelles and microemulsions, the critical Micelle Concentration (CMC) for surfactants, Solubilization and Formation of Microemulsions. **Synthesis of Nanoparticles from W/O Microemulsions:** Preparation of Nanoparticles of Metals, Metal Sulfides, Metal Salts, Metal oxides, Nanowires. **Synthesis of Organic Nanoparticles from O/W Microemulsions:** Styrene Latex NanoParticles, Methylmethacrylate Nanoparticles. Sol -Gel process for the fabrication of Glassy and Ceramic materials.

**SUGGESTED BOOKS**

1. Supramolecular Chemistry – concepts and perspectives by Jean-Marie Lehn
2. Principles and methods in Supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons
3. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
8. Photochemistry of Coordination compounds V.Balzani and Carassiti,academicpresss.
9. Elements of inorganic Photochemistry G.J.Ferrendi,Wiley,
14. Green Chemistry- An Introductory text by Mike Lancaster- RSC.
IC-25: Thermal Methods
Thermogravimetric analysis (TGA): Principle, Instrumentation, working function of each component, applications of TGA. Study of oxalates, nitrates and chromates by TGA. Determination of carbon black in polythene.
Differential scanning calorimetry (DSC): Principle, instrumentation, power compensated DSC instruments and Heat flow DSC instruments, Methodology, DSC experiment calibration and data analysis. Applications determination Glass transition temperatures and heat capacities, problems based on Thermal Techniques:
Thermometric titrations: Principle, apparatus, applications to acid base, precipitation, complexometric, redox and non-aqueous titrations.
Combined thermal instruments: Introduction to TGA/MS and TGA/FTIR, High resolution TGA, Microthermal analysis.

IC-26: Surface Analysis Methods/ Microscopic analysis
Introduction, types of surface measurements.
Photon Probe Techniques: X-Ray Photoelectron spectroscopy - Principle, Instrumentation, applications.
Ion Probe Techniques: Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation, applications. Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering, Principle, Instrumentation (static & dynamic), applications

IC-27: Advanced Separation Techniques
Separations by extraction: Solid phase extraction- Principle, methodology, applications. Solvent extraction of flow injection analysis. Applications to extractions of metal ions by chelating agents (Dithiazone, 8-hydroxy quinoline and cupferron). Organic reagents in Inorganic analysis - Theoretical basis for the use of organic reagents in inorganic analysis. Extraction of metal ions by the use of organic reagents – acetylacetone, thionyl-trifluoroacetone, tri-n-octyl phosphate oxide.
Affinity and chiral chromatography – Principle, technique, Instrumentation and applications.
Size Exclusion Chromatography – Principles of gel filtration Chromatography, Instrumentation, retention behavior, resolution, selection of gel type, applications, Ion exclusion – Principle and applications.
Supercritical fluid chromatography (SFC) – Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and applications of SFC.
GC-FT-IR: Instrumentation, Principles and Applications

IC-28: Optical Methods

SUGGESTED BOOKS

PAPER IV

CH(IC) 304T ( Elective IVb ): Nuclear Chemistry, Zeolites, Solid State, and Surface Chemistry

IC-29: Nuclear Chemistry
IC-30: Zeolites and Molecular Sieves
IC-31: Solid State Chemistry
IC-32: Surface Chemistry & Superconductors

IC-29: Nuclear Chemistry
Introduction: The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy.
Nuclear structure: Shell model-salient features, forms of the nuclear potential, magic numbers, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model.
Nuclear reactors :- General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials, reactor moderators and reflects, coolants, control materials, shield, regeneration and breeding of fissile matter, types of research reactors.
Nuclear reactions, fission and fusion, radio-analytical
Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of $\alpha$, $\beta$, $\beta^+$ and $\gamma$-decay, internal conversion, Auger effect. Radio isotopes & its applications.

IC-30: Zeolites and Molecular Sieves

**Introduction to porous materials:**
Classification into micro-, meso- and macro porous materials, the origin of pores and its significance, distinction from condensed materials.

**Zeolites:**
Definition, natural and synthetic zeolite or aluminosilicates, the primary and secondary building blocks, final framework structures, Lowensteins rule, sodalite and other structures, Nomenclature: Atlas of zeolite; structural distinctions, Novel zeolites, examples of small, medium, large and extra large pore zeolites; general properties and application of molecular sieves.

**Characterization of zeolite:**
XRD, SEM and other techniques; spectral techniques: FT-IR and solid-state NMR; sorption capacity, surface area by BET method, pore volume and pore structure, the origin of Brönsted and Lewis acidity in zeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

IC-31: Solid State Chemistry

Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones.
Structure of ionic Crystals & Compounds: Ionic Crystals with stoichiometry $MX$, Ionic Crystals with stoichiometry $MX_2$, spinel structure, perovskite structure. AB [nickel arsenide (NiAs)], $AB_2$[fluorite (CaF$_2$) and anti-fluorite structures, rutile (TiO$_2$) structure and layer structure [cadmium chloride and iodide (CdCl$_2$, CdI$_2$)].

**Crystal Defects and non-stoichiometry:**
Classification of Defects: subatomic, atomic and lattice defects in solids; Thermodynamics of vacancy in metals; Thermodynamics of Schottky defects in ionic solids ; Thermodynamics of Frenkel defects in silver halides; Calculation of number of defects and average energy required for defect, Other examples of defect structure; Non-stoichiometry and its classifications.

**Preparative method of solids:**
Introduction, Ceramic method, microwave synthesis, Precursor method, Hydrothermal method, Chemical vapour deposition (CVD) Method, Chemical vapour Transport, Choosing a method for solids. Crystal Growth: law governing nucleation; Growth of nuclei; Reaction between two solids; Improving the reactivity of solids; Zone refining method; Crystal growth.

IC-32: Surface Chemistry & Superconductors

**Surface Chemistry:**
Mechanism of catalytic reactions on the surfaces – diffusion of reactants to the surfaces, adsorption of reactants, reaction within the adsorbed layer, desorption of the products, diffusion of the products away from the surface; The mechanism of chemisorption on metals – The formation of chemisorptions layer, the character and nature of the chemisorption bond, the mechanism of chemisorptions for some gases; Nature of adsorbates on surfaces.

**Superconductors:**
Discovery of super conductors, Meissner effect, Type I and II conductors, Leavitation, BCS theory and Cooper pairs, High Tc Super Conductors, applications of super conductors.

SUGGESTED BOOKS

2. Nuclear and Radioactive chemistry; Friedlander, Kennedy and Miller; Chapters 8 and 9.
10. Superconductivity, Joi, Khachan & Stephen Bio Science, -----

LABORATORY COURSES (III Semester)

Paper CH (IC) 351: Synthesis and Characterization of Metal Complexes
Laboratory preparation and characterization of 3d transition metal complexes of tetrahedral, square planar and octahedral geometries.
1. VO(acac)₂
2. CoCl₂(Py)₂
3. Na[Cr(NH₃)₂(SCN)₄]
4. Prussian Blue, Turnbull’s Blue Complexes
5. K₃[Cr(C₂O₄)₃] 3H₂O : UV, IR, TGA and estimation of oxalate.
6. Solid phase synthesis of trans-bis(glycinato)copper(II): IR, estimation of Cu by iodometry
7. Fe(acac)₃: FTIR
8. Cis and trans [CoCl₂(en)₂]Cl : conversion of cis to trans and trans to cis by IR.
9. Potassium bis(peroxo)oxo(1,10-phenanthroline)vanadium(V) trihydrate: IR, TGA, estimation of vanadium and peroxide
10. Tetra-butylammoniumhexamolybdate(VI): IR, estimation of Mo
11. MnO₂ nano particles; SEM, SEM by adding CTAB

SUGGESTED BOOKS

Paper CH (IC) 352: Electro-analytical techniques

I Potentiometry
Potentiometric Titrations and Calculation of End Point Potentials for the following systems:
i) Fe²⁺ and VO³⁺ Mixture vs Ce⁴⁺
ii) Assay of sulphanilamide
iii) Silver electrode for silver assay
iv) Mixture of halide anions using Silver electrode
II pH-metry
1. Determination of CO$_3^{2-}$ and HCO$_3^-$ in a mixture
2. Determination of the dissociation constants of
   (i) Ethylenediamine (en)(H$_2$L) (ii) Glycine (HL)  (iii) Histidinemonohydrochloride (H$_2$L)
3. Determination of binary constants of i) Cu(II)-en and (ii) Ni(II)-His iii) Ni(II) – Gly Systems
4. Determination of stability constant of ternary (o-Phen-Ni(II)-His) system - Calculation of Log K.

III Conductometry:
1. Determination of the Composition of Cu(II)-oxine and Cu(II)-EDTA Complexes
2. Interaction of Pyrophosphate with Mg$^{2+}$, Ca$^{2+}$, Mn$^{2+}$ and Cu$^{2+}$
3. Determination of Aspirin with KOH

IV Ion selective electrodes method (Ionimetry)
1. Estimation of fluoride ion in water
2. Estimation of nitrate ion in water
3. Estimation of ammonia in water

V Polarography
1. Determination of $E_{1/2}$ of Cd$^{2+}$ and Pb$^{2+}$
2. Verification of Ilkovic equation by using Cd$^{2+}$ solution
3. Determination of Stability Constants of Cd$^{2+}$ and Pb$^{2+}$ complexes

VI Electrogravimetry
1. Determination of Copper and Nickel individually and in a Mixture

SUGGESTED BOOKS
IC-33: Multinuclear NMR

\(^{13}\text{C} \text{nmr spectroscopy: } \text{CW and PFT techniques. Types of } ^{13}\text{C} \text{ nmr spectra: undecoupled, proton-decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. } ^{13}\text{C} \text{ chemical shifts, factors affecting the chemical shifts.}

Chemical equivalence and magnetic equivalence. Virtual Coupling and its importance in study of Metal Complexes [Pd\{P(CH\textsubscript{3})\textsubscript{3}\}\textsubscript{2}]. Spin Dilute Systems-Satellites in Pt(II) Complexes cis-[Pt(P\textsubscript{3}Et\textsubscript{3})\textsubscript{2}Cl\textsubscript{2} ], Sn(CH\textsubscript{3})\textsubscript{4}. NMR Time Scale and its use in studying Stereo chemical Non –rigidity (PF\textsubscript{5}, [Rh(P\textsubscript{3}R\textsubscript{3})\textsubscript{3}].

Applications of \(^{1}H, ^{13}C, ^{19}F, ^{31}P \text{ and } ^{15}N \text{ to simple inorganic and Coordination Compounds - 1) } ^{1}H-\text{NMR: PtHCl(PEt\textsubscript{3})\textsubscript{2}, Pt(NH\textsubscript{3})\textsubscript{3}(CH\textsubscript{3})\textsubscript{3}, BH\textsubscript{4}-, NH\textsubscript{4}+; 2) ^{19}F: BF\textsubscript{4}, H\textsubscript{2}PF\textsubscript{3}; 3) ^{31}P: Mo(CO)\textsubscript{3}(P\textsubscript{3}Ph\textsubscript{3}), [Rh(P\textsubscript{3}Ph\textsubscript{3})Cl], trans-[PtCl\textsubscript{4}(PET\textsubscript{3})\textsubscript{2}]; 3) ^{31}PF\textsubscript{3}(^{14}NH\textsubscript{2})\textsubscript{2} 4) 13C; [^{1}h C\textsubscript{6}H\textsubscript{5}Ru(CO)\textsubscript{3}], Fe(CO)\textsubscript{5}, Fe\textsubscript{2}(CO)\textsubscript{9}, Fe\textsubscript{3}(CO)\textsubscript{12}, FeICp(CO)\textsubscript{12}, [^{13}C\textsubscript{15}N Co(DH)\textsubscript{5}Pyridine]. ^{13}C \{^{1}H\} \text{ NMR spectrum of } \sigma\text{ bonded C\textsubscript{6}H\textsubscript{5} ligand.}

IC-34: Advanced NMR techniques

Spin-Lattice (T\textsubscript{1}) and Spin-Spin Relaxation (T\textsubscript{2}). Spin Echo Polarization Transfer – Spin Echo Measurements. ^{13}C-NMR spectral editing techniques: Attached proton test (APT spectra) by Gated Spin Echo, Cross polarization, INEPT spectra, DEPT spectra (Distortionless enhancement by polarization transfer). INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment).

Two Dimensional NMR: Basic principles, Types of 2-D NMR ;i) J- resolved spectroscopy a) homo and b) heteronuclear J- resolved spectroscopy ii) Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY) and Hetero nuclear shift correlation spectroscopy (HETCOR) iii) NOESY (Nuclear Overhauser Enhancement Spectroscopy). HOESY (two dimensional heteronuclear NOE). Advantages of 2-D NMR

IC-35: Applications of ESR to Metal Complexes

Principle- Selection Rules – Instrumentation- Microwavesource (energy bands). Application of ESR to the study of simple free radicals: methyl (CH\textsubscript{3}), amine (NH\textsubscript{2}), diphenylpicrylhydrazyl,cyclopentadienyl (C\textsubscript{5}H\textsubscript{5}·), hydroxy methyl (CH\textsubscript{2}=OH·) radicals. Zero-Field Splitting (ZFS) - Effective Spin - Orbitally Non-degenerate and Degenerate States. ESR Spectra of d\textsuperscript{1}-d\textsuperscript{9} Transition Metal Complexes with examples. Interpretation of g in cubic, axial and rhombohedral geometries. Factors affecting g values. Calculation of g values with simple examples. Intensities of ‘g\textsuperscript{||}’ and g\textsuperscript{⊥} peaks. Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis –Salicyldalmine. [(NH\textsubscript{3})\textsubscript{2}Co O \textsubscript{2} Co (NH\textsubscript{3})\textsubscript{3}]\textsuperscript{5+}, Cu(II)- diethyldithiophosphinate, Vanadylldithiophosphinate, Copper(II) tetracyanophoryrin, Co(II)- phthalocyanine, K\textsubscript{2}[IrCl\textsubscript{6}]. Interpretation of ‘g’ and ‘A’ values from esr spectral data in- i) MnF\textsubscript{6}\textsuperscript{4-}, ii) CoF\textsubscript{6}\textsuperscript{4-}, and CrF\textsubscript{6}\textsuperscript{3-}. ESR spectra of dinuclear Cu (II) complexes.
IC-36 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy


Applications


Tin Compounds: Tin Halides and Organotin Compounds.

Iodine Compounds: Isomer Shifts of $^{127}$I and $^{129}$I - Applications to Alkali metal iodides and Molecular Iodine. Mossbauer spectra of IF$_6^-$ and IF$_6^{+}$

Nuclear Quadrupole Resonance Spectroscopy: Principle, nuclear quadrupole resonance experiment, Structural information from NQR spectra- PFCl$_4$, PCl$_4$Ph, Ga$_2$Cl$_7$ and TeCl$_4$ Interpretation of nuclear quadrupole coupling constants.

SUGGESTED BOOKS

2. S. Craddock, ELBS.

PAPER II

CH(IC) 402T: Bioinorganic Chemistry

IC-37: Metal ions Interactions with Nucleic acids and their constituents
IC-38: Transport of Electrons and Metal ions
IC-39: Metallo-Enzymes of Iron, Zinc and Nickel
IC-40: Metallo-Enzymes of Cobalt, Copper, Molybdenumand Manganese

IC-37: Metal ions Interactions with Nucleic acids and their constituents

IC-38: Transport of Electrons and Metal ions

IC-39: Metallo-Enzymes of Iron, Zinc and Nickel
Iron Enzymes: Structural and Mechanistic Aspects of Cytochrome P450, Cytochrome oxidase, Catalase and Peroxidase - Role of the Metal Ion.
Zinc Enzymes: Structural and Mechanistic Aspects of Carbonic Anhydrase, CarboxyPeptidase, Leucin – aminopeptidase, Thermolysin, Alcohol Dehydrogenase - Role of Zinc.
Nickel Enzymes: Urease, Hydrogenase and Factor F430: Reactions Catalyzed, Mechanistic Aspects.

IC-40: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese
Cobalt Enzymes: Cobalt in Vitamin B12 - Structural Features of Vitamin B12 with reference to coordination of Cobalt - Different Oxidation States of Cobalt - Various forms of Vitamin B12 and Active Enzyme forms - Types of Reactions Catalysed by i) Methyl Cobalamin ii) DeoxyadenosylCobalamin - Mechanism of the Methyl Malonyl CoA conversion to Succinyl CoA - Role of the Apoenzyme - Unique features of Cobalt to suit Vitamin B12.
Copper Enzymes: Types of Copper in Biological Systems - Structural and Mechanistic Aspects of Superoxide Dismutase, Laccase and Galactose oxidase.
Molybdenum Enzymes: Biological Roles and Mechanistic Aspects of Nitrogenase, Xanthineoxidase and Sulfite oxidase.
Manganese Enzymes: Arginase, Water – oxidase.

SUGGESTED BOOKS
2. Biochemistry - Mary K. Campbell. (added these books)
8. Advances in Inorganic Biochemistry, edited by G.L.Eichorn & Marzilli
IC-41: Metal complexes in Clinical Chemistry

IC-42: Metal complexes as Drugs and Anticancer agents

IC-43: Spectroscopic analysis of drug/metal complexes binding to DNA
Introduction to DNA binding studies. Cooperativity anti-cooperativity, the excluded site model. UV-Vis Absorption Spectroscopy and ligand/drug/metal complex DNA binding studies. Application of Fluorescence quenching in general and ligand/drug/metal complex DNA binding studies. Fluorescence titrations and binding constants. Salt back titrations interpretation of the data, the binding analysis, obtaining equilibrium binding isotherms. Dependence of K_{obs} on salt concentration, cation effects on ligand nucleic acid equilibria, Competitive effects of monovalent and divalent cations for binding. Record’s polyelectrolyte theory and its importance. Equilibrium dialysis. Partition analysis, competitive equilibrium dialysis to assess B & Z DNA binding. Competition dialysis to assess base and sequence specificity, viscosity studies. Tertiary structure of DNA, Supercoiled DNA(Form-I), Nicked DNA (Form-II) and Linear DNA(Form-III). DNA cleavage activity with ligand/metal complexes-Analysis by Gel electrophoresis.

IC-44: Applications of Nanomaterials
SUGGESTED BOOKS
5. Photoreactions of Metal complexes with DNA, A. Krisch – De Mesmacker et al.
8. Metal Complex -DNA Interactions, Editor(s): Nick Hadjiliadis, Einar Sletten, Copyright @ Blackwell Publishing Ltd.

PAPER III

CH(IC)403T (Elective IIIb ): Analytical Techniques -III

IC-45: Electroanalytical Methods
IC-46: Radiochemical Methods
IC-47: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry
IC-48: Industrial Analysis

IC-45: Electroanalytical Methods

Electrogravimetry: Basic principles of electrogravimetry, Instrumentation, electrogravimetry determination with constant applied voltage and at constant current. Applications of electrogravimetry. Problems based on effect of concentration on electrode potentials, calculation of theoretical cathode potential at the start of deposition, effect of pH in electrolytic separations.

Coulometry: Basic principles, Types of coulometers, constant current coulometric analysis, coulometric titrations – principle, circuit and cell for coulometry, Application to neutralization, Redox, precipitation, complexometric titrations, Advantages of coulometric titrations and errors. Controlled potential coulometry – Technique & applications of inorganic & organic compounds.

High Frequency Titrations: Introduction, Theory, Instrumentation, Applications, Advantages and disadvantages.
IC-46: Radiochemical Methods
Radioactive nucleotides, Instrumentation – measurement of alpha, Beta particles and Gamma radiation.
Radio tracers and tracer techniques, applications of Tracer techniques,
Neutron activation analysis: Neutron sources, interaction of neutrons with matter. Theory of activation methods, Experimental considerations, Nondestructive and destructive methods, applications.
Isotopic dilution analysis: Principles, theory and Applications.
Radiometric titrations: Principle, Procedure, advantages & disadvantages, applications to various types of titrations, problems based on the techniques.
Applications of Radio Chemical Methods in Biology, Agriculture and Environment

IC-47: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry

IC- 48: Industrial Analysis
Analysis of Ferroalloys: Analysis of steel - Molybdenum, Phosphorous.
Analysis of non- Ferrous alloys: Analysis of Tin, Zinc and Copper in Brass, Bronze. Analysis of Tin and lead in Solder.
Analysis of Oils & Fats: Theory, Melting point of fats, Chemical Characteristics: Saponification value, Iodine value, Thiocyanogen value, ketone or perfume rancidity.
Paints& Pigments: Constituents of Paints, Analysis of TiO₂ in Titanium dioxide pigments by XRD. Determination of Zn, Pb in Paint pigments by Polarographic method. Analysis of polyesters, acrylics by Gel permeation chromatography.

SUGGESTED BOOKS
IC-49: Clinical and Pharmaceutical Analysis


Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium in Vitamin D and Calcium formulations (Complexometry), Sulphanilamide (potentiometry), Pethidine hydrochloride (UV-Vis), Frusemide (UV-Vis), Aspirin, paracetamol and codeine in APC tablets (NMR), Phenobarbitone in tablets (IR), pivolic acid indipivefrin eye drops (GC), Assay of hydrocortisone cream. (HPLC). Impurity profiling of Propranolol (GC-MS), famotidine (LC-MS).

IC-50: Food and Agricultural analysis

Analysis of Chemical additives: Division of colour additives (Coal-tar dyes, vegetable colours and mineral colours). Chemical preservatives and synthetic sweetening agents (organic-ether extractable and non-ether extractable) SO$_2$, Sodium Benzoate, Sorbic acid, Benzoic acid.

Antioxidants: Types of Antioxidants used in foods, Analysis of Butylatedhydroxy toluene (BHT), propyl – gallates (PG), Octylgallates (GO), dodecyl gallates (DG) by TLC & GC.

Food adulteration: Common adulterants in food, contamination of food stuffs. Microscopic examinations for food adulterants.

Analysis of Soil – Determination of pH, conductivity, cation exchange capacity, total organic matter, nitrogen, phosphorous, potassium, S, Ca, Mg, Ca+Mg, Zn, Cu, Fe, Mn, B, Mo, Cd, Cr, Ni, Pb.

Analysis of Fertilizers – Moisture determination by Karl Fischer titration methods. Determination of Ammonical nitrogen and Ammonical nitrate nitrogen. Determination of total phosphates as P$_2$O$_5$. Estimation of potassium, Estimation of micronutrients by AAS.

Analysis of Pesticides: Analysis of Organo-chlorine pesticides (Cypermethrin) by Gas Chromatography. Determination of Malathion, Methyl parathion and DDT residues in vegetables and food grains.

IC-51: Analysis of Air and Water Pollutants

Air quality standards, sampling, analysis of air pollutants-SO$_2$ (UV-Vis, IR), H$_2$S (Spectrophotometry and Non-dispersive IR Spectrophotometry), NO-NOx (Chemiluminescence technique, Colorimetric technique- Saltzman method), CO & CO$_2$ (IR, AAS & GC), Hydrocarbons (GC, GC-MS), Aromatic hydrocarbons in automobile exhaust, petrol, air, O$_3$ (Chemiluminescence & Spectrophotometry), particulate matter analysis. Objectives of analysis, sampling, preservation and pre-concentration methods, physical analysis - colour, odour, temperature, pH, EC, redox potential, total desolved solids (turbidimetry), Chemical analysis of anions – CN$^-$, Cl$^-$, F$, NO_2^-$, NO$_3^-$ (spectrophotometry), SO$_4^{2-}$, PO$_4^{3-}$. 
Determination of BOD, COD, TOC & DO. Analysis of Toxic Metals: Hg, As, Pb, Cd, Be, Al, Cr (Atomic Absorption Spectroscopy and Spectrophotometry)

**IC-52: Drinking Water and Sewage Water Treatment**

**Hardness:** causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, Alkalinity of water and its estimation.

**Treatmet of Water for Municipal Supply:** Characteristics of potable water/Domestic water, WHO standards, and Indian Standards. Aeration, Sedimentation with coagulation, Filtration, Sterilization and Disinfection: Physical Methods-Boiling, Exposure to Sunlight, Disinfection with UV light, Chemical Methods – Ozonization, Chlorination, Breakpoint chlorination and Dechlorination

**Desalination of Brackish Water:** Treating saline water: distillation, electrodialysis, reverse osmosis (RO).

**Mineral Water and Purified Water:** Typical Manufacturing Process, Flow Sheet Diagram of Mineral Water Manufacturing Process, Purified Water-Purification methods-Distillation, Double distillation, Deionization - Co-current deionization, Counter-current deionization, Mixed bed deionization, Demineralisation, Uses of purified water- Laboratory use, Industrial uses and other uses; Health effects of drinking purified water

**Sewage Water Treatment:** Domestic sewage - Physical, Chemical, and Biological Characteristics of Domestic Sewage, Municipal sewage, Sewage Composition and Contaminants, Sewage Treatment - On-Site Sewage Treatment Systems and Off-Site Sewage Treatment Systems

**SUGGESTED BOOKS**

21. Handbook of Water and Wastewater Treatment Technologies, Nicholas P. Cheremisinoff, Published by Butterworth-Heinemann, 225 Wildwood Avenue, Woburn, MA 01801-2041
IC-49: Composite Materials
IC-50: Liquid Crystals
IC-51: Explosives and Propellants
IC-52: Fuels and Combustion

IC-49: Composite Materials


Ceramics: Plasticity of Clays, Whitewares or White-Pottery, Manufacture of White-Pottery, Glazing, Methods of glazing, Earthenwares and Stonewares.

IC-50: Liquid Crystals

IC-51: Explosives and Propellants
Explosives: Introduction, Classification of Explosives, Primary Explosives, Low Explosives, High Explosives, Precautions During Storage of Explosives, Blasting Fuses, Manufacture of Important Explosives-Lead azide, Diazonitrophenol (DDNP), Trinitrotoluene (TNT), Nitroglycerine (NG) or Glycerol trinitrate (GTN), Pentaerythritol tetranitrate (PETN) and RDX; Recent uses of Explosives

Propellants: Rocket Propellants - Introduction, Principle of Rocket Propulsion, Classifications of Propellants-Solid propellants, Composite propellants, Liquid Propellants, Mono-propellants, Bi-propellants; Differences between Solid propellants and Liquid Propellants

IC-52: Fuels and Combustion

Combustion:Combustion, Mass Analysis from Volume Analysis and Vice Versa, Analysis of Flue Gas
SUGGESTED BOOKS


Paper CH (IC) 451: Conventional Methods of Analysis

I. Titrimetry:
   1. Determination of Ca$^{2+}$, Mg$^{2+}$, CO$_3^{2-}$, HCO$_3^{-}$ in soil sample
   2. Determination of saponification value, iodine number, acid value and ester value of an oil sample (5-6 samples and comparative study)
   3. Determination of Ascorbic acid in Vit.C tablet by iodometry (2-3 samples)

II Water analysis:
   1. Determination of Dissolved Oxygen
   2. Determination of COD
   3. Determination of residual Chlorine in water by Iodometry
   4. Determination of Fluoride by Zirconium Alizarin Method
   5. Determination of Sulphate by spectrophotometry, turbidimetry or nephelometry

III Separation Methods
   1. Separation of Fe$^{3+}$ and Ni$^{2+}$ using tri-n-butyl phophite (TBP) from HCl medium (Solvent extraction)
   2. Determination of cations by paper chromatography; Co(II), Ni(II) and Cu(II)
   3. Separation of Fe(III) and Al(III) by column chromatography
   4. Separation of Fe$^{3+}$ and Ni$^{2+}$ using strongly basic anion resin.

SUGGESTED BOOKS

LABORATORY COURSES (IV Semester)
Paper CH (IC) 452: Spectroscopic techniques

I Spectrophotometry
1. Estimation of manganese.
2. Estimation of chromium.
3. Simultaneous determination of Manganese and Chromium in a mixture.
4. Determination of pKa of indicator (methyl orange/ methyl red)
5. Estimation of Nickel.
6. Determination of composition of Complex by Job’s Method and Mole ratio Method in the following:
   (i) Cu(II)-EDTA   (ii)Fe(II) - o-Phen

II Colorimetry
1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of creatinine
4. Determination of Paracetamol

III Fluorimetry
1. Determination of Riboflavin
2. Determination of Quinine Sulphate.

IV Flame photometry
1. Determination of Na
2. Determination of K
3. Determination of Ca
4. Determination of Li

V Atomic Absorption Spectroscopy
1. Determination of i) Fe, ii) Mg, iii) Cu, iv) Pb.

SUGGESTED BOOKS

   Text Book of Quantitative Inorganic Analysis Jafferyetal 4th edn. EdnElbs Publication
2. Quantitative Analysis by Day and Underwood Prentice Hall (India) VI Edn.
5. Medical Laboratory Technology – Mukherjee,McGraw Hills,1988
M.Sc. CHEMISTRY

ORGANIC CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR
2016 ONWARDS
M.Sc. CHEMISTRY (ORGANIC CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters
(for the batches admitted in academic year 2016 & later under CBCS pattern)
[Under Restructured CBCS Scheme]

Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G.BOS meeting held on 01-07-2017)

**SEMIESTER-III**

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* 15 marks for the written test and 5 marks for the assignment

**SEMIESTER - IV**

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OC-09: Synthetic Reagents-I  
OC-10: Synthetic Reagents-II  
OC-11: $^{13}$C NMR and 2D NMR spectroscopy  
OC-12: Conformational analysis (Cyclic systems ) and ORD  

**Paper-II CH (OC) 302T**: Modern Organic Synthesis  
OC-13: Asymmetric synthesis  
OC-14: Synthetic strategies  
OC-15: New Synthetic reactions  
OC-16: New techniques and concepts in organic synthesis  

**Elective-3A**  
**Paper-III CH (OC) 303T (CB1)**: Bioorganic Chemistry  
OC(CB1)-1: Carbohydrates  
OC(CB1)-2: Nucleic acids and Lipids  
OC(CB1)-3: Proteins and Enzymes  
OC(CB1)-4: Coenzymes and Vitamins  

**Elective-3B**  
**Paper-III CH (OC) 303T (CB2)**: Forensic Chemistry and Toxicology  
OC(CB2)-5: Forensic chemistry- I  
OC(CB2)-6: Forensic chemistry- II  
OC(CB2)-7: Forensic Toxicology-I  
OC(CB2)-8: Forensic Toxicology-II  

**Elective-4A**  
**Paper-IV CH (OC) 304T (CB3)**: Green chemistry and Organic materials  
OC (CB3) - 9: Principles of Green chemistry  
OC (CB3) - 10: Green Synthesis  
OC (CB3) - 11: Organic nanomaterials  
OC (CB3) - 12: Supramolecular chemistry  

**Elective-4B**  
**Paper-IV CH (OC) 304T (CB4)**: Pesticides  
OC (CB4) - 13: Introduction to pesticides  
OC (CB4) - 14: Synthetic insecticides  
OC (CB4) - 15: Natural insecticides & herbicides  
OC (CB4) - 16: Fungicides, and Rodenticides  

**LABORATORY COURSES**  
**Paper-V CH (OC) 351P**: Synthesis of organic molecules, isolation of natural products & TLC.  
**Paper-VI CH (OC) 352P**: Separation and identification of organic compounds & Column chromatography  

**Paper-I CH (OC) 401T**: Drug Design and Drug Discovery  
OC-17: Principles of Drug design and drug discovery  
OC-18: Lead modification and SAR Studies  
OC-19: QSAR studies and computer aided drug design  
OC-20: Combinatorial Synthesis  

**Paper-II CH (OC) 402T**: Drug synthesis and mechanism of action  
OC-21: Drugs acting on metabolic process, cell wall and specific enzymes  
OC-22: Drugs acting on genetic material and immune system  
OC-23: Drugs acting on receptors and ion channels  
OC-24: Chiral drugs  

**Elective-3A**  
**Paper-III CH (OC)-403T (CB1)**: Advanced Heterocyclic Chemistry  
OC (CB1) 17: Non aromatic heterocyclics & aromaticity  
OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms  
OC (CB1) 19: Heterocyclics with more than two hetero atoms  
OC (CB1) 20: Larger ring and other heterocycles  

**Elective-3B**  
**Paper-III CH (OC)-403T (CB2)**: Polymers, dyes and Pigments  
OC (CB2) 21: Polymers - I  
OC (CB2) 22: Polymers - II  
OC (CB2) 23: Dyes-I  
OC (CB2) 24: Dyes-II and pigments  

**Elective-4A (ID Paper)**  
**Paper-IV CH (OC) 404(CB3)T**: Advanced Natural Products  
OC(CB3)-25: Biosynthesis of natural products  
OC(CB3)-26: Structure determination of natural products -I  
OC(CB3)-27: Structure determination of natural products-II  
OC(CB3)-28: Total stereo selective synthesis of natural products  

**Elective-4B (ID Paper)**  
**Paper-IV CH (OC) 404 (CB4) T**: Biopharmaceutics and Pharmacodynamics  
OC(CB4)-29: Pharmacokinetics  
OC(CB4)-30: Pharmacodynamics  
OC(CB4)-31: Principles of Therapeutics  
OC(CB4)-32: Drug Interactions  

**LABORATORY COURSES**  
**Paper-V CH (OC) 451P**: Spectroscopic identification of organic compounds & practice of chemistry software programmes  
**Paper- VI CH (OC) 452P**: Synthesis and analysis of drugs
Paper-I CH (OC) 301T: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD
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M.Sc. CHEMISTRY (ORGANIC CHEMISTRY)
III SEMESTER SYLLABUS
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OC-09: Synthetic Reagents-I
OC-10: Synthetic Reagents-II
OC-11: $^{13}$C NMR and 2D NMR spectroscopy
OC-12: Conformational analysis (Cyclic systems) & ORD

OC-09: Synthetic Reagents I 15 Hrs

i) **Protecting groups:** a) Protection of alcohols by ether, silyl ether and ester formation
   b) Protection of 1,2-diols by acetal, ketal and carbonate formation
   c) Protection of amines by benzyl oxy carbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups.
   d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups.
   e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

ii) **Organometallic Reagents:** Preparation and application of the following in organic synthesis:
   1) Organolithium
   2) Organomagnesium reagents
   3) Organoboron compounds in C-C bond formation
   4) Organosilicon reagents: reactions involving β-carbocations and α-carbanions,
      utility of trimethyl silyl halides, cyanides and triflates.

iii) **Carbonyl methylenation:**
   a) Phosphorousylide mediated olefination
      1) Witting reaction,
      2) Horner-Wordsworth-Emmons reaction.
   b) Titanium-carbene mediated olefination
      1) Tebbe reagent,
      2) Petasis reagent
      3) Nysted reagent.

iv) **Carbene insertions:** Rh based carbene complexes, cyclopropanations.

v) **C-H Activation:** Introduction, Rh catalysed C-H activation.

OC-10: Synthetic Reagents II 15 Hrs

i) **Oxidations:**
   a) Oxidation of active C-H functions: DDQ and SeO$_2$.
   b) Alkenes to diols: Prevost and Woodward oxidation
   c) Alcohol to carbonyls: Cr$^{VI}$ oxidants (Jones reagent, PCC, PDC)
   IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation
   d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) **Reductions:**
   a) Catalytic hydrogenation: Homogenous (Wilkinson’s catalytic hydrogenation) and heterogeneous catalytic reduction.
   b) Non-metallic reductions: Diimide reduction
c) Dissolving metal reductions: Birch reduction.
   d) Nucleophilic metal hydrides: LiAlH$_4$, NaBH$_4$, and their modifications.
   e) Electrophilic metal hydrides: BH$_3$, AlH$_3$ and DIBAL.
   f) Use of tri-n-butyl tin hydride: Radical reductions.

OC-11: $^{13}$C NMR and 2D NMR spectroscopy 15 Hrs

i) $^{13}$C NMR spectroscopy:
   Introduction, Types of $^{13}$C nmr spectra: undecoupled, proton-
decoupled and off-resonance decoupled (ORD) spectra. $^{13}$C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ($^{13}$C, $^{13}$C J) and heteronuclear ($^{13}$C, $^1$H J and $^{13}$C, $^2$H J) coupling. Applications of $^{13}$C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. $^{13}$C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY ($^1$H-$^1$H COSY), TOCSY (Total Correlation Spectroscopy), HeteroCOSY ($^1$H,$^{13}$C COSY,HMQC), long range $^1$H,$^{13}$C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

OC-12: Conformational analysis (Cyclic systems) & ORD 15 Hrs
Conformational analysis (Cyclic systems)
Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthol), cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halocyclohexanones, cycloheptane. Stereo chemistry of bicyclo[3,3,0]octanes, hydridanones, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. ($\text{oxidation, }$S$_\text{N}$2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.


Recommended Books:
1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
6. Organic synthesis by Robert E Ireland
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahuwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome
15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
20. Basic one and two-dimensional NMR spectroscopy by Horst Frieboe
21. NMR spectroscopy by H. Gunther
22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen
24. Stereochemistry: Conformation & Mechanism by P S Kalsi
25. The third dimension in organic chemistry, by Alan Bassendale
28. Optical rotatory dispersion by C Djerassi
29. Optical rotatory dispersion and circular dichroism by P Crabbe
30. Mechanism and Structure in Organic chemistry by S Mukherjee

Paper II– CH (OC) 302T: Modern Organic Synthesis
OC-13: Asymmetric synthesis
OC-14: Synthetic strategies
OC-15: New Synthetic reactions
OC-16: New techniques and concepts in organic synthesis

OC-13:- Asymmetric synthesis 15 Hrs
Introduction: Brief revision of classification of stereo selective reactions
Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.
Prochiral nomenclature: Pro chirality and Pro-R, Pro-S, Re and Si.
Conditions forstereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.
Analytical methods: % Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.
Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram’s rule and Felkin-Anh model.
Chiral auxiliary controlled asymmetric synthesis: α-Alkylation of chiral enolates, Evan’s oxazolidinone, 1, 4-Asymmetric induction and Prelog’s rule.
Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC₂ BH and IPCBH₂.
Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate& achiral aldehydes ) its explanation by Zimmerman-Traxelmodel.

OC-14: Synthetic Strategies 15 Hrs
Order of events: S-Salbutamol, Propoxyxaine.
One group C-C and C-X disconnections: Introduction One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols,ethers and sulphides.
Two group C-C and C-X disconnections: Introduction Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.
Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.
Control in carbonyl condensations: oxanamide and mevalonic acid.
Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, longifoline.
1. **Metal mediated C-C and C-X coupling reactions:** Suzuki, Heck, Stille, Sonogishira crosscoupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

2. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurry reactions, Julia-Lythgoe olefination and Peterson’s stereoselective olefination.

3. **Multicomponent Reactions:** Ugi, Passerini, Biginelli, Bergman and Mannich reactions.

4. **Ring Formation Reactions:** Pausan-Khand reaction, Nazerov cyclisation.

5. **Click Chemistry:** Click reaction, 1,3-dipolar cycloadditions.

6. **Metathesis:** Grubb’s 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

7. **Other important synthetic reactions:** Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

**OC-16: New techniques and concepts in organic synthesis 15 Hrs**

1. **Techniques in peptide synthesis:** Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2. **Solid phase oligodeoxynucleotide synthesis:** Phosphotriester, phosphitetriester and phosphoramidite pathway

3. **Oligosaccharide synthesis:** Glycosidation: cyclic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, convergent and linear oligosaccharide synthesis.

4. **Phase Transfer catalysis:** Onium and crown ethers as PTC.

5. **Tandem synthesis:** Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, electrocyclic-Diels Alder reaction.

6. **Baldwin Rules:** Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

7. **Chiron approach in organic synthesis:** Nature’s chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonyycin from D-glucose, S-(-)-ipsenol from S-leucine.

8. **Determination of absolute configuration:** Mosher’s method.

**Recommended Books:**

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moscher
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Aten
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
13. Name reactions by Jie Jacob Li

**Elective-3A**

**Paper-III CH (OC)303T (CB1): Bioorganic Chemistry**
OC(CB1)-1: Carbohydrates

OC(CB1)-2: Nucleic acids & lipids

OC(CB1)-3: Proteins and Enzymes

OC(CB1)-4: Coenzymes and Vitamins
Coenzymes: Introduction. Co-factors - cosubstrates - prosthetic groups. Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of i) nicotinamide adenine dinucleotide / their phosphates (NAD), NADH, NADP$^+$, NADPH) ii) Flavin adenine nucleotide FAD, FADH$_2$ and iii) Flavin mononucleotide (FMN, FMNH$_2$) lipoic acid, biotin, tetrahydrofolate and ubiquinone. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl
methionine (SAM) and uridine diphosphosugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.  


**Reference Books:**
2. Carbohydrate Chemistry by Barton Volumes
3. Carbohydrate chemistry by G.J.Boons
4. The chemistry of natural products:vol.V - carbohydrates by S.F.Dyke
5. Organic Chemistry by McMurry
6. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
7. LehningerPrinciples of Biochemistry by D L Nelson and M MCoxon
8. Outlines of Biochemistry by Conn and Stumpf
9. Enzyme structure and mechanism by Fersht and Freeman
10. Enzymes for green organic synthesis by V.K.Ahuwalia
12. Principles of biochemistry by Horton &others.
13. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugasand Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian& others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg.

**Elective-3B**
OC(CB2)-5: Forensic chemistry-I
Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methods and instrumental techniques
Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) _ Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) – Natural products (tobacco, tea, sugars, rubber) – Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P-Aminophenol, and Nitrobenzene etc. with reference to forensic work.

OC(CB2)-6: Forensic chemistry-II

OC(CB2)-7: Forensic Toxicology-I
Toxicology- Introduction- History- Scope- Areas of Toxicology- Role of forensic toxicologist- Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation of toxicological exhibits in fatal and survival cases- Storage of samples- Signs and symptoms of poisoning- Toxicological investigation/examination of poisoned death- Interpretation of toxicological data- Courtroom testimony in toxicological cases. Case Histories.

OC(CB2)-8: Forensic Toxicology-II
Recommended books:
12. Wilson and Wilson’s Comprehensive Analytical Chemistry Volumes
13. Standard Methods of Chemical Analysis
14. AOAC: Official Methods of Analysis
22. Laboratory procedure Manual, Forensic Toxicology: DFS, 2005
26. Eckert; An Introduction to Forensic Science, CRC Press
Elective-4A

Paper-IV CH (OC) 304T (CB3): Green chemistry and Organic materials

OC (CB3) -9: Principles of Green chemistry
OC (CB3) -10: Green Synthesis
OC (CB3) -11: Organic nanomaterials
OC (CB3) -12: Supramolecular chemistry

OC (CB3)-9: Principles of Green Chemistry 15 Hrs
Green chemistry: Introduction
Principles of Green Chemistry: Designing a Green Synthesis using these principles; Prevention of Waste/by-products; maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy); prevention/minimization of hazardous/toxic products; designing safer chemicals; selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis: energy requirements for reactions - use of microwaves, ultrasonic energy in organic synthesis; prevention of unnecessary derivatization - careful use of protecting groups; use of catalytic reagents in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

OC (CB3) -10: Green Synthesis 15Hrs
i) Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations
a) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.
b) Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes.
ii) Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound-Cannizaro reaction, Reformatsky reaction and Strecker synthesis.
iii) Organic Synthesis in Green Solvents: introduction
a) Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and dihydroxylation reactions.
iv) Green Catalysts in organic synthesis: introduction
a) Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction
b) Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions.

OC (CB3) -11: Organic Nanomaterials 15Hrs
Introduction: The ‘top-down’ approach, the ‘bottom-up’ approach and Nanomanipulation.
Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.
New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs)and Graphenes.
Structures of aromatics belts, nano car and molecular machines.
Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures)
Natural Benzhetrazoles and their synthetic modifications as optoelectronic molecules.

OC (CB3) -12: Supramolecular Chemistry
15Hrs
Introduction: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions), Ionophore and molecular receptors.
Host-Guest Chemistry: Lock and key analogy, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcrirands.
Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.
Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral framework, Chiral receptor from Kemp’s triacid. Chiral receptors for tartaric acid.

Recommended books:
6. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH
8. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
10. Stereochemistry of organic compounds -Principles & Applications by D Nasipuri
11. Nanochemistry by G.B. Sergeev; Elsevier
Elective-4B
Paper-IV CH (OC) 304T (CB4): Pesticides

OC(CB4)- 13: Introduction to pesticides
OC(CB4)- 14: Synthetic insecticides
OC(CB4)- 15: Natural insecticides & herbicides
OC(CB4)- 16: Fungicides, and Rodenticides

**OC (CB4)-13: Introduction to pesticides** 15 Hrs

i) **Definition** Classification and importance of pesticides

ii) **Pest control**: Different methods – chemical – insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents.

   a) **Biological** – pheromones: Definition and classification, synthesis of Disparlure, Exobrevicomin, Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants.


   c) Moulting hormones: Structural formulae and mode of action of ecdysones


iii) **Environmental pollution from pesticides**

iv) **Integrated pest management**.

v) Pesticide formulations: Dusts, Granules, Wettable powders, Emulsions and Aerosols.

**OC (CB4)- 14: Synthetic insecticides** 15 Hrs

i) **Organochlorine insecticides** - synthesis and mode of action of methoxychlor, perthan, Dicofol, Heptachlor, Dieldrin and Endosulfan.

ii) **Organophosphorous insecticides** – synthesis and mode action of Phosphoric acid derivatives, phosphorothioates, Dichlorophos, parathion, Zolone, Aninphomethyl, TEPP and Sachradan.

iii) **Carbamate insecticides** – synthesis and mode of action of carbamyl, Furadan, Baygon, Aldicarb and Zectron.

iv) Formulation and residue analysis of organochlorine, organophosphorous and carbamate insecticides.

**OC (CB4)- 15: Natural insecticides and herbicides** 15 Hrs

i) **Insecticides of plant origin** – synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine. Main constituents Neem - structural formula of Azadirachtin. Synthesis of polygodial and warburganol (Antifeedants).


iii) **Concept of Bioinsecticides** – Bacillus thuringiensis.

iv) **Concept of pro-insecticides** - structure and mode of action of pro-pheromones and pre-pro-insecticides.

   v) **Herbicides** – synthesis, applications and mode of action of the following

   a) Aryloxyalkyl carboxylic acid derivatives: 2,4-D, MCPA, 2,4,5-T and 2,4,5-TP

   b) Carbamates - propham and chloropham, c) Urea derivatives - Monuron and diuron, d) Aliphatic acids - Dalapon, TCA,

   c) Aromatic acids - 2,3,6-TBA, Dicamba and Amiben, f) Nitrogen heterocyclic derivatives - Simazine, Atrazine, Amitrole, Maleic hydrazide, Diquat and paraquat, g) Phenols - PCP and Dinoseb, h) Benzonitrile compounds
OC (CB4)-16: Fungicides, and Rodenticides 15 Hrs

i) Fungicides –classification, synthesis application and mode of action of the following classes:
   a) Carbamates
   b) Quinones –chloranil, Dichlone, and Benquinox
   c) perchloromethylmercaptan derivative –captan, folpet, Difolatan and Mesulfan
   d) Benzimidazoles –carbendazim, Benomyl and Thiabandazole

ii) Rodenticides, a) Anticoagulents –synthesis and application of warfarin, Coumachlor, Vacor,
    Coumatetralyl, Dicoumarol and Bromidiolen, b) Acute poisons – application of
    pindone, Ratindan, Sodium Fluoroacetate, Barium fluoroacetate, Antu, Tetramine,
    pindone and castrix.

Reference books:
1) Naturally occurring insecticides: M. Jacobson and D. G. Crosby.
2) Insecticides for future: Jacobson
3) Insect juvenile hormone chemistry and action: J. J. Mann and M. Beroza
4) Polygodial and warburganal. Terpenoid antifeedants part-II rec, Tran, chin 106
5) Insect antifeedants: S. V. ley & P. L. Toogood, chemistry in Britain, Jan 1990, P. 31
6) Synthesis of Insecticides: Metcalf
7) Fungicides-Frear
8) Fungicides-Nene
9) Residue reviews vol. 36: Melnikov
10) Safer insecticides: E. Hodgson
11) Crop protection agents from Nature: Leonard G Copping
12) Biofertilizers and Bioinsecticides: A. M. Deshmukh
13) Insecticides and Fungicides: U Sriramulu.
14) Organo chlorine insecticides: persistent organic pollutants: F. Moriary
15) Herbicides: P. C. Kearney & D. D. Kaufman
16) Analytical Method for pesticides: Z. Weig (Vol III)
17) Pesticide formulations: Van Valkenburg
18) Insecticides: A. S. Tahori
19) Herbicides, fungicides, formulation chemistry: A. S. Tahori
20) Environmental pollution by pesticides: C. A. Edwards
21) Pesticides management and insecticide resistance: Watson and brown
22) Organo phosphorous pesticides: M. eto
**Laboratory courses:**

**Paper CH (O) 351P: Synthesis of organic molecules, isolation of natural products & TLC**

(A) **Laboratory synthesis of the following compounds:**
2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker-Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4-Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzillic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin (NaBH₄ reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

(B) **Isolation of the following natural products:**
Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

(C) **Thin layer chromatography:** Thin layer chromatography: Determination of purity (All the above preparations), monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the Rf values of known standards.

**Paper CH (O) 352P: Separation and identification of organic compounds & Column chromatography**

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5% aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 09 mixtures should be separated and analyzed by these procedures.

**Cannizzaro reaction:** 4-Chloro benzaldehyde as substrate and separation of the resulting two component mixture

Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed.

**Column chromatography:** Separation of a mixture of ortho and para-nitroanilines and any one of the two component mixture using silica gel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC.

**Recommended Books:**
1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin
Paper-I CH (OC) 401T: Drug Design and Drug Discovery
OC-17: Principles of Drug design and drug discovery
OC-18: Lead modification and SAR Studies
OC-19: QSAR studies and computer aided drug design
OC-20: Combinatorial Synthesis

Paper-II CH (OC) 402T: Drug synthesis and mechanism of action
OC-21: Drugs acting on metabolic process, cell wall and specific enzymes
OC-22: Drugs acting on genetic material and immune system
OC-23: Drugs acting on receptors and ion channels
OC-24: Chiral drugs

Elective-3A Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry
OC (CB1) 17: Non aromatic heterocyclics & aromaticity
OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms
OC (CB1) 19: Heterocyclics with more than two hetero atoms
OC (CB1) 20: Larger ring and other heterocycles

OC (CB2) 21: Polymers - I
OC (CB2) 22: Polymers - II
OC (CB2) 23: Dyes - I
OC (CB2) 24: Dyes - II and pigments

Elective-4A Paper-IV CH (OC) 404(CB3)T: Advanced Natural Products
OC(CB3)-25: Biosynthesis of natural products
OC(CB3)-26: Structure determination of natural products - I
OC(CB3)-27: Structure determination of natural products - II
OC(CB3)-28: Total stereo selective synthesis of natural products.

Elective-4B Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics
OC(CB4)-29: Pharmacokinetics
OC(CB4)-30: Pharmacodynamics
OC(CB4)-31: Principles of Therapeutics
OC(CB4)-32: Drug Interactions

Laboratory courses
Paper-VCH (OC) 451P: Spectroscopic identification of organic compounds & practice of chemistry software programmes
Paper-VI CH (OC) 452P: Synthesis and analysis of drugs
Paper-1 CH(OC) 401T: Drug Design and Drug Discovery

OC-17: Principles of Drug design and drug discovery
OC-18: Lead modification and SAR Studies
OC 19: QSAR studies and computer aided drug design
OC 20: Combinatorial Synthesis

**OC- 17: Principles of Drug design and drug discovery** 15 Hrs
Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore -structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g. Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

**OC-18: Lead modification and SAR Studies** 15 Hrs
SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs.

**OC-19: QSAR studies and computer aided drug design** 15 Hrs
QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constants($\sigma$), lipophilicity constant($\pi$), steric effects and Taft’s constant, linear and nonlinear relationship between biological activity. Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig’s plot, Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).

**Computer aided drug design:** Introduction, active site, allosteric binding site, use of grids in docking, rigid docking, flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.
OC-20: Combinatorial Synthesis 15Hrs


Reference books
1. Burger’s medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
5. Principles of medicinal chemistry. by William Foye
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistty Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11. Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishansingh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotechnology By Roger A. Sheldon

**Paper-II CH (OC) 402T: Drug synthesis and mechanism of action**

OC-21: Drugs acting on metabolic process, cell wall and specific enzymes
OC-22: Drugs acting on genetic material and immune system
OC-23: Drugs acting on receptors and ion channels
OC-24: Chiral drugs

**OC-21: Drugs acting on metabolic process, cell wall and specific enzymes**
Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.
a) Drugs acting on metabolic process:
Antifolates – Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone.
Diaminopyrimidines - trimethoprim, bacterial resistance to sulfonamides and drug synergism
c) Drugs acting on specific enzymes: \( \text{H}^+ / \text{K}^+ \)-ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

**OC-22: Drugs acting on genetic material and immune system**
Drugs acting on genetic material: Introduction, classification and mechanism of action.
b) DNA-Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Timidazole.
c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.
d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.
f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifaxymcins and partial synthesis of Rifampicin.
g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

**OC-23: Drugs acting on receptors and ion channels**
Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.
Drugs acting on receptors:
a) Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin.
β-Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabutalin, Propranolol and Atenolol.


c) Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.


f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen.

Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca$^{2+}$, Na$^{+}$ and Cl$^{-}$ channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

OC-24: Chiral drugs
Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer’s rule. Role of chirality on biological activity: Distomers – a) with no side effects b) with undesirable side effects c) both isomers having independent therapeutic value d) combination products having therapeutic advantages e) metabolic chirality inversion.


Reference Books:
2. Introduction to Medicinal chemistry. By Graham Patrick.
8. Drug design By E.J. Arienes.
10. Medicinal chemistry An introduction By Gareth Thomas.
13. Medicinal Chemistry By Ashutoshkar.
17. Top Drugs: Top synthetic routes By John Saunders.
18. Chirotechnology By Roger A. Sheldon.
Elective-3A
Paper-III CH (OC)-403T (CB1): Advanced Heterocyclic Chemistry
OC (CB1) 17: Non aromatic heterocyclics & aromaticity
OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms
OC (CB1) 19: Heterocyclics with more than two hetero atoms
OC (CB1) 20: Larger ring and other heterocycles

OC (CB1) 17: Nonaromatic heterocyclics & Aromaticity 15 Hrs
Different types of strains, interactions and conformational aspects of nonaromatic heterocycles. Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and thietanes
Aromaticity: Introduction, Aromatic and anti aromatic compounds. Criteria for aromaticity. Huckel’s 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes.

OC (CB1) 18: Five and six membered heterocyclics with two hetero atoms 15 Hrs
Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine, Pyrazine, Oxazine, thiazine, benzimidazole, benzoazole and benzthiazole.

OC (CB1) 19: Heterocyclics with more than two hetero atoms 15 Hrs
Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoies, 1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5- oxadiazole, 1,2,3-thiadiazoles, 1,3,4-thiadiazoles, 1,2,5-thiadiazoles, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Synthesis of Caffeine, theobromine and theophylline.

OC (CB1) 20: Larger ring and other Heterocycles 15 Hrs

Recommended Books:
1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule & K. Mills
5. Heterocyclic Chemistry, J.A.Joule & Smith
7. The aromaticity III level, units 17-19 British open university volumes
8. Aromatic character and aromaticity by G.M.Badger
9. Non-benzenoid aromatic compounds by D.Ginsberg
10. Nonbenzenoid compounds by Lloy
Elective-3B
OC (CB2) 21: Polymers- I
OC (CB2) 22: Polymers- II
OC (CB2) 23: Dyes-I
OC (CB2) 24: Dyes-II and pigments

OC (CB2) 21: Organic Polymers - 115 Hrs

OC (CB2) 22: Organic Polymers - II 15 Hrs
a) Functional polymers:
   i) Electrically conducting polymers: Introduction, basic principles. Brief description of polyanilines, polypyrroles, polyacetylenes, polythiophenes and their applications.
   ii) Photoconductive polymers: Liquid crystal polymers, smectic, nematic and cholesteric structures, ion-exchange polymers – cationic, anionic exchange polymers and their uses.
   iii) Smart materials: Uses in sensing device and communication networks.


c) Fire retarding polymers and photonic polymers.
   Polymers in biomedical application, artificial organs and controlled drug delivery.

OC (CB2) 23: Dyes – I 15 Hrs
Synthetic and Natural dyes
Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromospheres and auxochromes with suitable examples, Witt’s theory, Armstrong’s theory, Baeyer’s theory, Nietzki’s theory, Waston’s theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methane dyes[malachite green, rosiniline, para aniline blue, crystal violet methyl violet, hydroxytriphenyl methane dyes, Aurin, chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.

OC (CB2) 24: Dyes–II and Pigments 15 Hrs
a) Introduction to Fluorescence dyes
yields and factors affecting them. Synthesis of Fluorescent aromatic hydrocarbons and Fluorescent heteroaromatic compounds.


**Reference Books**
1. Organic polymer chemistry by K.J. Sanders
3. The elements of Polymer Science and Engineering by A. Rudin
4. Principles of Polymer Chemistry by A. Ravve
5. Polymer Science by V.R. Gowariker, N.V. Viswanathan and J. Sreedhar
6. Polymer Chemistry by C.E. Carraher, Jr.
8. Polymer Chemistry, B. Vollmert
11. Color and constitution of organic molecules by J. Griffiths
15. Introduction to Fluorescence Sensing, Springer 2009, by A.P. Demchenko
16. Natural Dyes and their Applications in Textiles by M.L. Gulrajani, IIT Delhi
17. Handbook on Natural Dyes for Industrial Applications by P. S. Vankar, National Institute of Industrial Research
Elective-4A(ID Paper)
Paper-IVCH (OC) 404(CB3)T: Advanced Natural Products

OC(CB3)-25: Biosynthesis of natural products
OC(CB3)-26: Structure determination of natural products-I
OC(CB3)-27: Structure determination of natural products-II
OC(CB3)-28: Total stereo selective synthesis of natural products.

**OC(CB3)-25: Biosynthesis of natural products 15 Hrs**

**OC(CB3)-26: Structure determination of natural products-I 15 Hrs**
Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

**OC(CB3)-27: Structure determination of natural products-II 15 Hrs**
Spectroscopic techniques IR, UV, \(^1\) Hnmr, \(^13\)Cnmr, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

**Study of the following solved problems:** Mass, IR, \(^1\)H, \(^13\)C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of menthol, APT of apparicine,

Heteronuclear 2D-J resolved spectrum of stricticine, NOESY of buxaquamarine, HETEROCOSY of strictanol, 2D-INADEQUATE of α-picoline and β-methyl tetrahydrafuran.

**OC(CB3)-28: Total stereoselective synthesis of natural products. 15 Hrs**
Nicalou’s synthesis of Dynemicin A, Corey’s synthesis of prostaglandins (E2, F2α) and paeoriflorin, Sharpless synthesis of L-hexoses, Nicolaous synthesis of taxol, Danishefsky synthesis of indolizomycin, Takasago synthesis of menthol, Hoffmann-LaRoche synthesis of Biotin.
Reference books:
1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser arid Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo
11. Alkaloids by Pelletier
12. Total synthesis of Natural Products by Apsimon Vol 1-5
13. Biosynthesis by Geismann
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster
Elective-4B(ID Paper)
Paper-IV CH (OC) 404(CB4)T: Biopharmaceutics and Pharmacodynamics

OC(CB4)-29 : Pharmacokinetics
OC(CB4)-30 : Pharmacodynamics
OC(CB4)-31 : Principles of Therapeutics
OC(CB4)-32: Drug Interactions

OC(CB4)-29: Pharmacokinetics.
Introduction and importance of ADME studies of drugs. Routes of administration .
i)Absorption: Definition, absorption of drugs across the membranes. Physico chemical factors affecting the drug absorption (emphasis on pH partition hypothesis and Drug Dissolution).

OC(CB4)-29: Pharmacodynamics.

OC(CB4)-30: Principles of Therapeutics
Plasma Drug concentration vs Time profile,Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen, Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plama concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

OC(CB4)-31: Drug Interactions.
Introduction, classification, Mechanisms of drug interactions.– pharmacokinetic interactions(alteration of gastrointestinal absorption, compexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic effects, alteration of electrolyte levels, interactions involving adnergenic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol( Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking( Theophylline, Diazepam, a Tri cyclic antidepressants), food ( Bronchodaliators, Diuretics, ACE Inhibitors, Anti coagulants,Tetracyclines) on drug action.
Reference books:
1. Pharmacokinetics. By Shobha Rani
2. Elements of Pharmacology. By Gandhi, Desani & Goyal.
5. Biopharmaceutics and pharmacokinetics By Brahmanikar
6. Pharmacology By Lippincot
8. Comprehensive pharmacy review by Leon Shargel
9. Hospital and clinical pharmacy
11. Introduction to Medicinal chemistry. By Patrick.
12. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
**Laboratory courses**

Paper CH (OC) 451P: Spectroscopic identification of organic compounds & practice of chemistry software programmes

1. Identification of unknown organic compounds by interpretation of IR, UV, $^1$H -NMR, $^{13}$C NMR, and mass spectral data (two examples with 2D-NMR). A minimum of 30 representative examples should be studied.

2. **Chemistry software programmes:** Chem Draw, analysis of IR and NMR using ACD/Id NMR processor. EXCEL: Drawing graphs, Molecular docking.

Paper CH (OC) 452P: Synthesis and analysis of drugs

(A) **Laboratory Synthesis of the following drugs:**
Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, Fluorescien, 4-Aminobenzene sulphonamide, antipyrine and phenothiazine

(B) **Estimation of the following drugs:**
Aspirin (titrimetry), Ibuprofen (titrimetry), Analgin (titrimetry), Chloride in Ringer’s lactate (argentometry), ascorbic acid (titrimetry, Iodometry and Cerimetry), colorimetry, Isoniazid (Iodometry), Riboflavin (colorimetry), Zn ions in Bactracin Zinc, Ca$^{2+}$ ions in Calcium gluconate injection (complexometry), Riboflavin (UV-Visible Spectrophotometer).

**Reference books:**
1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster
M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY SPECIALISATION)

SYLLABUS OF III & IV SEMESTERS

REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR

2016 ONWARDS
M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)  
Syllabus for III and IV SEMESTERS  
(For the batch admitted in the academic year 2016 and later under the CBCS pattern)  
[Under Restructured CBCS Scheme]  
Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits  

(Approved in the P.G.BOS meeting held on 01-07-2017)

### SEMESTER-III

<table>
<thead>
<tr>
<th>Paper</th>
<th>Instruction Hrs/Week</th>
<th>Internal Assessment marks*</th>
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* 15 marks for the written test and 5 marks for the assignment

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* 15 marks for the written test and 5 marks for the assignment

Grand total all 4 semesters: 2400 marks and 96 credits
### III SEMESTER SYLLABUS

<table>
<thead>
<tr>
<th>Paper-I CH(PhC)301T: Basics of Pharmaceutical Chemistry</th>
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<tbody>
<tr>
<td>PhC 10: Rheology and micromeritics</td>
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<td>PhC 11: Physical pharmacy</td>
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<td>PhC 12: Introduction to pharmaceutics</td>
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<th>Paper-II CH(PhC) 302T: Pharmacokinetics and Pharmacodynamics</th>
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<td>PhC 13: Pharmacokinetics</td>
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**Elective-3A**

- Paper-IIIC(PhC) 303T(CB1): Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD
- PhC(CB1)-1: Synthetic Reagents-I
- PhC(CB1)-2: Synthetic Reagents-II
- PhC(CB1)-3: $^{13}$C NMR and 2D NMR spectroscopy
- PhC(CB1)-4: Conformational analysis (Cyclic systems) & ORD

**Elective-3B**

- Paper-III CH(PhC) 303T(CB2): Pharmaceutical Inorganic and Analytical Chemistry
- PhC(CB2)-5: Inorganic pharmaceuticals-I
- PhC(CB2)-6: Inorganic and Radio pharmaceuticals-II
- PhC(CB2)-7: Limit tests
- PhC(CB2)-8: Biochemical analysis

**Elective-4A**

- Paper IV CH(PhC) 304T(CB3): Modern Organic Synthesis
- PhC(CB2)-9: Asymmetric synthesis
- PhC(CB2)-10: Synthetic strategies
- PhC(CB2)-11: New Synthetic reactions
- PhC(CB2)-12: New techniques and concepts in organic synthesis

**Elective-4B**

- Paper IV CH(PhC) 304T(CB4): Herbal drugs, synthetic pharmaceuticals and IPM
- PhC(CB4)-13: Herbal Drugs
- PhC(CB4)-14: Synthetic pharmaceuticals -I
- PhC(CB4)-15: Synthetic pharmaceuticals –II
- PhC(CB4)-16: Intellectual Property Management

### IV SEMESTER SYLLABUS

<table>
<thead>
<tr>
<th>Paper-I CH(PhC) 401T: Drug Design and Drug Discovery</th>
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<tbody>
<tr>
<td>PhC-17: Principles of Drug design and drug discovery</td>
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<tr>
<td>PhC-18: Lead modification and SAR Studies</td>
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<tr>
<td>PhC-19: QSAR studies and computer aided drug design</td>
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<td>OC 20: Combinatorial Synthesis</td>
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<table>
<thead>
<tr>
<th>Paper-II CH(PhC) 402T: Drug synthesis and mechanism of action</th>
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<tbody>
<tr>
<td>PhC-21: Drugs acting on metabolic process, cell wall and specific enzymes</td>
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<td>PhC-22: Drugs acting on genetic material and immune system</td>
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<td>PhC-23: Drugs acting on receptors and ion channels</td>
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<td>PhC-24: Chiral drugs</td>
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</table>

**Elective-3A**

- Paper III CH(PhC)403T(CB1): Medicinal natural products and drug analysis
- PhC(CB1)-17: Medicinal natural products
- PhC(CB1)-18: Spectroscopic analysis of drugs
- PhC(CB1)-19: Titrimetric analysis of drugs
- PhC(CB1)-20: XRD and chromatographic analysis of drugs

**Elective-3B**

- Paper-III CH(PhC) 403T(CB2): Industrial Pharmaceutical Chemistry
- PhC(CB2)-21: Unit Process |
- PhC(CB2)-22: Industrial Synthesis
- PhC(CB2)-23: Quality Control and Quality Assurance
- PhC(CB2)-24: Effluents of Industrial Units and their purification

**Elective-4A (ID Paper)**

- Paper IV CH(PhC) 404T(CB3): Biopharmaceutical Chemistry
- PhC(CB3)-25: Enzymes – Enzyme Immobilisation
- PhC(CB3)-26: Microbial Transformations
- PhC(CB3)-27: Pharmaceuticals From Fermentation Technology
- PhC(CB3)-28: Pharmaceuticals From Recombinant DNA Technology

**Elective-4B (ID Paper)**

- Paper IV CH(PhC) 404T(CB4): Biomolecules and Molecular Modelling
- PhC(CB4)-29: Nucleic acids
- PhC(CB4)-30: Proteins:
- PhC(CB4)-31: Molecular Modelling
- PhC(CB4)-32: Modelling Biomolecules

### LABORATORY COURSES

<table>
<thead>
<tr>
<th>Paper-V CH(PhC) 351: Qualitative Analysis of Organic Mixtures</th>
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<tbody>
<tr>
<td>Paper-VI CH (PhC) 352: Spectroscopic identification of organic compounds and Chromatography</td>
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<tr>
<td>Paper-V CH (PhC) 451P: CH (PhC) 451P: Synthesis of drug molecules and QSAR studies</td>
</tr>
<tr>
<td>Paper- VI CH (PhC) 452P: Titrimetric &amp; Instrumental Drug analysis</td>
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**M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)**

**III SEMESTER SYLLABUS**

(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

**PAPER- I**

**CH (PhC) 301T BASICS OF PHARMACEUTICAL CHEMISTRY**

**PhC 9:** Introduction to I.P, B.P & USP monographs, Errors in pharmaceutical analysis and statistical validation.

**PhC 10:** Rheology and micromeritics

**PhC 11:** Physical pharmacy

**PhC 12:** Introduction to pharmaceutics

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**PhC 9: Introduction to I.P, B.P & USP monographs, Errors in pharmaceutical analysis and statistical validation.**  
15hrs


**PhC 10: Rheology and Micromeritics**  
15hrs


**Micromeritics** Introduction, particle size analysis- concepts of particle size, size distribution, mean size of particulate system, methods of particle size analysis (sieving, microscopic method, sedimentation methods, electrical sensing zone method, optical sensing zone and light diffraction method).

**PhC 11: Physical Pharmacy**  
15hrs

Physical properties of drug molecules: Dielectric constant, Induced polarization, refractive index, molar refraction, optical rotation, Colligative properties.

**PhC 12: Introduction to pharmaceutics**


**Recommended text books:**
1. Practical pharmaceutical chemistry. By A.H.Backette, J.B.Stenlake, Part-A & B.
2. Pharmaceutical analysis by Ashtoshkar
3. Fundamentals of analytical chemistry by Skoog & West
4. Physical Pharmacy by AN.Martin,J, Swarlbick etal
5. Physical pharmaceutics by Shotton and Ridgeway
7. Text book of physical pharmaceutics by Subramaniyan
8. Essentials of Physical chemistry and pharmacy by Arnikar & Kadam
9. Introduction to pharmaceuticals by Mittal
10. Pharmaceutical dosage forms and drug delivery systems by Ansel
11. Introduction to Pharmaceuticals by Gupta, Volume I & II.
12. Modern pharmaceutics by Banker and Rhode

**References:**
1. British Pharmacopoeia vol I,II
2. Indian Pharmacopoeia vol I,II
3. Bently’s Text book of pharmaceutics by Rowlins
4. The science and practice of pharmacy by Remington

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**PAPER-II CH (PhC) 302T PHARMACOKINETICS AND PHARMACODYNAMICS**

**PhC 13: Pharmacokinetics**
**PhC 14: Pharmacodynamics**
**PhC 15: Principles of Therapeutics**
**PhC 16: Drug Interactions**

**PhC 13: Pharmacokinetics**

**PhC14: Pharmacodynamics**  
15hrs  

**PhC15: Principles of Therapeutics**  
15hrs  
Plasma Drug concentration vs Time profile, Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph). Peak plasma concentration, time of peak concentration. Therapeutic range. Steady state concentration, onset of action, onset of time, duration of action, intensity of action. LD50, ED50. Therapeutic objective. Dosage regimen. Design of dosage regimes: Dose size, dosing frequency, drug accumulation during multiple dosing, time to reach steady-state during multiple dosing, average concentration and body content on multiple dosing to steady state, loading dose, maintenance dose, maintenance of drug within the therapeutic range, design of dosage regimen from plasma concentration. Kinetics of fixed dose, fixed time interval regimes. Modification to dosage regime: Dosing of drugs in obese patients, dosing of drugs in Neonates, infants & children, dosing of drugs in geriatrics (elderly), dosing of drugs in Hepatic disease, dosing of drugs in renal disease.

**PhC16: Drug Interactions.**  
15hrs  
Introduction, classification, Mechanisms of drug interactions.– pharmacokinetic interactions(alteration of gastrointestinal absorption, compexation and adsorption, alteration of distribution, alteration of metabolism and alteration of excretion) & pharmacodynamic interactions (antagonistic effects, synergistic effects, alteration of electrolyte levels, interactions involving adrenergic system, alteration of receptor site interaction and antibiotic combinations). Influence of alcohol( Anti biotics, Anti coagulants, Anti histamines, Anti psychotic drugs, sedatives and Hypnotics), smoking( Theophylline, Diazepam, and T ri cyclic antidepressants), food ( Bronchodaliators, Diuretics, ACE Inhibitors, Anti coagulants,Tetracyclines) on drug action.

**Recommended text books:**
1. Pharmacokinetics. By Shobha Rani  
2. Elements of Pharmacology. By Gandhi,Desani & Goyal.  
5. Biopharmaceutics and pharmacokinetics By Brahmanikar  
6. Pharmacology By Lippincot  
8. Comprehensive pharmacy review by Leon Shargel  
9. Hospital and clinical pharmacy  
11. Introduction to Medicinal chemistry. By Patrick.  
12. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.  
PAPER III -CH (PhC) 303T(CB1): Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD

PhC-(CB1) -1: Synthetic Reagents-I
PhC-(CB1) -2: Synthetic Reagents-II
PhC-(CB1) -3: $^{13}$C NMR and 2D NMR spectroscopy
PhC-(CB1) -4: Conformational analysis (Cyclic systems) & ORD

PhC-(CB1) -1: Synthetic Reagents I
15 Hrs

i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation
b) Protection of 1,2-diols by acetal, ketal and carbonate formation
c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups.
d) Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung) groups.
e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

ii) Organometallic Reagents: Preparation and application of the following in organic synthesis:
1) Organo lithium
2) Organo copper reagents
3) Organo boranes in C-C bond formation
4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.

iii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination 1) Witting reaction,

iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.

v) C-H Activation: Introduction, Rh catalysed C-H activation.

PhC-(CB1) -2: Synthetic Reagents II
15 Hrs

i) Oxidations: a) Oxidation of active C-H functions: DDQ and SeO$_2$. b) Alkenes to diols: Prevost and Woodward oxidation
c) Alcohol to carbonyls: Cr$^{VI}$ oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation
d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinsons’s catalytic hydrogenation) and heterogeneous catalytic reduction.
b) Non-metallic reductions: Diimide reduction
c) Dissolving metal reductions: Birch reduction.
d) Nucleophilic metal hydrides: LiAlH$_4$, NaBH$_4$, and their modifications.
e) Electrophilic metal hydrides: BH$_3$, AlH$_3$ and DIBAL.
f) Use of tri-n-butyl tin hydride: Radical reductions.

PhC-(CB1) -3: $^{13}$C NMR and 2D NMR spectroscopy
15 Hrs

i) $^{13}$C NMR spectroscopy: Introduction, Types of $^{13}$C nmr spectra: undecoupled, proton-decoupled and off-resonance decoupled (ORD) spectra. $^{13}$C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ($^{13}$C, $^{13}$C J) and heteronuclear ($^{13}$C,$^1$H J and $^{13}$C,$^2$H J) coupling. Applications of $^{13}$C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. $^{13}$C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY ($^1$H-$^1$H COSY) , TOCSY (Total Correlation Spectroscopy)
Spectroscopy), Hetero COSY (\( ^1\text{H},^{13}\text{C}\) COSY, HMOC), long range \( ^1\text{H},^{13}\text{C}\) COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

**PhC-(CB1) -4: Conformational analysis (Cyclic systems) AND ORD**

**15 Hrs**

**Conformational analysis (Cyclic systems)** Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cycloheptane. Stereo chemistry of bicyclo [3,3,0] octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.

(oxidation, S\(_{\text{N}}\)2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

**Optical Rotatory Dispersion (ORD) and CD Spectroscopy:** Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

**Recommended Books:**

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
6. Organic synthesis by Robert E Ireland
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome
15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
20. Basic one and two-dimensional NMR spectroscopy by Horst Frieben
21. NMR spectroscopy by H.Gunther
22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
24. Stereochemistry: Conformation & Mechanism by P S Kalsi
25. The third dimension in organic chemistry, by Alan Bassendale
28. Optical rotatory dispersion by C Djerassi
29. Optical rotatory dispersion and circular dichroism by P Crabbe
30. Mechanism and Structure in Organic chemistry by S Mukherjee

Paper III  CH (PhC) 303T (CB2)  PHARMACEUTICAL INORGANIC AND ANALYTICAL CHEMISTRY

PhC (CB2) -5 : Inorganic pharmaceuticals
PhC (CB2) -6 : Inorganic and Radio pharmaceuticals
PhC (CB2) -7 : Limit tests
PhC (CB2) -8 : Biochemical analysis

PhC (CB2) -5 : Inorganic pharmaceuticals 15hrs

PhC (CB2) -6: Inorganic and radio pharmaceuticals 15hrs

PhC (CB2) -7: Biochemical analysis 15hrs
   Principles and practical aspects of i) Microbiological assay- Zone inhibition method, serial dilution method (eg: antibiotics); ii) Competitive protein binding assay (eg. testosterone); iii) Radioimmuno assay(eg. morphine, insulin); iv) Radioreceptor assay(eg. benzodiazepine); v) Enzyme linked immunosorbent assay (eg. cocaine, opiates, ); vi) Flourescence immuno assay(eg. galactosyl umbelliferone drug, cortisol).vii) Test for pyrogens.
**PhC (CB2) -8 : Limit tests**


**Recommended text books:**

1. Vogel’s text book of quantitative chemical analysis
2. Pharmaceutical analysis By Chapman
3. Pharmaceutical analysis By Ashtoshkar
4. Inorganic pharmaceutical chemistry By Chatwal
5. Inorganic pharmaceutical chemistry By Mohammadali
6. Inorganic pharmaceutical and medicinal chemistry By Quadri and Quadri

**References**

1. Practical pharmaceutical chemistry. By A.H.Backette, J.B.Stenlake.
2. British Pharmacopoeia vol I,II
3. Indian Pharmacopoeia vol I,II
4. Pharmaceutical analysis. By Takeru,Higuchi
5. Pharmaceutical analysis By. David G.Watson
7. The science and practice of pharmacy by Remington

**Paper IV -CH (PhC) 304T (CB3): Modern Organic Synthesis**

**PhC (CB3)-9: Asymmetric synthesis**

**PhC (CB3)-10: Synthetic strategies**

**PhC (CB3)-11: New Synthetic reactions**

**PhC (CB3)-12: New techniques and concepts in organic synthesis**

**PhC (CB3)-9:- Asymmetric synthesis**

**Introduction:** Brief revision of classification of stereo selective reactions

**Prostereoisomerism:** Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

**Prochiral nomenclature:** Pro chiraility and Pro-R, Pro-S, Re and Si.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivityy.

**Analytical methods:** % Enantiomeric excess and diastereomeric excess. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiralderativating agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

**Chiral Substrate controlled asymmetric synthesis:** Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram’s rule and Felkin-Anh model.

**Chiral auxiliary controlled asymmetric synthesis:** α-Alkylation of chiral enolates, Evan’s oxazolidinone, 1, 4-Asymmetric induction and Prelog’s rule..
Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC₂ BH and IPCBH₂.

Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphin catalyst.

Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate & achiral aldehydes ) its explanation by Zimmerman-Traxel model.

PhC (CB3)-10: Synthetic Strategies 15 Hrs


Order of events: S-Salbutamol, Propoxycaine.

One group C-C and C-X disconnections: One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

Two group C-C and C-X disconnections: Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds. Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations: oxanamide and mevalonic acid.

Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, longifoline.

PhC (CB3)-11: New Synthetic reactions 15 Hrs


2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson’s stereoselective olefination.


5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.

6. Metathesis: Grubb’s 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

PhC (CB3)-12: New techniques and concepts in organic synthesis 15Hrs

1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

2. Solid phase oligodeoxynucleotide synthesis: Phospho triester, phosphtie triester and phosphoramidite pathway
3. **Oligosaccharide synthesis:** Glycosidation: cyclic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.

4. **Phase Transfer catalysis:** Onium and crown ethers as PTC.

5. **Tandem synthesis:** Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, electrocyclic-Diels Alder reaction.

6. **Baldwin Rules:** Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

7. **Chiron approach in organic synthesis:** Nature’s chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-ipsenol from S-leucine.

8) **Determination of absolute configuration:** Mosher’s method.

**Recommended Books:**

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moscher
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng

**Paper IV - CH(PhC) 304T (CB4): Herbal drugs , synthetic pharmaceuticals and IPM**

**PhC (CB4)-13: Herbal Drugs**

**PhC (CB4)-14 : Synthetic pharmaceuticals -I**

**PhC (CB4)-15 : Synthetic pharmaceuticals --II**

**PhC (CB4)-16: Intellectual Property Management**

**PhC (CB4)-13: Herbal Drugs** 15hrs

PhC (CB4)-14: Synthetic pharmaceuticals –I 15hrs
Synthesis and pharmacological activity of the following drugs. Diclofenac (anti-inflammatory), Tinidazole (anti-amebic), Pheniramine (anti-histamine), Ciprofloxacin (anti-bacterial), Cloxacillin, Cephalexin (anti-biotics), Miconazole (anti-fungal), Cisplatin (anti-neoplastic), Ethambutal (anti-tubercular) and Enalapril (anti-hypertensive).

PhC (CB4)-15: Synthetic pharmaceuticals-II 15hrs
Benzocaine (localanesthetic), Phenobarbitone, Nitrazepam (Hypnotic) Isoprenalin (sympathomimetic) Celecoxib (anti-inflammatory), Procainamide (cardiovascular), Omeprazole (antiulcer), 5-Floro uracil (anticancer), Ciprofloxacin, norfloxacin (antibacterials), Lamivudine (anti-AIDs) and Clofazimine (anti leprosy and anti T.B).

PhC (CB4)-16: Intellectual Property Management 15hrs
Introduction, Intellectual property-meaning of patent, definition, object of patent law, salient features of IPA 1970, Patentable invention, procedure for patentship, application, examination, exclusive marketing rights, opposition, grant and seal, patent addition, amendment in application, restoration of lapsed patent, surrender, revocation, register of patents, powers of controller, non-patentable inventions, transfer of patent, use of inventions by Government, Infringement, Reliefs, Patents (amendment) Act- 1999 and 2002(briefly) and any further amendments on that date. Case Laws-relating to Pharmaceuticals and drugs.

Recommended text books:

1. Natural products. By P.S.Kalsi
5. May’s chemistry of synthetic drugs. Hand Book of Reagents for organic synthesis. By Reich,Rigby
6. The organic chemistry of Drug synthesis. vol 1-6 By Ledneicer etal.
7. Top Drugs: The synthetic routes. J.Saunders
8. Organic natural products By Barton and Ollis
9. Organic natural products by OP Agarwal
10. Natural products. By P.S.Kalsi
11. Organic natural products By Barton and Ollis
13. Intellectual property rights by N.K.Acharya
14. Law relating to patents, trademarks, Copyright designs and geographical indications by B.L.Wadehra
B Laboratory work

PAPER V–(PhC-351 P): Qualitative Analysis of Organic Mixtures.
Separation and identification of organic compounds:

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, dil hydrochloric acid, 5 % aqueous sodium bicarbonate and sodium hydroxide solutions, checking the purity of two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 10 mixtures should be separated and analyzed by these procedures.

Paper VI (PhC-352 P): Spectroscopic identification of organic compounds and Chromatography
Identification of unknown organic compounds by interpretation of IR, UV, $^1$H NMR, $^{13}$C NMR and mass spectra. A minimum of 30 representatives

Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions and column chromatographic separations, identification of unknown organic compounds by comparing the Rf values of known standards, and preparative TLC for separation of mixtures.

Paper chromatography- Separation and identification of amino acids by ascending and radial paper chromatography.

Separation / Purification by column chromatography: Separation of a mixture of ortho and para-nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.
M.Sc. CHEMISTRY (PHARMACEUTICAL CHEMISTRY)
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016 -2017 under the CBCS pattern)

Paper-1 CH (PhC) 401T: Drug Design and Drug Discovery
PhC-17: Principles of Drug design and drug discovery
PhC-18: Lead modification and SAR Studies
PhC 19: QSAR studies and computer aided drug design
PhC 20: Combinatorial Synthesis

PhC- 17: Principles of Drug design and drug discovery 15 Hrs
Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore -structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

PhC-18: Lead modification and SAR Studies 15 Hrs
SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs.

PhC-19: QSAR studies and computer aided drug design 15Hrs
QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft’s constant, linear and nonlinear relationship between biological activity Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig’s plot, Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).
Computer aided drug design: Introduction, active site, allosteric binding site, use of grids in docking, rigid docking, flexible docking and induced fit docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.
**PhC-20: Combinatorial Synthesis**


**Recommended books**

1. Burger’s medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman.
8. Drug design by E.J.Arienes.
13. Medicinal Chemistry By Ashtoshkar.
14. Medicinal Chemistry By Chatwal.
17. Top Drugs: Top synthetic routes By John Saunders.
18. Chirotechnology By Roger A. Sheldon.

**Paper-II CH (PhC) 402T: Drug synthesis and mechanism of action**

PhC-21: Drugs acting on metabolic process, cell wall and specific enzymes
PhC-22: Drugs acting on genetic material and immune system
PhC-23: Drugs acting on receptors and ion channels
PhC-24: Chiral drugs
PhC-21: Drugs acting on metabolic process, cell wall and specific enzymes 15hrs
Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a) Drugs acting on metabolic process:
Antifolates – Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone.
Diaminopyrimidines - trimethoprim, bacterial resistance to sulfonamides and drug synergism


PhC-22: Drugs acting on genetic material and immune system 15hrs
Drugs acting on genetic material: Introduction, classification and mechanism of action.


b) DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.


f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Drugs acting on immune system: Introduction to immune system. Immunosupressing agent-structural formula of Cyclosporin. Immunoenhancers-use of vaccines and structural formula of levamisol.

PhC-23: Drugs acting on receptors and ion channels 15hrs
Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:


c) Dopamine receptors: Introduction and classification. Dopamine receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen

Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca$^{2+}$, Na$^+$ and Cl$^-$ channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

**PhC-24: Chiral drugs**

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer’s rule. Role of chirality on biological activity: Distomers – a) with no side effects b) with undesirable side effects c) both isomers having independent therapeutic value d) combination products having therapeutic advantages e) metabolic chirality inversion.


**Recommended Books:**

2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
10. Medicinal chemistry An introduction By Gareth Thomas
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotecchnology By Roger A. Sheldon
Paper III -CH(PhC) 403T(CB1): Medicinal natural products and drug analysis
PhC(CB1) 17 : Medicinal natural products
PhC(CB1) 18 : Spectroscopic analysis of drugs
PhC(CB1) 19 : Titrimetric analysis of drugs
PhC(CB1) 20 : XRD and chromatographic analysis of drugs

PhC(CB1) 17 : Medicinal natural products 15hrs
Glycosides: Source, Isolation, structure determination, Synthesis of Streptomycin, stereochemical structures and pharmacological activity of Digitoxin and Digoxin.
Prostaglandins: Introduction, Classification, Source, Isolation, structure determination, and synthesis of \( \text{PGE}_2 \). Stereochemical structures and pharmacological activity of Prostacyclin and Thromboxane.

PhC(CB1) 18: Spectroscopic analysis of drugs 15hrs
\(^1\)H-NMR spectrometry: Quantitative analysis of (i) Aspirin – paracetamol - caffeine tablets.
Atomic emission spectroscopy (Flame photometry): Principle, instrumentation. Applications—Determination of calcium in magnesium chloride for dialysis, determination of the concentration of potassium in haemodialysis solution.
Spectrofluorimetry: Theory, instrumentation, applications—determination of proflavin hemisulphate in proflavin cream, determination of ethinyloestradiol in tablets.
**PhC(CB1) 19 : Titrimetric analysis of drugs** 15hrs

**PhC(CB1) 20: XRD and Chromatographic analysis of drugs** 15hrs
X-ray Diffraction studies: Polymorphism, Miller indices, Bragg’s equation. Experimental methods- the rotating crystal method, oscillating crystal method, powder method, indexing the reflections, systemic absences and applications.

**Size-exclusion Chromatography:** Principle, Instrumentation, stationary phases, retention behavior, applications: determination of relative component composition. Determination of molecular weight, eg. Corticotrophin and insulin.

**Capillary electrophoresis:** Types of Electrophoresis, Electro osmotic flow, instrumentation, control of separation, applications: Separation of Atenolol and related impurities, analysis of non steroidal anti inflammatory drugs.

**Super Critical fluid Chromatography:** Principle, super critical fluids, instrumentation, stationary phases, mobile phases, and detectors.

**Recommended books:**
1. Natural products. By P.S.Kalsi
2. Organic natural products By Barton and Ollis
3. Organic natural products by OP Agarwal
4. Natural products. By P.S.Kalsi
5. Medicinal natural products by Dewick
7. Steroid chemistry. By Kalsi
10. Analytical chemistry by Christian
11. Fundamentals of analytical chemistry by Skoog, West, Holler
12. Vogel’s text book of quantitative chemical analysis
13. Quantitative analysis by Day & Underwood
14. Pharmaceutical analysis By Ashtoshkar
15. Analytical chemistry by open learning by Clive Watson
16. Physical chemistry by Atkins
17. Physical chemistry by Glasstone
18. Solid state chemistry by West
19. Instrumental methods of analysis by Willard
References
22. Pharmaceutical analysis By. David G.Watson
23. Instrumental methods of chemical analysis By Sharma
24. Analytical chemistry By Harris

Paper III CH(PhC) 403T(CB2) INDUSTRIAL PHARMACEUTICAL CHEMISTRY

PhC(CB2)-21: Unit Process
PhC(CB2)-22 : Industrial Synthesis
PhC(CB2)-23: Quality Control and Quality Assurance
PhC(CB2)-24: Effluents of Industrial Units and their purification

PhC 21:: Unit Processes 15hrs
Concept of unit processes in systematization of chemical reactions, explanation of one example each for unit processes: Thermodynamic and kinetic aspects of Alkylation, amination, (by ammonolysis, reduction), esterification, halogenation, hydroformylation, hydrogenation, nitration, oxidation and reduction. Mechanistic aspects of carbonylation, carboxylation, condensation, dehydration, diazotization, disproportionation, hydration, hydrolysis, hydroxylation, sulphonation and acetylation.

PhC 22: Industrial Synthesis 15hrs
Introduction to pharmaceutical manufacturing - raw materials, detailed manufacturing procedure, therapeutic function, common name, chemical name, structural formulae of the following drugs. Acyclovir, alprazolam, Ibuprofen, cimetidine, sulphamethoxazole, ciprofloxacin, chloramphenicol maleate, licocaine, ethambutal hydrochloride, 5-fluorouracil, furazolidine.

PhC 23:: Quality Control and Quality Assurance 15hrs
Introduction, concepts and significance, Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, blind samples in control.
PhC 24: Effluents Of Industrial Units And Their Purification 15hrs
Introduction to industrial effluents. Classification of effluents. Classification of basic methods of purifying effluents. i) Purification of suspended and emulsified impurities by mechanical method. ii) Purification of dissolved impurities- a) from mineral matter by ion exchange, reverse osmosis, electrical and reagent methods. b) From organic matter by destructive methods, biological oxidation, ozonization, chlorination, extraction, adsorption and ion exchange) Purification of gases by desorption method. iii) Purification by elimination and destruction- by thermal destruction, burying and pumping into depth of oceans.

Recommended text books:
1. Industrial chemistry By B.K.Sharma
2. Bulk drug manufacture. Profile
3. Environmental chemistry By B.K.Sharma
4. Unit processes in chemical engineering By Groggins
5. Unit processes in chemical engineering By Drydens
6. Pharmaceutical manufacturing encyclopedia vol I&II

Paper IV CH(PhC) 404(CB3) T BIOPHARMACEUTICAL CHEMISTRY (ID Paper)
PhC(CB3) 25 :Enzymes – Enzyme Immobilisation
PhC(CB3) 26: Microbial Transformations
PhC(CB3) 27: Pharmaceuticals From Fermentation Technology
PhC(CB3) 28: Pharmaceuticals From Recombinant DNA Technology

PhC(CB3) 25 : Enzymes – Enzyme Immobilisation 15hrs
Introduction; Classification and nomenclature of enzymes; mechanism of enzyme action- lock and key model; induced fit model; enzyme kinetics-initial velocity, effect of enzyme concentration substrate concentration (Michaels- Menton equation Lineweaver-Berk representation), effect of pH, temp.; Enzyme inhibition- irreversible, reversible(competitive, non-competitive and uncompetitive). Immobilization of enzymes- adsorption method, chemical binding method, cross binding method, entrapping method, effect of immobilization on kinetics and properties of enzyme applications and production of penicillin’s , steroids, L-DOPA

PhC(CB3) 26:Microbial Transformations 15hrs
Introduction; methods used in biotransformation process- fermentation, analysis and isolation of product and selection of organisms. biotransformations with special reference to steroids and sterols- hydroxylation, dehydrogenation, hydrogenation, epoxidation, ring A aromatization, synthetic routes. Biotransformations with reference to prostaglandins -synthhesis of PGE1 and sulprostone

PhC(CB3) 27 :Pharmaceuticals From Fermentation Technology 15hrs
Introduction; development of industrial microorganisms-mutatoins, selectioni of mutants, selection of secondary metabolite producing mutants, catalyst screening, industrial fermentation (brief discussion only), maintainance of aseptic conditions, oxygen transfer; applications; b-lactam antibiotics- penicillins, streptpmycin, tetracyclins, chloramphenicol, vitamins- vit.B2, vit C, ergot alkaloids.
**PhC(CB3) 28: Pharmaceuticals From Recombinant DNA Technology**  
*15hrs*

Introduction; oligonucleotide synthesis, restriction enzymes, recombinant DNA technology using plasmids, phase and cosmids; polymerase chain reaction principle, components technique method, Sanger’s method automated DNA sequencing. Applications - Insulin, human growth hormone, vaccines, interferons, novel enzymes.

**Recommended books:**
5. Pharmaceutical Biotechnology. By Kor and Hal Kari
6. An introduction to biotransformation in organic chemistry By James R. Hanson
7. Biotransformation by Faber
8. Goodmann & Gilman’s “The pharmacological basis of therapeutics.”

**Paper IV CH(PhC) 404(CB4)T: BIOMOLECULES AND MOLECULAR MODELLING**
*(ID Paper)*

**PhC (CB4)-29: Nucleic acids**


**PhC (CB4)-30: Proteins**


**PhC (CB4)-31: Molecular Modelling**

PhC (CB4)-32: Modelling Biomolecules

Introduction to modeling biomolecules, Protein structure prediction – Protein folding, secondary structure prediction, sequence alignment, the inverse folding problem. Modelling by homology – the alignment, construction of the frame work, selecting variable regions, side chain placement. Validation of protein models – Ramachandran plot. Molecular modeling in drug discovery, 3D pharmacophores and detection methods, molecular docking, Denovo ligand design.

Recommended Books
7. Introduction to drug design. By Silverman
8. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.

References:
1. Drug design By E.J. Arienes
2. Jenkin’s quantitative pharmaceutical chemistry By Knevel and Dryden
3. Recent advances in Bioinformatics By IA.Khan and A Khanum
4. Computational chemistry By GH. Grant and WG. Richards
5. Molecular modeling By Hans Dieter Holtje and Gerd Folkers
6. Molecular modeling By Leach
7. Computational Chemistry by Jenson

Laboratory work

PAPER-V: PhC-451P Synthesis of drug molecules and QSAR studies

(A) Synthesis of drug molecules

2-Phenyl indole, (Fischer Indole Synthesis), 7- Hydroxy-3-methylflavole (Baker-Venkatraman Reaction), 2, 5-Dihydroxy acetopheneone(Fries reaction), 4-ChloroToluene(Sandmeyer reaction), 7-Hydroxy Coumarin(Pechman synthesis), vanillyl alcohol form vanillin(NaBH4 Reduction) , Benzylc acid rearrangement, Beckmann rearrangement, Phenytoin, Fluorescein, 6-Methyl Uracil, Benzocaine, 4-Aminobenzene Sulphonamide, Phenacetin, phenothiazine, Tolbutamide

(B) Prepration of Pharmaceutical formulations
(i) Sulpha ointment  (ii) salicylin ointment (iii) Benadryl Cough syrup
(C) QASR problems based on logP, \( \pi \) ans \( \sigma \) parameters.

**PAPER-VI: PhC-452P Titrmetric & Instrumental Drug analysis**

Assay of Aspirin, (Acid-base titrations).
Assay of Chloride in Ringers lactate (Precipitation titrations).
Assay of Codiene phosphate syrup
Assay of Acorbic acid in raw material by iodometry
Assay of Calcium in Calcium tablets (single tablet method)
Assay Zinc in Bacitracin zinc
Assay of Ethambutol in Ethambutol tablets
Assay of Amlodipine in Amlodipine tablets
Assay of Ampicillin in Ampicillin Capsules.
Tests for hardness of tablets, Friability, Disintegration tests for uncoated, coated and enteric coated tablets, capsules.
Colorimetric estimation of dextrose in dextrose injection.
Conductometric assay of Aspirin
Assay of Riboflavin in tablets by UV-Visible Spectrophotometry
Dissolution profile of paracetamol
Determination of sodium and potassium ions in pharmaceuticals by flamephotometry
Determination of quinine sulphate by florimetry.
Potentiometric estimation of Sulphanilamide
M.Sc. CHEMISTRY

PHYSICAL CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR
2016 ONWARDS
### M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY SPECIALISATION)

**Syllabus for III and IV Semesters**  
(for the batches admitted in academic year 2016 & later under CBCS pattern)

[Under Restructured CBCS Scheme]

Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G. BOS meeting held on 01-07-2017)

#### Semester - III (Physical Chemistry)

[Under CBCS Scheme]

(for the batches admitted in academic year 2016 & later under CBCS pattern)

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#### Semester - IV (Physical Chemistry)

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Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits
M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2016 & later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY
PC - 09: Applications of Schrödinger equation
PC - 10: Angular momentum & approximate methods
PC - 11: Bonding in molecules
PC - 12: Group theory

PAPER – II CH (PC) 302T : SPECTROSCOPY AND LASERS
PC- 13 : Physical principles of spectroscopy and Vibrational spectroscopy
PC- 14 : NMR , NQR and Mossbaur Spectroscopy
PC- 15 : X-ray Spectroscopy & Diffraction techniques
PC - 16 : Lasers in Chemistry

ELECTIVE 3A
PAPER III CH (PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS
PC(CB1)-1 : Applied kinetics
PC(CB1)-2 : Applied Electrochemistry
PC(CB1)-3 : Types of materials, conducting organics and NLO materials
PC(CB1)-4 : Radiation effects

ELECTIVE–3B
PC-(CB2)- 5:Bioenergetics and physical properties of biopolymers
PC-(CB2)- 6:Biological membranes and binding of ligands by biopolymers
PC-(CB2) - 7: DNA, genes and cloning
PC-(CB2) - 8: Bioinformatics

ELECTIVE–4A
PAPER-IV CH(PC) 304T(CB3): Polymer Chemistry
PC-(CB3)-9: Polymerization and Kinetics of polymerization
PC-(CB3)-10: Structure and properties of polymers
PC-(CB3)-11: Processing of Polymers
PC-(CB3)-12: Functional polymers

ELECTIVE –4B
Paper IV CH(PC) 304T(CB4): Environmental Chemistry
PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

LABORATORY COURSES

Paper-V CH (PC) 351 P: Chemical Kinetics
Paper-VI CH(PC) 352P: Instrumentation
M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in the academic year 2016 and later under CBCS pattern)

PAPER-I CH(PC) 401T(CB1): Thermodynamics, Chemical Kinetics and Electrochemistry
PC- 17. Statistical Thermodynamics
PC- 18. Non-equilibrium Thermodynamics
PC- 19. Chemical Kinetics-II
PC- 20. Electrochemistry-II

PAPER-II CH(PC) 402T: Supramolecular Chemistry, Photo Chemistry and Computational Chemistry
PC- 21: Supramolecular Chemistry
PC- 22: Photochemistry-II
PC- 23: Computational Chemistry
PC- 24: Theoretical treatment of bio polymers

ELECTIVE–3A
PAPER-III CH(PC) 403 T(CB1) : Catalysis
PC-(CB1)-17: Homogeneous catalysis
PC-(CB1)-18: Surface Chemistry and Micellar catalysis
PC-(CB1)-19: Heterogeneous catalysis
PC-(CB1)-20: Phase transfer, Anchored and Photo catalysis

ELECTIVE–3B
Paper IV CH(PC) 403 T(CB2) : Dynamics of chemical reactions and Sensors
PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects
PC-(CB2)-23: Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

ELECTIVE –4A (ID PAPER)
PAPER-IV CH(PC) – 404T(CB3) : Computational Chemistry and It’s Applications
PC(CB3)-25: Computational Chemistry – I
PC(CB3)-26: Computational Chemistry – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

ELECTIVE –4B (ID PAPER)
PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry
PC(CB4)-29: Water And Waste Water Treatment
PC(CB4)-30: Corrosion And Its Control
PC(CB4)-31: Energy Sources:
PC(CB4)-32 Engineering Materials.

ELECTIVE –4C (ID PAPER)
PAPER-IV CH(PC) 405T(CB5): Sugar Chemistry and Sugar Technology
PC(CB5)-33: Advanced Sugar Chemistry
PC(CB5)-34: Sugar and Sugar byproducts
PC(CB5)-35: Methodology used in Sugar Analysis
PC(CB5)-36: Sugar Technology and Management

LABORATORY COURSES
Paper-V CH (PC) 451P: Chemical Kinetics
Paper-VI CH (PC) 452P: Instrumentation
M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY Specialization
(for the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY

PC -09: Applications of Schrödinger equation
PC -10: Angular momentum and approximate methods
PC -11: Bonding in molecules
PC -12: Group theory

PC–09: Applications of Schrödinger equation (15 hrs)


Atomic and molecular term symbols.
Atoms in external field, Zeeman and anomalous Zeeman effect.

PC–10: Angular momentum and approximate methods (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of $L^2$ and $L_z$ and the eigen values. Magnitude and orientation of angular momentum vectors.


Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals ( STOs ).
**PC–11: Bonding in molecules** (15 hrs)


Concept of hybridization – sp, sp², and sp³ hybrid orbitals.

Semiempirical MO methods. The Hückel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Introduction to extended Hückel Theory, extension of the Hückel’s approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: H₂ + F₂ → 2HF reaction. 2NO → N₂ + O₂ reaction.

**PC–12: Group theory** (15 hrs)


Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.


**Books suggested:**

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
5. Coulson’s Valence, R. McWeeny, ELBS
PC-13: Physical principles of spectroscopy and Vibrational spectroscopy: (15 Hrs)


PC-14: NMR, NQR and Mossbaur Spectroscopy. (15hrs)


Two dimensional nmr spectroscopy:
Principles of 2D nmr - Graphical representation of 2D nmr spectra – Homonuclear $¹H J, δ$ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional $¹H, ¹H$ shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine.

The nuclear overhauser effect(NOESY). Two dimensional nuclear overhauser spectroscopy(NOESY). Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splitting.

Mossbauer Spectroscopy - Mossbauer effect – Recoil energy, typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – $⁵⁷Fe$ – Mossbauer spectra of $Fe^{2+}$ and $Fe^{3+}$ (paramagnetic) and $Fe^{3+}$ (magnetic) compounds.

PC-15: X-ray Spectroscopy and Diffraction techniques: (15 hrs)

X-ray fluorescence (XRF) : Experimental method, Processes in X-ray fluorescence, K-emission spectrum of tin, L-emission spectrum of gold.

X-ray absorption: Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.


**PC-16: Lasers in Chemistry:** (15 hrs)


Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.


**Books suggested:**

1. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
9. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley-VCH publishers
10. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
15. Atkin’s Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
17. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd.
ELECTIVE 3A

PAPER III CH(PC) 303T(CB1) : APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS

PC(CB1)-1 : Applied kinetics
PC(CB1)-2 : Applied Electrochemistry
PC(CB1)-3 : Types of materials, conducting organics and NLO materials
PC(CB1)-4 : Radiation effects

PC(CB1)-1: Applied kinetics (15 hrs)


Batch reactors (BR): General features. Design equations for a BR. Material and energy balances. Isothermal operation, constant-density system.


Comparisons of ideal reactors for a single reaction. Single-vessel comparisons. BR and CSTR. BR and PFR. Numerical examples.

PC(CB1)-2: Applied Electrochemistry (15 hrs)

Batteries: Battery parameters. Energy density, power density and Ragone plot. Measures of battery performance. Primary and secondary batteries. Zn/MnO₂, lead-acid and Ni-Cd batteries and Lithium cells; Lithium-thionylchloride cell and lithium-ion battery.


Photovoltaic cells: Semiconductor based photoelectrochemical cells. Electrochemical energy from solar energy.


Electro-organic synthesis: Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon. Reduction of nitro compounds.
PC(CB1)-3: Types of materials, Conducting Organics and NLO materials (15 hrs)

Classification of materials – metals, ceramics, polymers, composites, semiconductors and biomaterials.

Glassy state – glass formers and glass modifiers, applications
Ceramics – criteria for determining the crystal structure of ceramic materials – examples.
Composites – particle reinforced and fibre reinforced composites.

Preparative methods of solid materials - Ceramic method (Solid State method), co-precipitation as a precursor to solid state reaction, solutions and gels (Zeolite synthesis), crystallization from melts: Czochralski method, Kyropolous method; vapour phase transport method, modification of existing structure by ion-exchange and interaction reactions.

Conducting organics – Fullerenes, alkali metal doped fullerides, fullerenes as superconductors

PC(CB1)-4: Radiation effects 15hrs


Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations, Use of radiation for food preservation and sterilization.

Books suggested:
1. Introduction to Chemical reaction Engineering and Kinetics, R. W. Missen, C. A. Mims & B. A. Saville, John Wiley
2. Chemical Reaction Engineering, O. Levenspiel, John Wiley
4. Elements of Chemical Reaction Engineering, H. Scott Fogler, Prentice Hall (page-114)
5. Modern Electrochemistry 2B, Bockris & Reddy, Plenum
6. Industrial Electrochemistry, D. Pletcher, Chapman & Hall
7. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi
8. Electrochemistry – B K Sharma
9. Fundamental principles of Modern Electroplating, Lowenheim, John Wiley
10. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons
11. Solid state chemistry and applications. A.R.West, John Wiley & Sons
12. New directions in solid state chemistry. CNR Rao and Gopalakrishnan, Cambridge University Press
13. Principles of the Solid State, H. V. Keer, New Age International

ELECTIVE –3B

Paper III CH(PC) 303T(CB2) : BIOPOLYMER CHEMISTRY

PC(CB2)-5: Bioenergetics & physical properties of biopolymers
PC(CB2)-6: Biological membranes & binding of ligands by biopolymers
PC(CB2)-7: DNA, genes and cloning
PC(CB2)-8: Bioinformatics

PC(CB2)-5: Bioenergetics and physical properties of biopolymers (15 hrs)


Viscometry: Molecular weights. Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers. Light scattering method.


PC(CB2)-6: Biological membranes and binding of ligands by biopolymers (15 hrs)

Binding of ligands and metal ions to macromolecules – one and n-equivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of $H^+$ and $CO_2$. Bohr effect.

**PC(CB2)-7: DNA, genes and cloning** (15 hrs)

Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA.


Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.


**PC(CB2)-8: Bioinformatics** (15 hrs)

Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment.

General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB - Organism Specific Databases examples - E. Coli, Yeast, Oryza.

Introduction to Proteins - primary, secondary, tertiary and quaternary structures.

Structure databases – PDB, MMDB, CSD. Homology modeling – Flow chart, structure refinement - Ramachandra Plot.

**Books suggested:**

4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books
ELECTIVE 4A

Paper IV CH(PC) 304T(CB3) : POLYMER CHEMISTRY

PC(CB3)-9: Polymerization and Kinetics of polymerization
PC(CB3)-10: Structure and properties of polymers
PC(CB3)-11: Processing of Polymers
PC(CB3)-12: Functional polymers

**PC(CB3)-9: Polymerization and Kinetics of polymerization** (15 hrs)

Classification of polymers. Types of polymerization.

Kinetics and mechanism of free radical polymerization. Degree of polymerization, kinetic chain length and chain transfer coefficient – Trommsdorff effect. Effect of pressure and temperature on chain polymerization.

Kinetics and mechanism of cationic, anionic polymerization, coordination polymerization, linear stepwise polymerization.


Polymerization in homogeneous and heterogeneous systems. Techniques of polymerization-Bulk, solution, suspension and emulsion polymerizations.

**PC(CB3)-10: Structure and properties of polymers** (15 hrs)

Polymer solutions:


Mechanical properties of polymers:


The glassy state – glass transition temperature Tg of polymers. Factors influencing Tg. Glass transition temperature and melting point.

Molecular weight distribution – measurement of molecular weights by end group analysis, osmometry and GPC.
PC(CB3)-11: Processing of Polymers (15hrs)

General applications of Polymers. Polymer Additives - Fillers, plasticizers, lubricants, catalysts, stabilizers, colorants, antioxidants, flame retardants.

Processing techniques of polymers - one dimensional coating - Adhesives, Lamination; extrusion- calendering and thermoforming; Molding of Polymers- Process, advantages and limitations of Compression molding, Injection Molding, Extrusion Molding, Blow Molding.

Casting - Types, Vacuum Casting, Potting, Encapsulation, Film Casting,


Processing of fiber reinforced Composites- Pultrusion technique, prepreg production processes, filament winding.

PC(CB3)-12: Functional polymers (15hrs)

Smart materials – Their uses in sensing devices and in communication networks.

Electrically conducting polymers- Introduction, basic principles and their applications. Brief description of polyanilines, polypyrrole, polyacetylene and polythiophene.

Photoconductive polymers, Liquid crystal polymers – smectic, nematic and cholesteric structures, Ionic exchange polymers- Cationic and anionic exchange polymers and their uses.

Biodegradable polymers- Definition, classification, applications. Brief description of polyhydroxyalkanoates, polycaprolactone, polylactic acid and polyvinylalcohol.


Fire retarding polymers, photonic polymers.

Polymers in biomedical applications – artificial organs and controlled drug delivery.

Books suggested:

1. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
4. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and professional
6. Polymer Chemistry, B. Vollmert, Springer publishers
7. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
ELECTIVE 4B

Paper IV CH(PC) 304T(CB4) : ENVIRONMENTAL CHEMISTRY

PC(CB4)-13: Pollution in Atmosphere
PC(CB4)-14: Pollution in Hydrosphere
PC(CB4)-15: Heavy Metal and Radiochemical Pollution.
PC(CB4)-16: Analysis of Air, Water and Metal Pollutants

PC(CB4)-13: Pollution in Atmosphere


Carbon Monoxide: Sources and Sinks, Concentration Profile, Effects on Human Health, Control of CO Emissions.

Nitrogen Oxides (NO\textsubscript{x}): Reactions Leading to Formation of NO\textsubscript{x}, Sources and Sinks, Concentration Profile, Harmful Effects of NO\textsubscript{x} on Human Beings, Plants, Materials and Control of NO\textsubscript{x} Emissions.

Sulphur Oxides (SO\textsubscript{x}): Reactions Leading to Formation of SO\textsubscript{x}, Sources of SO\textsubscript{x}, Harmful Effects on Human Beings, Plants and Materials - Control of SO\textsubscript{x} Emissions - Acid Rain: Formation and Toxic Environmental Effects.

Particulate Matter: Sources, Inorganic and Organic Particulate Matter - Effects on Human Beings, Materials and Climate - Control of Particulate Emissions.

Hydrocarbons: Sources - Types of Polluting Hydrocarbons - Hydrocarbons and Photochemical Smog Formation - Harmful Effects of Photochemical Smog - Control of Hydrocarbon Emissions.

Green House Effect: Causes, Consequences and Abatement of Green House Effect - Ozone Depletion - Mechanism, Causes, Consequences and Abatement of Ozone Depletion - Bhopal Gas Tragedy and Sevozo Disaster.

PC(CB4)-14: Pollution in Hydrosphere


PC(CB4)-15: Heavy Metal and Radiochemical Pollution.


Mercury: Sources of Pollution. Speciation and Environmental Forms of Mercury - Biochemical Effects of Different Species of Mercury - Minamata Bay Episode as a Case Study of Mercury Poisoning.
Arsenic: Sources of Pollution - Speciation and Environmental Chemistry of Arsenic - Biochemical Effects of Different Species of Arsenic.

Lead: Sources of Lead Pollution - Speciation and Pathways of Lead in Environment - Biochemical Effects of Lead.

Cadmium: Sources of Pollution – Speciation - Biochemical Effects of Cadmium Poisoning.

Radiochemical Pollution: Sources, Chemical Changes due to Radiation on Water.


**PC(CB4)-16: Analysis of Air, Water and Metal Pollutants**

Air Quality Standards - Sampling (Particulates and Gaseous Pollutants) - Analysis of Pollutants: SO\(_2\) (Modified West-Gaeka Spectrophotometric Method, Pulsed Fluorescence Spectrometry), H\(_2\)S (Spectrophotometry – Ethelyne Blue Method), NO-NOx (Chemiluminescence Technique, Colorimetric Technique- Saltzman Method) – CO (NDIR Spectrometry, GC), Hydrocarbons (Ionization Analysis), Aromatic Hydrocarbons in Automobile Exhausts, Petrol, Air, O\(_3\) (Chemiluminiscene and Spectrophotometry) - Particulate Matter Analysis (High Volume Method).

Water Sampling, Preservation and Preconcentration Methods and Physical Analysis - Colour, Odour, Temperature, pH, EC, Redox Potential and Total Dissolved Solids (Turbidimetry). Chemical Analysis of Anions: CN\(^-\), Cl\(^-\), F\(^-\) (Spectrophotometry, Ion Selective Potentiometry and Titrimetry), NO\(_2^-\) and NO\(_3^-\) (Spectrophotometry), SO\(_4^{2-}\), PO\(_4^{3-}\), HCO\(_3^-\), CO\(_3^{2-}\), Hardness of Water (Titrimetry), Ammonical Nitrogen (Spectrophotometry) - Determination of DO, BOD, COD, TOC in Water.

**Books Suggested:**

2. Principles of Environmental Chemistry, Stanley E. Manahan 2nd Ed.
4. Environmental Pollution Analysis, S.M. Khopkar Wiley Eastern Ltd. 1995
6. Text Book of Environmental Chemistry, Ayodhya Singh, Campus Books International publishers
7. Chemistry of the Environment, II Edn Thomas G.Spiro William M.Stigliani
III SEMESTER PRACTICALS

CH (PC) 351 P: Paper-V (Chemical Kinetics) 9 hrs/week

Note: The data obtained in all the experiments are to be analyzed by the students both by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.

♦ Study of peroxydisulphate – iodide reaction:
  1. Individual orders of the reactants by initial rate and isolation methods
  2. Effect of temperature on reaction rate
  3. Effect of ionic strength on reaction rate

♦ Study of peroxydisulphate – iodide clock reaction:
  1. Individual orders of the reactants
  2. Effect of ionic strength on uncatalyzed and Cu(II)-catalyzed reactions

♦ Study of acetone – iodine reaction by titrimetry
  1. Order w.r.t. [iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H+]

CH (PC) 352 : Paper-VI (Instrumentation) 9 hrs/week

Conductometry:

♦ Conductometric titrations:
  1. Mixture of strong and weak bases vs strong acid
  2. Mixture of strong and weak acids vs weak base
  3. Mixture of strong acid, weak acid and CuSO4 vs strong base
  4. Mixture of halides (chloride + iodide) vs AgNO3
  5. Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and Trichloroacetic acid
  6. and their mixtures vs strong base
  7. Precipitation titration: K2SO4 vs BaCl2

♦ Dissociation constants of weak acids
♦ Effect of solvent on dissociation constant of a weak acid
♦ Verification of Onsager equation
♦ Composition of Cu(II) – tartaric acid complex by Job’s method

pH metric:

♦ pH – metric titrations:
  1. Monobasic acids vs strong base
  2. Dibasic acid vs strong base
  3. Tribasic acid vs strong base
  4. Mixture of strong and weak acids vs strong base

♦ Determination of dissociation constants of monobasic/dibasic acids by Albert- Serjeant method
♦ Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane
♦ Determination of pKa and pKb of glycine (calculation using a computer program)
♦ Determination of stability constant of a metal complex

Suggested books:
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav
M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(For the batches admitted in academic year 2016 and later under CBCS pattern)

PAPER I CH(PC)401: Thermodynamics, Chemical kinetics and Electrochemistry

PC-17 : Statistical Thermodynamics
PC-18 : Non-equilibrium Thermodynamics
PC-19 : Chemical Kinetics-II
PC-20 : Electrochemistry -II

PC -17: Statistical Thermodynamics


The relation between equilibrium constant and partition function- derivation.

Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

PC-18: Non-equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states. Entropy production in irreversible processes. Entropy production in heat flow and entropy production in material flow.

Fluxes and forces. Linear flux-force relations. Phenomenological equations and coefficients. Microscopic reversibility. Onsager reciprocal relations.


Irreversible thermodynamics as applied to biological systems - examples.

Application to thermoelectric circuits. Seebeck and Peltier effect.
**PC-19: Chemical kinetics – II:**

(15hrs)


**PC –20 : Electrochemistry – II**

(15 hrs)


**Books suggested:**

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
3. Statistical Thermodynamics, M. C. Gupta, New Age International
4. Atkin’s Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
7. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition
8. Physical chemistry by Puri and Sharma, Vishal Publishing Co.
11. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
17. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi

**PAPER- CH(PC) 402T: SUPRAMOLECULAR CHEMISTRY, PHOTO CHEMISTRY AND COMPUTATIONAL CHEMISTRY**

PC-21 : Supramolecular Chemistry  
PC-22 : Photochemistry  
PC-23 : Computational Chemistry  
PC-24 : Theoretical treatment of bio polymers

**PC-21: Supramolecular Chemistry**


- Molecular receptors for alkali metal ions, ammonium ions, anions and neutral molecules. Crown ethers, cryptands, spherands, calixaranes, and cyclodextrins - their selectivity, macrocyclic, and template effects. Fullerenes as supramolecules.

Threading of a linear molecule through a cyclic molecule – creation of Rotaxanes and Catenanes.

- Thermodynamics of host-guest complexation. Enthalpy and entropy contributions. Complexation free energies.
- Supramolecular catalysis- Crownether supported alkaline earth metal ions as catalysts, cyclodextrins and calixaranes as catalysts in chemical reactions. Transport of ions across membranes by biological molecules.
- Molecular electronic devices: Molecular wires, molecular switches and machines.

**PC-22: Photochemistry – II**


- P-type delayed fluorescence. The experimental study of photochemical reactions: Product analysis, chemical methods in the study of intermediates, spectroscopic methods, ESR and CIDNP, rate coefficients for photochemical processes and identification of excited states.

- Electronic transitions in transition metal complexes. Ligand field (LF) and charge transfer (CT) electronic states. Ru(bpy)$_3^{2+}$ as sensitizer for photoredox reactions, examples. Photochemical cleavage of water.
**PC-23: Computational treatment of many electron systems**  
(15hrs)


**PC-24: Theoretical treatment of biopolymers**  
(15 hrs)

Types of biopolymers. Methods of determining size and shape of biopolymers - mean molecular masses, colligative properties, sedimentation, viscosity, light scattering methods.

Chain conformation and configuration of poly peptides. Random coils and measures of size – contour length, rms separation, radius of gyration, constrained chains.


**Books suggested:**

2) Piet W. N. M. van Leeuwen, Supramolecular Catalysis, Wiley-VCH Verlag GmbH & Co.
4) Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House
5) Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science
6) Quantum Chemistry, I. N. Levine, Prentice Hall
7) Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press
8) Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons
10) Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover publishers
11) Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications
12) Physical Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books Ltd.


14) Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill
15) Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company
16) Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall
18) Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books

ELECTIVE –3A:

PAPER III CH(PC)- 403T(CB1): CATALYSIS

PC(CB1)-17: Homogeneous catalysis
PC(CB1)-18: Surface Chemistry & Micellar catalysis
PC(CB1)-19: Heterogeneous catalysis
PC(CB1)-20: Phase transfer, Anchored & Photo catalysis

PC(CB1)-17: Homogeneous catalysis

Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.


PC(CB1)-18: Surface Chemistry and Micellar catalysis


Adsorption. Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption.


Surface films. Monometallic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between H₂(g) and N₂(g) catalyzed by surfaces to give NH₃(g).

Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

**PC(CB1)-19: Heterogeneous catalysis**

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts, supported metal catalysts and non-metallic catalysts. Co-precipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods.


**PC(CB1)-20: Phase transfer, Anchored and Photo catalysis**


Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Crown ethers: Crown ethers as phase transfer catalysts(PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC’s viz., quaternary ammonium salts and crown ethers.

Anchored catalysis: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- application of intercalated clay catalysts in hydrogenation reactions.

Photo catalysis: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.
Books suggested:
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
4. Catalysis, J. C. Kuriacose, Macmillan
5. Colloidal and surface chemistry, M. Satake, Y. Hayashi, Y. Mido, S.A. Iqbal and M.S. Sethi
15. Physical Chemistry of surfaces, A.W. Adamson and A.P. Gast, Wiley

ELECTIVE–3B

PAPER IV CH(PC) 403 T(CB2) : Dynamics of Chemical Reactions And Sensors

PC-(CB2)-21: MO and VB theory of reactivity
PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects
PC-(CB2)-23: Nucleophilic, electrophilic and free radical reactivity
PC-(CB2)-24: Sensors

PC-(CB2)-21: Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity 15 Hrs

**PC-(CB2)-22: Kinetic, isotopic, structural, solvent, steric and conformational effects** 15 Hrs


**PC-(CB2)-23: NUCLEOPHILIC, ELECTROPHILIC AND FREE RADICAL REACTIVITY** 15 Hrs


**PC-(CB2)-24: Chemical, Electrochemical and Bio Sensors** 15hrs

Books suggested:

5. Physical Organic chemistry, N.S.Isaacs
6. Supramolecular Chemistry - concepts and perspectives by J M .Lehn,

ELECTIVE –4A (ID PAPER)

PAPER III CH(PC)- 403T(CB3): MOLECULAR MODELING AND IT’S APPLICATIONS

PC(CB3)-25: Molecular Modeling – I
PC(CB3)-26: Molecular Modeling – II
PC(CB3)-27: Drug Design Methods I - Ligand Based
PC(CB3)-28: Drug Design Methods II - Structure Based.

PC(CB3)-25: Molecular Modeling – I (15hrs)

Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems; Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.

Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

PC(CB3)-26: Molecular Modeling – II (15hrs)

Force Field Equation in Energy minimization (Energy as function of r, θ, ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods ; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.
PC(CB3)-27: Drug Design Methods I - Ligand Based

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters; Electronic effects, Hydrophobicity, Steric Factors - Taft's Steric factor, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topleiss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, r^2, r^2%, F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

PC(CB3)-28: Drug Design Methods II - Structure Based.


Books suggested:

2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press.
ELECTIVE –4B (ID PAPER)

PAPER-IV CH(PC) 404T(CB4): Engineering Chemistry

PC(CB4) -29: Water And Waste Water Treatment
PC(CB4) -30: Corrosion And Its Control
PC(CB4) -31: Energy Sources
PC(CB4)- 32 Engineering Materials

PC(CB4) -29: Water and waste water treatment (15 hrs)

PC(CB4) -30: Corrosion and its control: (15 hrs)

PC(CB4) -31: Energy sources: (15 hrs)

Non conventional energy resources: Nuclear fuels- nuclear reactor, nuclear fission, nuclear fusion, sources of nuclear fuels, disposal of radio active wastes, reprocessing of nuclear fuels. solar, hydro, wind, tidal energies. Bio fuels, H₂ as a non polluting fuel.
PC(CB4) -32: Engineering materials.  
(15 hrs)

Cement: composition of Portland cement, analysis, setting and hardening of Portland cement (reactions), decay of cement concrete, lime, manufacture, types of lime, plaster of paris

Lubricants: Criterion of a good lubricant, classification of lubricants: petroleum oils, fixed oils, synthetic lubricants, semisolid lubricants, solid lubricants. Properties of lubricants: cloud point, pour point, flash and fire point, viscosity.


Conductors and insulators: Classification of insulators, characteristics of thermal and electrical insulators and super conductors (Nb-Sn alloy, YBa$_2$Cu$_3$O$_{7-x}$) applications.

Composite materials: Advantageous properties of the composites, classification, mechanism of strengthening, mechanism of hardening of particle reinforcement, fabrication of the composites.

Liquid crystals: Characteristics of liquid crystal orders, physical properties of liquid crystals, classification of Liquid crystals, types of mesophases chemical nature of Liquid crystals, applications of Liquid crystals, future of liquid crystals.

Books suggested:

ELECTIVE–4C (ID PAPER)

PAPER-IV CH(PC) 404T(CB5): Sugar Chemistry AND Sugar Technology

PC(CB5) -33: Advanced Sugar Chemistry
PC(CB5) -34: Sugar & Sugar byproducts
PC(CB5) -35: Methodology used in Sugar Analysis
PC(CB5)- 36: Sugar Technology and Management

PC(CB5) -33: Advanced Sugar Chemistry:  
(15 hrs)


PC(CB5) -34: Sugar & Sugar byproducts:  
(15 hrs)


PC(CB5) -35: Methodology used in Sugar Analysis:  
(15 hrs)


PC(CB5) -36: Sugar Technology and Basic Principles of Management:  
(15 hrs)

Management: Concept and philosophy of management in major and small-scale industries. Location of factory site and Lay out of plant. Joint stock companies. Co-operative Societies. Production management and control. Personnel administration, purchases and sales, organization and control.

**Books suggested:**
1. Cane Sugar Hand Book, Maede & Chen, John Wiely & Sons
3. Text Book of Sugar Chemistry and Sugar Technology, Mathur
4. Text Book of Sugar Byproducts, Morris Patrov
5. A Hand Book of Qualitative and Quantitative Organic Analysis, H. J. Clark, Orient Longman
6. Text Book of Biochemistry, Lehninger
7. Analysis of Sugars, Pleus
8. Text Book of Sugar Technology, Hugot
9. Instrumental Methods in Sugar Industry, Eckman
10. Principles of Instrumental Analysis, Skoog and West
12. Advanced Sugar Chemistry, R. S. Shellaxberges
13. Sugar, John Yulkin, Jack Edelman, Liesel Hough

**IV SEMESTER PRACTICALS**

**Note:** The data obtained in all the experiments are to be analyzed by the students both by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.

**CH (PC) 451P: Paper-V (Chemical Kinetics) 9hrs/week**

- **Study of acetone-iodine reaction by spectrophotometry**
  1. Order w.r.t. [iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H+]

- **Study of peroxydisulphate – iodide reaction by colorimetry**

- **Study of saponification of ethyl acetate by conductometry:**
  1. Overall order of the reaction
  2. Order w.r.t. [ethyl acetate]
  3. Order w.r.t. [NaOH]

- **Study of solvolysis of t-butylchloride by conductometry:**
  effect of solvent dielectric constant/polarizability (methanol/water mixture) on the rate of solvolysis

- **Study of oxidation of primary alcohols by dichromate by spectrophotometry:**
  Application of Taft equation
Spectrophotometry:
- Estimation of Cu(II) using EDTA
- Estimation of Fe(III) using thiocyanate
- Estimation of Fe(II) using 1,10-phenanthroline
- Estimation of Fe(III) in tap water using thiocyanate by standard addition method
- Simultaneous determination of dichromate and permanganate in a mixture
- Spectrophotometric titrations: Cu(II) vs EDTA
  Fe(II) vs 1,10-phenanthroline
- Composition of Cu(II) – EDTA complex by Job’s method
- Composition of Fe(II) – phenanthroline complex –Job’s method, mole ratio, slope ratio method.
- Determination of composition and Gibbs energy of formation of Fe(III)–salicylic acid complex
- Determination of $pK_a$ of methyl red indicator
- Estimation of Mn(II) by spectrophotometry using periodate.

Potentiometry:
- Potentiometric titrations:
  1. Weak acids vs strong base and calculation of dissociation constants
  2. Mixture of strong and weak acids vs strong base
  3. Dibasic acid vs strong base
  4. Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)
     - Fe(II) vs MnO$_4^-$
     - Fe(III) vs EDTA
     - Mixture of halides vs AgNO$_3$
     - Mixture of KI and KSCN vs AgNO$_3$

Polarography:
- Estimation of Pb$^{2+}$, Cd$^{2+}$ and Ni$^{2+}$ separately and in a mixture.

Suggested books:
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B.Yadav
M.Sc. CHEMISTRY

PHYSICAL ORGANIC CHEMISTRY SPECIALISATION
SYLLABUS OF III & IV SEMESTERS
REVISED AS PER NEW (CB) SYLLABUS

FOR STUDENTS ADMITTED FROM THE YEAR
2016 ONWARDS
M.Sc. CHEMISTRY (PHYSICAL ORGANIC CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters
(for the batches admitted in academic year 2016 & later under CBCS pattern)
[Under Restructured CBCS Scheme]
Grand total marks and credits (all 4 semesters) 2400 marks – 96 credits

(Approved in the P.G.BOS meeting held on 01-07-2017)

Semester - III

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(Choice based paper (CB) = Paper offered by the same Department or other Department in the Science faculty)

*15 marks for written test and 5 marks for assignment

Grand total (all 4 semesters) 2400 marks and 96 credits
M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
Syllabus for III Semester
(For the batch admitted during the academic year 2016 onwards under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper I- CH(PO) 301T: Quantum Chemistry and Group Theory
PO- 09: Applications of Schrödinger equation
PO- 10: Angular momentum & approximate methods
PO- 11: Bonding in molecules
PO- 12: Group Theory

Paper II– CH (PO) 302T: Conformational Analysis, Asymmetric Synthesis, Synthetic Strategies and Advanced NMR spectroscopy
PO- 13: Conformational Analysis (Cyclic Systems) and ORD
PO- 14: Asymmetric synthesis
PO- 15: Synthetic Strategies
PO- 16: $^{13}$C NMR and 2D NMR spectroscopy

Elective-3A
Paper-III-CH(PO) 301T(CB1): Spectroscopy, Photochemistry and Statistical Thermodynamics
PO-(CB1)1: Physical principles of spectroscopy & Vibrational spectroscopy
PO-(CB1)2: X-Ray Spectroscopy & Diffraction techniques
PO-(CB1)3: Chemical kinetics II
PO-(CB1)4: Statistical Thermodynamics

Elective–3B
Paper-III CH (PO) 303T(CB2):Biopolymer Chemistry
PO-(CB2)-5:Bioenergetics & physical properties of biopolymers
PO-(CB2)-6:Biological membranes & binding of ligands by biopolymers
PO-(CB2)-7: DNA, genes & cloning
PO-(CB2)-8: Bioinformatics

Elective-4A
Paper IV- CH(PO) 304(CB3)T: Modern Organic Synthesis
PO-(CB3)-9: Synthetic Reagents I
PO-(CB3)-10 Synthetic Reagents II
PO-(CB3)-11: New Synthetic reactions
PO-(CB3)-12: New techniques and concepts in organic synthesis

Elective–4B
Paper-IV CH(PO)304T(CB4): Organic materials, Dyes and Pigments
PO (CB4)-13: Organic Nanomaterials
PO (CB4)-14: Supramolecular Chemistry
PO (CB4)-15: Dyes – I
PO (CB4)-16: Dyes–II and Pigments

LABORATORY COURSES
Paper-V (Lab)-CH(PO) 351: Chemical Kinetics
Paper-VI(Lab)-CH(PO) 352: Synthesis of Organic compounds and Chromatography
M.Sc. PHYSICAL ORGANIC CHEMISTRY   SPECIALIZATION
IV SEMESTER SYLLABUS

(For the batch admitted during the academic year 2016 under the CBCS pattern)

[Under Restructured CBCS Scheme]

PAPER-1 CH(PO) 401T: Non-equilibrium thermodynamics, NMR, NQR and Mossabaur Spectroscopy, Electrochemistry & Lasers
PO-17: Non-equilibrium Thermodynamics
PO-18: NMR, NQR and Mossbauer Spectroscopy
PO-19: Electrochemistry II
PO-20: Lasers in Chemistry

Paper-II CH(PO) 402T: Medicinal Chemistry and Biomolecules
PO-21: Principles of Drug design and drug discovery
PO-22: Lead modification and SAR Studies
PO-23: QSAR studies
PO-24: Biomolecules

Elective–3a
PAPER –III CH (PO) 403T(CB1) : Catalysis
PO(CB1)- 17 : Homogeneous catalysis
PO(CB1)- 18 : Surface Chemistry & Micellar catalysis
PO(CB1)- 19 : Heterogeneous catalysis
PO(CB1)- 20 : Phase transfer , Anchored & Photo catalysis

Elective –3b
PAPER-III CH(PO) – 403T(CB2) : Molecular modeling and It’s Applications
PO(CB2)-21: Molecular Modeling – I
PO(CB2)-22: Molecular Modeling – II
PO(CB2)-23: Drug Design Methods I - Ligand Based

Elective-4a(ID Paper)
Paper-IV CH (PO) 404T(CB3)T: Five and six membered heterocycles, Carbohydrates and Proteins, Structure determination of natural products and Green chemistry
PO-(CB3 )- 25: Five and six membered heterocycles with two hetero atoms
PO-(CB3 )- 26: Carbohydrates and proteins
PO-(CB3) - 27: Structure determination of natural products by chemical and spectral methods
PO-(CB3) - 28: Green chemistry

Elective-4b(ID Paper)
Paper IV- CH(PO) 404(CB4)T: Forensic Chemistry and Toxicology
PO-(CB4)29: Forensic Chemistry-I
PO-(CB4)30: Forensic Chemistry-II
PO-(CB4)31: Forensic Toxicology-I
PO-(CB4)32: Forensic Toxicology-II

LABORATORY COURSES
Paper-VII–(LAB)CH (PO) 451 P :Instrumentation
Paper-VIII–(LAB) CH (PO) 452P : Separation, identification and spectral analysis of organic
compounds

M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
III SEMESTER SYLLABUS
(For the batch admitted during the academic year 2016 under the CBCS pattern)
[Under Restructured CBCS Scheme]

Paper I- CH(PO) 302T: Quantum Chemistry and Group Theory
PO- 09: Applications of Schrödinger equation
PO- 10: Angular momentum & approximate methods
PO- 11: Bonding in molecules
PO- 12: Group Theory

PO- 09: Applications of Schrödinger equation (15 hrs)


Atomic and molecular term symbols.
Atoms in external field, Zeeman and anomalous Zeeman effect.

PO- 10: Angular momentum & approximate methods (15 hrs)

Angular momentum operators. Commutation relations of angular momentum operators and their consequence. Eigen functions of L² and Lz and the eigen values. Magnitude and orientation of angular momentum vectors.


Multielectron atoms. The Hartree-Fock self-consistent field method. Basis functions. Slater-type orbitals ( STOs ).
**PO-11: Bonding in molecules**  
(15 hrs)


Concept of hybridization – $sp$, $sp^2$, and $sp^3$ hybrid orbitals.

Semiempirical MO methods. The Hückel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π-electron charges and bond orders. Simplification of secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Introduction to Extended Hückel Theory, extension of the Hückel’s approach to molecules containing heteroatoms. Orbital symmetry and reactivity: $H_2 + F_2 \rightarrow 2HF$ reaction. $2NO \rightarrow N_2 + O_2$ reaction.

**PO-12: Group theory**  
(15 hrs)


Symmetry operations forming a group. Classes of symmetry operations. Matrix representation of symmetry operations and point groups. Generation of representations for point groups. Reducible and irreducible representations.

The Great Orthogonality theorem (proof not required) and its consequences. Relation between reducible and irreducible representations. Character tables. Construction of character tables for $C_{2v}$, $C_{2v}$, and $C_{3v}$ groups.


**Books suggested:**
1. Quantum Chemistry, Ira N. Levine, Prentice Hall
5. Coulson’s Valence, R. McWeeny, ELBS
Paper II– CH (PO) 302T: Conformational Analysis, Asymmetric Synthesis, Synthetic Strategies and Advanced NMR spectroscopy

PO- 13: Conformational Analysis (Cyclic Systems ) and ORD
PO- 14: Asymmetric synthesis
PO- 15: Synthetic Strategies
PO- 16: $^{13}$C NMR and 2D NMR spectroscopy

**PO-13: Conformational analysis (Cyclic systems) and ORD** 15 Hrs

**Conformational analysis (Cyclic systems)**

Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3 -alkyl ketone effect), 2-halocyclohexanones, cycloheptane . Stereo chemistry of bicycle [3,3,0] octanes,hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinolineand quinolizidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes. (oxidation, $S_N2$ reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

**Optical Rotatory Dispersion (ORD) and CD Spectroscopy:** Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule. Application of the rules to the study of absolute configuration and conformations of organic molecules.

**PO-14: Asymmetric synthesis** 15 Hrs

**Introduction:** Brief revision of classification of stereo selective reactions

**Prostereoisomerism:** Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

**Prochiral nomenclature:** Pro chirality and Pro-R, Pro-S, Re and Si.

Conditions for steroeselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.

**Analytical methods:** % Enantiomeric excess and diastereomeric excess. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

**Chiral Substrate controlled asymmetric synthesis:** Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram’s rule and Felkin-Anh model.

**Chiral auxiliary controlled asymmetric synthesis:** $\alpha$-Alkylation of chiral enolates, Evan’s oxazolidinone, 1, 4-Asymmetric induction and Prelog’s rule.

**Chiral reagent controlled asymmetric synthesis:** Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC$_2$ BH and IPCBH$_2$.

**Chiral catalyst controlled asymmetric synthesis:** Sharplessepoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphincatalyst.

**Asymmetric aldol reaction:** Diastereoselective aldol reaction (achiral enolate and achiral aldehydes ) its explanation by Zimmerman-Traxelmodel.
PO-15: Synthetic Strategies 15 Hrs


Order of events: S-Salbutamol, Propoxycaine.

One group C-C and C-X disconnections: Introduction. One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.

Two group C-C and C-X disconnections: Introduction. Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.

Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations: oxanamide and mevalonic acid.

Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, Longifoline.

PO-16: $^{13}$C NMR and 2D NMR Spectroscopy 15 Hrs

i) $^{13}$C NMR spectroscopy: Introduction, Types of $^{13}$Cnmr spectra: undecoupled, proton-decoupled and off-resonance decoupled (ORD) spectra. $^{13}$C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ($^{13}$C, $^{13}$C J) and heteronuclear ($^{13}$C,$^{1}$H J and $^{13}$C, $^{2}$H J) coupling. Applications of $^{13}$C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. $^{13}$C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY ($^{1}$H-$^{1}$H COSY), TOCSY (Total Correlation Spectroscopy), HeteroCOSY ($^{1}$H,$^{13}$C COSY,HMQC), long range $^{1}$H,$^{13}$C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Recommended Books:
1. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
2. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
3. Stereochemistry: Conformation & Mechanism by P S Kalsi
4. The third dimension in organic chemistry, by Alan Bassendale
7. Asymmetric synthesis by Nogradi
8. Asymmetric organic reactions by J D Morrison and H S Moscher
10. Stereo differentiating reactions by Izumi
11. Some modern methods of organic synthesis by W Carruthers
12. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
13. Organic synthesis by Michael B Smith
14. Organic Synthesis-The disconnection approach by S Warren
15. Organic Synthesis by C Willis and M Willis
16. Problems on organic synthesis by Stuart Warren
17. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
18. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
19. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
20. Organic Spectroscopy by William Kemp
21. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
22. Modern NMR techniques for chemistry research by Andrew B Derome
23. NMR in chemistry - A multinuclear introduction by William Kemp.
24. Spectroscopic identification of organic compounds by P S Kalsi
25. Introduction to organic spectroscopy by Pavia
27. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
28. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
29. NMR spectroscopy by H. Gunther

ELECTIVE-3A

Paper-III-CH(PO) 301T(CB1): Spectroscopy, Electrochemistry and Statistical Thermodynamics
PO-(CB1)1: Physical principles of spectroscopy & Vibrational spectroscopy
PO-(CB1)2: X-Ray Spectroscopy & Diffraction techniques
PO-(CB1)3: Electrochemistry – II
PO-(CB1)4: Statistical Thermodynamics

PO-(CB1)1: Physical principles of spectroscopy & Vibrational spectroscopy (15 Hrs)
Interaction of electromagnetic radiation with matter. Absorption and emission of radiation.
Induced absorption, spontaneous emission and stimulated emission. Oscillator strength, transition
moment integral. Selection rules, Spectrum of formaldehyde. Factors affecting width and intensity
of spectral lines -Line width and natural line broadening, doppler broadening. Intensity of spectral
lines.
Infrared spectroscopy- Anharmonic oscillator. Morse potential energy diagram.
Vibration – rotation spectroscopy, P, Q, R branches. Vibration – rotation spectra of polyatomic
molecules – linear, symmetric top and asymmetric top molecules. Principles of FTIR.
Raman spectroscopy- Classical and quantum theories of Raman effect. Pure rotational, vibrational
and vibrational – rotational Raman spectra. Selection rules. Depolarization factors of Raman lines
and their relevance. Instrumentation. Typical applications of Raman spectroscopy – Strucure
determination of XY₄ molecules, Phase transitions.
**PO-(CB1)2: X-ray Spectroscopy and Diffraction techniques:** (15 hrs)


X-ray absorption: Absorption techniques, Absorption edge fine structure (AEFS spectra) and extended X-ray absorption fine structure (EXAFS) spectra.


**PO-(CB1)3: Chemical Kinetics II** (15 hrs)

**Reactions in solution:** Factors affecting reaction rates in solution. Effect of pressure on rate of reaction. Diffusion controlled reactions. Influence of dielectric constant and ionic strength on ion-ion, ion-dipole and dipole-dipole reactions. Primary and secondary salt effects. Kinetic isotope effects: Primary and secondary isotope effects. Solvent isotope effects.

**Fast reactions:** Flow methods and the stopped-flow technique. The fluorescence technique. Shock tube method. Relaxation methods (T-jump and P-jump). Kinetic equations for chemical relaxation.


**PO-(CB1)4: Statistical Thermodynamics** (15 hrs)


The relation between equilibrium constant and partition function- derivation.
Basic ideas of Bose-Einstein statistics and Fermi-Dirac statistics and comparison of these with Maxwell-Boltzmann statistics.

Books suggested:
1. Modern Spectroscopy, J. M. Hollas, John Wiley & sons
2. Fundamentals of Molecular Spectroscopy, Banwell&McCash
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill
18. Atkin’s Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
20. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley
21. Statistical Thermodynamics, M. C. Gupta, New Age International
22. Atkin’s Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press

ELECTIVE –3B

Paper III CH(PO) 303T(CB2) : Biopolymer Chemistry
PO(CB2)-5: Bioenergetics & physical properties of biopolymers
PO (CB2)-6: Biological membranes & binding of ligands by biopolymers
PO (CB2)-7: DNA, genes & cloning
PO (CB2)-8: Bioinformatics

PO(CB2)-5: Bioenergetics & physical properties of biopolymers (15 hrs)

Molecular weights of biopolymers. Viscometry, Use of viscometry in the study of ligand binding to DNA. Separation/molecular weight studies of biopolymers. Sedimentation: Sedimentation velocity.

**PO(CB2)-6: Biological membranes & binding of ligands by biopolymers** (15 hrs)


Binding of ligands and metal ions to macromolecules – one and n-equivalent binding sites per molecule. Allosteric interactions – Oxygen binding to myoglobin and hemoglobin – Cooperative and non-cooperative binding. Hill equation and Hill plots. Transport of H⁺ and CO₂. Bohr effect.

**PO(CB2)-7: DNA, Genes & Cloning** (15 hrs)
Watson –Crick model of DNA. Types of DNA chains – linear, circular and supercoiled DNA. Types of RNA. Secondary structure of t-RNA.

Genes and genome: Gene expression. Transcription and translation (general principles only). Codons and the genetic code.

Sequence analysis of DNA by the Sanger chain-termination method.

Introduction to biotechnology and recombinant DNA technology. Molecular cloning. Restriction endonucleases and cloning vectors. Steps involved in the construction of recombinant DNA. DNA hybridization and hybridization probes.


**PO(CB2)-8: Bioinformatics** (15 hrs)
Introduction: Use of informatics and computers in biology. Homology as descendants of common ancestors, statistical analysis of sequence alignment.

General purpose Databases for Comparative Genomics: COGs, KEGG, MDGB - Organism Specific Databases examples - E. Coli, Yeast, Oryza.


**Books suggested:**

4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books

ELECTIVE – 4A

Paper IV – CH (PO) 304T(CB3): Modern Organic Synthesis
PO-(CB3)-09: Synthetic Reagents I
PO-(CB3)-10: Synthetic Reagents II
PO-(CB3)-11: New Synthetic reactions
PO-(CB3)-12: New techniques and concepts in organic synthesis

PO-(CB3)-09: Synthetic Reagents I

i) Protecting groups: a) Protection of alcohols by ether, silyl ether and ester formation b) Protection of 1,2-diols by acetal, ketal and carbonate formation c) Protection of amines by benzylxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups. d) Protection of carboxyls by acetal, ketal and thiol acetal (Umpolung) groups. e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.

ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organo lithium 2) Organo copper reagents 3) Organo boranes in C-C bond formation 4) Organo silicon reagents: reactions involving β-carbocations and α-carbanions, utility of trimethyl silyl halides, cyanides and triflates.


iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.

v) C-H Activation: Introduction, Rh catalyzed C-H activation.

PO-(CB3)-10: Synthetic Reagents II

i) Oxidations: a) Oxidation of active C-H functions: DDQ and SeO₂. b) Alkenes to diols: Prevost and Woodward oxidation c) Alcohol to carboxyls: Cr⁶⁺ oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.

ii) Reductions: a) Catalytic hydrogenation: Homogenous (Wilkinson’s catalytic hydrogenation) and heterogeneous catalytic reduction. b) Non-metallic reductions: Diimide reduction c) Dissolving metal reductions: Birch reduction. d) Nucleophilic metal hydrides: LiAlH₄, NaBH₄, and...
their modifications. e) Electrophilic metal hydrides: BH₃, AlH₃ and DIBAL. f) Use of tri-n-butyl tin hydride: Radical reductions.

PO-(CB3)-11: New Synthetic reactions 15 Hrs
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurry reactions, Julia-Lythgoe olefination and Peterson’s stereoselective olefination.
5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.
6. Metathesis: Grubb’s 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.
7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

PO-(CB3)-12: New techniques and concepts in organic synthesis 15 Hrs
1. Techniques in peptide synthesis: Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.
2. Solid phase oligodeoxynucleotide synthesis: Phosphotriester, phosphotriester and phosphoramidite pathway.
3. Oligosaccharide synthesis: Glycosidation: cyclohexane ion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, convergent and linear oligosaccharide synthesis.
4. Phase Transfer catalysis: Onium and crown ethers as PTC.
5. Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, electrocyclic-Diels Alder reaction.
8. Determination of absolute configuration: Mosher’s method.

Recommended Books:
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken.
13. Organic Reactions and their mechanisms by P.S.Kalsi
14. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar

ELECTIVE –4B

Paper-IV CH(PO)304T(CB4): ORGANIC MATERIALS, DYSES AND PIGMENTS

PO (CB4)-13: Organic Nanomaterials
PO (CB4)-14: Supramolecular Chemistry
PO (CB4)-15: Dyes – I
PO (CB4)-16: Dyes–II and Pigments

PO (CB4)-13: Organic Nanomaterials 15Hrs

Introduction: The ‘top-down’ approach, the ‘bottom-up’ approach and Nanomanipulation.
Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles.
New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs)and Graphenes.
Structures of aromatics belts, nano car and molecular machines.
Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures) Natural Benz heterazoles and their synthetic modifications as optoelectronic molecules.

PO (CB4)-14: Supramolecular Chemistry 15Hrs

Introduction: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions),Ionophore and molecular receptors.
Host-Guest Chemistry: Lock and key analogy, Structures and applications of Cryptands,Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.
Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications.
Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral frame work, Chiral receptor from Kemp’s triacid. Chiral receptors for tartaric acid.

PO (CB4)-15: Dyes – I 15 Hrs

Synthetic and Natural dyes:Introduction, nomenclature and classification of synthetic dyes. Color and constitution - chromospheres and auxochromes with suitable examples, Witt’s theory, Armstrong’s theory, Baeyer’s theory, Nietzki’s theory, Waston’s theory, Modern theories, Valence Bond Theory and Molecular orbital theory. Chemistry and synthesis of triphenyl methane dyes malachite green, rosaniline, para aniline blue, crystal violet methyl violet, hydroxytriphosphynl methane dyes, Aurin,chrome violet], Azo dyes - types of azo dyes, synthesis of acidic and basic azo dyes, mono azo, di azo, tri azo and poly azo dyes. Chemistry and synthesis of cyanine dyes. Natural dyes – structure determination and synthesis of alizarine, Quinazarin and Indigo.
PO (CB4)-16: Dyes–II and Pigments 15 Hrs


Recommended Books
2. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
5. Stereochemistry of organic compounds - Principles & Applications by D Nasipuri
6. Nanochemistry by G.B. Sergeev; Elsevier
9. Color and constitution of organic molecules by J.Griffiths
Klaus Hunger
13. Introduction to Fluorescence Sensing, Springer 2009, by A P Demchenko
14. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
15. Handbook on Natural Dyes for Industrial Applications by P. S. Vankar, National Institute of Industrial Research
SEMESTER III LABORATORY COURSES

PAPER V (Lab)-CH(PO) 351P: Chemical Kinetics
1. Study of peroxydisulphate-iodide reactions;
   ➢ Individual orders of the reactants by isolation and initial rate methods
   ➢ Effect of temperature on reaction rate
   ➢ Effect of ionic strength on reaction rate
   ➢ clock reaction
2. Study of saponification of ethyl acetate by conductometry:
   a). Overall order of the reaction b). Order w. r. to ethylacetate  c).Order w.r. to NaOH
3. Study of acetone-iodine reaction by colorimetry/spectrophotometry
   a).Order w.r.t. iodine  b).Order w.r.t. acetone  c). Order w.r.t. [ H+] 
4. Study of oxidation of primary alcohols using dichromate by spectrophotometry:
   Application of Taft equation.
5. Study of solvolysis of t-butylchloride by conductometry: effect of solvent dielectric constant/polarizability (methanol/water mixture) on the rate of solvolysis.
Note: The Data obtained in all the experiments are to be analysed by the students both by the usual graphical methods and by regression (linear/nonlinear) techniques using a PC.

Suggested books:
2. Senior practical physical chemistry.  B. D. Khosla, V.C. Garg, Adarsh Gulati
5. Practical in Physical Chemistry: P.S. Sindhu
6. Advanced Practical Physical chemistry: J.B. Yadav

PAPERVI -CH(PO)352P: Synthesis of Organic compounds and Chromatography
1. Laboratory synthesis of the following compounds: 2-Phenyl indole (Fischer- Indole synthesis), 2,5-Dihydroxy acetophenone (Fries reaction), 7-hydroxy coumarin (Pechmann synthesis), Photodimerization of maleic anhydride, Benzanilide (Beckmann rearrangement), Benzilic acid from benzoin (rearrangement), Vanillylalchohol from vanillin (NaBH4 reduction), 4-Nitoacetanilide from acetanilide, Benzimidazoles and Benzimidazolines by reaction of o-phenylenediamine with aromatic aldehydes and carboxylic acids.
2. Thin layer chromatography : Thin layer chromatography: Determination of purity( All the above preparations), monitoring the progress of chemical reactions (any of the four above preparations), identification of unknown organic compounds by comparing the Rf values of known standards.
3. Separation/Purification by column chromatography: Separation of a mixture of ortho and para-nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC. Purification of commercial sample of anthracene by column chromatography (using silica gel as adsorbant and n-hexane as eluent).

Suggested books:
2. Unitized experiments in organic chemistry by R Q Brewster and others.
3. Handbook of organic analysis by H T C Clarke.
M.Sc. PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
IV SEMESTER SYLLABUS
(For the batch admitted during the academic year 2017 onwards under the CBCS pattern)
[Under Restructured CBCS Scheme]

PAPER-1 CH(PO) 401T: Non-equilibrium thermodynamics, NMR, NQR and Mossabaur Spectroscopy, Electrochemistry & Lasers

PO-17: Non-equilibrium Thermodynamics
PO-18: NMR, NQR and Mossbaur Spectroscopy
PO-19: Electrochemistry II
PO-20: Lasers in Chemistry

PC-17 Non-equilibrium Thermodynamics (15hrs)


PC-18: NMR, NQR and Mossbaur Spectroscopy. (15hrs)

Principle of nmr. Derivation of $h \nu = g \beta H$. Larmor precessional frequency- spin-spin splitting (AX) - Quantitative treatment (proof for J= distance between two successive nmr spectral lines) – Instrumentation - CW instrument and FT instrument.

Two dimensional nmr spectroscopy: Principles of 2D nmr-Graphical representation of 2D nmr spectra – Homonuclear $^1$H J, δ spectroscopy-its application for mixture analysis- (for instance mixture analysis of n-butyl bromide and n-butyl iodide) - The COSY experiment. Two dimensional $^1$H, $^1$H shift correlations. COSY spectra of an AX system, o-nitroaniline, alanine, glutamic acid and arginine.

The nuclear overhauser effect(NOESY). Two dimensional nuclear overhauser spectroscopy(NOESY). Nuclear Quadrupole Resonance: Quadrupole nuclei and quadrupole moments-prolate and oblate nuclear charge distributions-energies of quadrupolar transitions-electric field gradient, coupling constants and splitting.

Mossbauer Spectroscopy - Mossbauer effect – Recoil energy, typical Mossbauer spectrum - isomer shift – quadrupole splitting – magnetic hyperfine interaction – $^{57}$Fe – Mossbauer spectra of Fe$^{2+}$ and Fe$^{3+}$ (paramagnetic) and Fe$^{3+}$ (magnetic) compounds.
**PC –19: Electrochemistry – II**  
(15 hrs)


**PC 20: Lasers in Chemistry:**  
(15 hrs)


Practical lasers. Solid-state lasers, gas lasers, chemical and excimer lasers. Examples.


**Books suggested:**

1. Atkin’s Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
2. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books
5. Advanced physical chemistry by Gurru and Gurtu.
6. Physical chemistry by Puri and Sharma.
7. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley & sons
9. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
10. NMR basic principles - Atta-ur-Rahman, Springer publisher
12. Physical chemistry by Puri and Sharma.
16. Introduction to Electrochemistry, S. Glasstone.
18. Lasers in Chemical and Biological Sciences, S. Chopra & H. M. Chawla, Wiley Eastern Ltd

Paper-II CH(PO) 402T: Medicinal Chemistry and Biomolecules

PO-21: Principles of Drug design and drug discovery
PO-22: Lead modification and SAR Studies
PO-23: QSAR studies
PO-24: Biomolecules

PO-21: Principles of Drug design and drug discovery
Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead- screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug – receptor interactions and their theories – Occupancy theory, Induced – fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Principles of design of agonists (e.g. Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril). Drug discovery without lead – serendipity- Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

PO-22: Lead modification and SAR Studies
SAR: Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine, salbutamol, cimitidine and captopril. Structure- Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs. Introduction of combinatorial chemistry, a brief outline of methods of parallel and mixed combinatorial synthesis.

PO-23: QSAR studies and computer aided drug design
QSAR: Introduction, physicochemical properties - pKa, electronic effects and Hammett constants(σ), lipophilicity constant(π), steric effects and Taft’s constant, linear and nonlinear relationship between biological activity. Lipophilicity Substituent constants. Lipinski rule of five.
Hansch analysis, Craig’s plot, Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine, design of Crizotinib).

Computer aided drug design: Introduction, active site, allosteric binding site, use of grids in docking program - rigid docking, flexible docking of ligands. Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

**PO-24: Biomolecules**

15 Hrs


2. **Nucleic acids:** Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA. Replication, transcription and translation. Genetic code. Protein biosynthesis. Chemical Synthesis of nucleotides.

3. **Lipids:** Lipid structure- acylglycerols, phosphoglycerides and sphingolipids. Biosynthesis and chemical Synthesis of lipids.

**Recommended books**

1. Burger’s medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
5. Principles of medicinal chemistry. by William Foye
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
10. Medicinal chemistry An introduction by Garreth Thomas
11. Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishansingh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotechnology By Roger A. Sheldon
23. Enzyme structure and mechanism by Fersht and Freeman
24. Bio-Organic chemistry by HennanDugas
25. Nucleic acids in Chemistry and Biology by G M Blackbum MI Gait
26. LehningerPrinciples of Biochemistry by D L Nelson and M M Cox
27. Outlines of Biochemistry by ConnardStumpf

ELECTIVE –3A

PAPER III CH(P)- 403T(CB1): CATALYSIS

PC(CB1)-17: Homogeneous catalysis
PC(CB1)-18: Surface Chemistry & Micellar catalysis
PC(CB1)-19: Heterogeneous catalysis
PC(CB1)-20: Phase transfer , Anchored & Photo catalysis

PC(CB1)-17: Homogeneous catalysis. (15 hrs)
Introduction to catalysis. Types of catalysis, characteristics of catalyst, catalyst supports, promoters, general mechanism of catalysis, equilibrium treatment and steady state treatment. Activation energies of catalyzed reactions.

Acid-base catalysis, specific acid-base catalysis, general acid base catalysis, mechanism of acid base catalysis, catalytic activity and acid-base strength- Bronsted relationships.


PC(CB1)-18: Surface Chemistry & Micellar catalysis (15hrs)

Adsorption. Types of adsorption, factors effecting adsorption, Chemistry and thermodynamics of adsorption. Determination of heats and entropies of adsorption.


Surface films. Monometallic surfaces and bimetallic surfaces. Experimental techniques for the study of monolayer films. States and reaction in monomolecular films. Reaction between H₂(g) and N₂(g) catalyzed by surfaces to give NH₃(g).

Counter ion binding to micelles. Thermodynamics of micellization. Phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

**PC(CB1)-19: Heterogeneous catalysis**

Heterogeneous catalysis. Broad categories of catalysts – metals, bimetals, semiconductors, insulators, zeolites, oxides, nano materials.

Preparation of metal catalysts, supported metal catalysts and non-metallic catalysts. Co-precipitation, Impregnation, sol-gel method, deposition-precipitation, hydrothermal synthesis, pulsed laser methods, plasma chemical methods, chemical vapor deposition methods


Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

**PC(CB1)-20: Phase transfer, Anchored & Photo catalysis**

*Phase-transfer catalysis (PTC)*: Principles of phase-transfer catalysis. PTC classification. Role of water in phase-transfer catalyzed reactions. Factors influencing the rate of PTC reactions.

Inverse phase transfer catalysis. Mechanism of nucleophilic displacement reactions.

Crown ethers: Crown ethers as phase transfer catalysts(PTC) in the reaction of alkyl halides with super oxide. Permanganate oxidation of alkenes and phenols in presence of PTC’s viz., quarternary ammonium salts and crown ethers.

*Anchored catalysis*: Definition and examples of anchored catalysis- organic polymers, inorganic oxides and clays as supports. Structure of montmorillonite anchored catalysts- HEW structure and EF structure. Montmorillonite anchored catalysts- application of intercalated clay catalysts in hydrogenation reactions.

*Photo catalysis*: Photocatalytic effect, metal semiconductor systems as photo catalysts, nature of the metal loaded, extent of metal loading, nature of semiconductor, doped semiconductors, coupled Semiconductors. Application of photocatalysis for splitting of water by semiconductor particles, removal of organic and inorganic pollutants, for oxidation and reduction of organic compounds.
Books suggested:
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill
4. Catalysis, J. C. Kuriacose, Macmillan

ELECTIVE – 3B

PAPER-3 CH(PO) – 403T(CB2) : Molecular Modeling & It’s Applications
PO(CB2)-21: Molecular Modeling – I
PO(CB2)-22: Molecular Modeling – II
PO(CB2)-23: Drug Design Methods I - Ligand Based

PC(CB2)-21: Molecular Modeling – I (15hrs)
Introduction to Molecular Modeling, Single molecule calculations, assemblies of molecules and reactions of molecules - Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix - Potential energy surface - Conformational search; Global minimum, Local minimum, Conformational analysis of ethane.
Force field ; Features of Molecular Mechanics, Bonded and Non-bonded interactions, Bond Stretching, Angle Bending, Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms), Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions), Hydrogen Bonding Interactions.

PC(CB2)-22: Molecular Modeling – II (15hrs)
Force Field Equation in Energy minimization (Energy as function of r, θ, ω) - Introduction to Derivative Minimization Methods (First Order Minimization), Types of energy minimization Methods; Steepest Descent, Conjugate Gradient, Conformational Search procedures - Geometry optimization procedures - Molecular Dynamics: Introduction, description of Molecular Dynamics, basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method, Qualitative exposure to Molecular Dynamics Simulations.

**PC(CB2)-23: Drug Design Methods I - Ligand Based**

(15hrs)

Lead Molecule - Structure Activity Relationship (SAR), Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR - Physicochemical parameters; Electronic effects, Hydrophobicity, Steric Factors Taft’s Steric function, Molar Refractivity, Verloop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bioisosteres - Hansch model, Free-Wilson model for QSAR equations - Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, r^2, r%^2, F) - Examples for linear and non-linear equations - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR.

**PC(CB2)-24: Drug Design Methods II - Structure Based.**

(15hrs)


**Books suggested:**

2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press

**Elective – 4A (ID Paper)**
Paper-IV CH (PO) 404T(CB3): Five and six membered heterocycles, Carbohydrates and proteins, structure determination of natural products and Green chemistry

PO-(CB3) - 25: Five and six membered heterocycles with two hetero atoms
PO-(CB3) - 26: Carbohydrates and proteins
PO-(CB3) - 27: Structure determination of natural products by chemical and spectral methods
PO-(CB3) - 28: Green chemistry

PO-(CB3) - 25: Five and six membered heterocycles with two hetero atoms 15 Hrs
Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

PO-(CB3) - 26: Carbohydrates and proteins 15 Hrs
Carbohydrates: Determination of the relative and absolute configuration in D(+)-glucose and D(-)-fructose. Proof for the ring size of D(+)-glucose. 4C1 and 4C4 conformations of D-glucose. Occurrence, importance and synthesis of monosaccharides containing functional groups such as amino, halo and sulphur. Structure elucidation and synthesis of sucrose. Conformational structures of D(+)-ribose, 2-deoxy-D-ribose, sucrose, lactose maltose and cellobiose. Structural features of starch, cellulose and chitin.

PO-(CB3) - 27: Structure determination of natural products by chemical and spectral methods 15 Hrs
i) Determination of structure of morphine by chemical methods and spectral methods (IR, UV, 1H-NMR, 13C-NMR)
ii) Determination of structure of reserpine by chemical methods and spectral methods (IR, UV, 1H-NMR, 13C-NMR and Mass)
iii) Determination of structure of abeitic acid by chemical methods and spectral methods (IR, UV, 1H-NMR, INEPT, DEPT, HOMOCOSY, HETEROCOSY and Mass)
iv) Determination of structure of geraneol by chemical methods and spectral methods (IR, UV, 1H-NMR, INEPT, DEPT, HOMOCOSY, HETEROCOSY, 2D-INADEQUATE, NOE and Mass)

PO-(CB3) - 28: Green chemistry 15 Hrs
2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation, Dihydroxylation (Syn- & Anti-)
3. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects.
   a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.
   b) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions.
   c) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, OrthoesterClaisen rearrangement, Diels- Alder reaction, decarboxylation.
   d) Microwave assisted reactions under PTC conditions:

4. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.

5. Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker’s Yeast.


**Recommended Books:**

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule&K.Mills
5. Heterocyclic Chemistry, J.A.Joule& Smith
8. Carbohydrate Chemistry by Barton Volumes
9. Carbohydrate chemistry by G.J.Boons
10. The chemistry of natural products: Vol.V - carbohydrates by S.F.Dyke
12. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
13. NMR in chemistry - A multinuclear introduction by William Kemp
14. Introduction to organic spectroscopy by Pavia
15. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
16. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
17. NMR spectroscopy by H.Gunther
18. Textbook of organic chemistry, Vol II by I L Finar
19. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
20. An introduction to the chemistry of terpenoids and steroids, by William templeton
21. Steroids by Fieser arid Fieser
22. Alkaloids by Manske
23. Alkaloids by Bentley
24. The chemistry of terpenes by A Pinder
25. The terpenes by Simenson
26. Terpenoids by Mayo
27. Alkaloids by Pelletier
28. Total synthesis of Natural Products by Apsimon Vol 1-5
29. Principles of organic synthesis 3rd Ed. R O C Norman and J M Coxen
30. One and two dimensional nmr spectroscopy by Atta Ur Rahman
32. New trends in green chemistry By V.K. Ahulwalia and M. Kidwai.

ELECTIVE-4B(ID PAPER)

Paper-IV CH (PO) 404T (CB4): Forensic Chemistry & Toxicology
PO-(CB4)29: Forensic chemistry- I
PO-(CB4)30: Forensic chemistry- II
PO-(CB4)31: Forensic Toxicology-I
PO-(CB4)32: Forensic Toxicology-II

PO-(CB4)29: Forensic chemistry- I
15 Hrs
Forensic Chemistry - Introduction - Types of cases / exhibits - Preliminary screening - presumptive tests (colour and spot tests) - Examinations procedures involving standard methods and instrumental techniques
Qualitative and quantitative forensic analysis of inorganic and organic material - Chemical fertilizers (N,P,K) - Insecticides (Endosulfan, Malathion, Carbaryl) - Metallurgical analysis (Fe, Cu, Zn, Au, Ag) – Natural products (tobacco, tea, sugars, rubber) – Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids, Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chloride, Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether Organic chemicals like Acetanilide, P- Aminophenol, and Nitrobenzene etc. with reference to forensic work.

PO-(CB4)30: Forensic chemistry- II
15 Hrs

PO-(CB4)31: Forensic Toxicology-I
15 Hrs
Toxicology- Introduction - History- Scope- Areas of Toxicology- Role of forensic toxicologist- Poisons- Classification of poisons- Types of poisoning- Sample collection and preservation of toxicological exhibits in fatal and survival cases - Storage of samples- Signs and symptoms of poisoning- Toxicological investigation/examination of poisoned death - Interpretation of toxicological data- Courtroom testimony in toxicological cases. Case Histories.
**PO-(CB4)32: Forensic Toxicology-II**

15 Hrs


**Recommended books:**

12. Wilson and Wilson’s Comprehensive Analytical Chemistry Volumes
13. Standard Methods of Chemical Analysis
14. AOAC Official Methods of Analysis
22. Laboratory procedure Manual, Forensic Toxicology DFS, 2005
26. Eckert; An Introduction to Forensic Science, CRC Press
SEMESTER IV LABORATORY COURSES

PAPER VII (Lab)-CH(PO) 451P: Instrumentation

I. Conductometry:

Conductometric titrations:
 a) Mixture of strong and weak bases vs strong acid
 b) Mixture of strong and weak bases vs weak base
 c) Mixture of strong acid, weak acid and CuSO4 vs strong base 
 d) Formic acid, acetic acid, chloro acetic acid, dichloro acetic acid and trichloro acetic acid and their mixtures vs strong base
 e) Precipitation titration: K\(_2\)SO\(_4\) vs BaCl\(_2\)

II. pH – metry:

1. Preparation of a) phosphate  b) acetate  and c) borate buffers
2. pH-metric titrations of
   a) monobasic acids vs strong base
   b) dibasic acids vs strong base
   c) tribasic acids vs strong base
   d) mixture of strong and weak acids vs strong base
3. Determination of dissociation constant of monobasic/dibasic acids by Alber-Serjeant method.
4. Determination of dissociation constant of acetic acid in DMSO, acetone and dioxane.
5. Determination of pKa and pKb of glycine (calculation using a computer program)

III. Spectrophotometry:

1. Estimation of a) Cu(II) using EDTA
   b) Fe(III) using thiocyanate
   c) Fe(II) using 1,10-phenanthroline
   d) Fe(III) in tap water using thiocyanate by standard addition method
   e) dichromate and permanganate simultaneously in a mixture
2. Spectrophotometric titrations: 
   a) Cu(II) vs EDTA
   b) Fe(II) using 1,10-phenanthroline
   c) Mixture of Cu(II) and Bi(III) vs EDTA
3. Determination of composition of
   a) Cu(II)-EDTA complex by Job’s method
   b) Fe(II)-phenanthroline complex- by Job’s method or mole ratio /slope ratio method
4. Determination of pKa of methyl red indicator

IV Potentiometry:

1. Potentiometric titrations:
   a) Weak acid vs strong base and calculation of dissociation constants
   b) Mixture of strong and weak acids vs strong base
c) Dibasic acid vs strong base
d) Fe(II) vs Ce(IV) and calculation of formal redox potentials of Fe(II)/Fe(III)
e) Fe(II) vs MnO4-
f) I – vs MnO4-
g) Fe(II) vs EDTA
h) Mixture of halides vs AgNO3
i) Mixture of KI and KSCN vs AgNO3
2. Determination of temperature dependence of e.m.f of a cell
3. Determination of formation constant of silver-ammonia complex
4. Determination of solubility product
5. Determination of mean ionic activity coefficient of HCl

Suggested Books:
1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
4. Practical in Physical Chemistry: P.S. Sindhu
5. Advanced Practical Physical Chemistry: J.B.Yadav

Paper VIII –(LAB) CH (PO) 452P : Separation, identification and spectral analysis of organic compounds

1. Separation of two component mixtures by chemical methods and their identification by chemical reactions – separation by using solvent ether, dil. hydrochloric acid, 5% aqueous sodium bicarbonate and sodium hydroxide solutions, checking the purity of the two components by TLC, identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 6 mixtures should be separated and analyzed by these procedures.
2. Separation of three component mixtures by chemical method. A minimum of 2 mixtures should be separated.
3. Identification of unknown organic compounds by interpretation of IR, UV, 1H nmr, 13C nmr and mass spectra. A minimum of 15 representative examples should be studies.

Suggested Books:
1. The systematic identification of organic compounds by R L Shriner, R C Fusion and D Y Curtin
3. Unitized experiments in organic chemistry by R Q Brewster and others
4. Handbook of organic analysis by HTC Clarke
5. Practical Organic Chemistry by Mann and Saunders
### FIVE YEAR INTEGRATED COURSE (FYIC)

**SYLLABUS FOR IX NAD X SEMESTER**

**Semester IX**

<table>
<thead>
<tr>
<th>Subject Code</th>
<th>Subject</th>
<th>Instruction Hrs /Week</th>
<th>Internal Assessment. Marks</th>
<th>Max Marks Sem. Exams</th>
<th>Duration of Sem. Exam. Hrs</th>
</tr>
</thead>
<tbody>
<tr>
<td>FYIC-T901</td>
<td>Inorganic Chemistry</td>
<td>4 Hrs</td>
<td>20</td>
<td>80</td>
<td>3</td>
</tr>
<tr>
<td>FYIC-T902</td>
<td>Organic Chemistry</td>
<td>4 Hrs</td>
<td>20</td>
<td>80</td>
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#### PRACTICALS

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**Total** 34+2 hrs 80 620

**Semester X**

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**Total** 600
SEMESTER –IX

Paper-I FYIC 901 INORGANIC CHEMISTRY
(Bonding, Group Theory and its Applications)

IC-01: Group Theory, Normal mode analysis and Spectral Activity
IC-02: MOT of Metal Complexes
IC-03: Electronic Spectroscopy of Metal Complexes
IC-04: IR and Raman Spectroscopy

Paper II FYIC 902 ORGANIC CHEMISTRY

OC-01: New synthetic reactions
OC-02: Pericyclic reactions
OC-03: Photochemistry
OC-04: 13C NMR spectroscopy

Paper III FYIC 903 PHYSICAL CHEMISTRY

PC-01: Applications of Schrödinger equation
PC-02: Chemical Kinetics-II
PC-03: Electrochemistry -II
PC-04: Bonding in molecules

Paper-IV FYIC 904 GENERAL CHEMISTRY
(ANALYTICAL TECHNIQUES, SPECTROSCOPY and GREEN CHEMISTRY)

GC-01: Atomic Spectroscopy
GC-02: CD, ORD and 2D NMR techniques
GC-03: Diffraction Methods
GC-04: Green Chemistry
**SEMESTER-IX**

**PAPER I: FYIC 901: Bonding, Group Theory and its Applications**

IC-01: Group Theory, Normal mode analysis and Spectral Activity
IC-02: MOT of Metal Complexes
IC-03: Electronic Spectroscopy of Metal Complexes
IC-04: IR and Raman Spectroscopy

**IC-01: Group Theory, Normal Mode Analysis and Spectral Activity** *(15 hours)*

Group Multiplication Tables – Properties of a Group-Subgroups-Classes of Symmetry Elements. Representation of Symmetry Elements: Simple Matrices, Block-Factorization, Matrix Representation of $E, C_n, S_n, i$ and $\sigma$ Elements –Matrix Representation of $C_{2v}, C_{3v}$ and $C_{2h}$ point groups. Character of a Matrix and a Representation, Reducible and Irreducible Representations, Properties of Irreducible Representations, Construction of Character Tables for some simple Point Groups: $C_{2v}, C_{3v}$ and $C_{2h}$ – Mulliken Symbolism for Irreducible Representations - Standard Reduction Formula – Direct Products.

**Normal Modes analysis & Spectral Activity:** Number, Type and Symmetry – Symmetry of Normal Modes of Molecules: Cartesian and Internal Coordinate Methods of Analysis – Normal Mode Analysis of Molecules with Cnv ($n=2,3$), C2h, D2h, Td and Oh Point Groups – Internal Coordinates and Redundancy (Qualitative concept) – Infrared and Raman Activity of Normal Modes (Infinite Groups Excluded)

**IC-02: Molecular Orbital Theory of Metal Complexes** *(15 hours)*

Symmetry Classification of Metal and Ligand Orbitals in Cubic and Non-Cubic Environments: Octahedral, Tetrahedral, Square Planar, Square Pyramidal, Trigonal Bipyramidal Geometries – Concept of Ligand Group Orbitals – Construction of Molecular Orbital Energy Level Diagrams for Octahedral, Tetrahedral and Square Planar Metal Complexes with Sigma ($\sigma$) and Pi ($\pi$) Bonding Contribution from the Ligands.

**IC-03: Electronic Spectroscopy of Metal Complexes** *(15 hours)*


**IC-04: Infrared and Raman Spectroscopy** *(15 hours)*

SUGGESTED BOOKS
7. Molecular Symmetry, Schoenland
8. Electronic Spectroscopy, A. B. P. Lever
9. Introduction to Ligand fields, B. N. Figgis
10. Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto
11. Infrared spectroscopy of Inorganic Compound, Bellamy
OC 01- New synthetic reactions
OC 02- Pericyclic reactions
OC 03-Photochemistry
OC 04- 13C NMR spectroscopy

OC-01: New synthetic reactions: (15 hours)
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson’s stereoselective olefination.
5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.
6. Metathesis: Grubb’s 1\textsuperscript{st} and 2\textsuperscript{nd} generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.
7. Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

OC-02: Pericyclic reactions (15 hours)
Introduction, Classification of pericyclic reactions,
Electrocyclic reactions: con rotation and dis rotation. Electrocyclic closure and opening in 4n and 4n+2 systems.
Cycloaddition reactions: suprafacial and antara facial additions in 4n and 4n+2 cycloadditions.
Sigmatropic reactions: \([i, j]\) shifts- suprafacial and antarafacial shifts, Cope and Claisen rearrangement reactions.
Molecular orbitals: ethylene, 1, 3-butadiene, 1, 3, 5-hexatriene, allyl cation, allyl radical, pentadienyl cation, pentadienyl radical.
Frontier Molecular Orbital (HOMO-LUMO) approach-concept: Framing Woodward-Hofmann selection rules for all the pericyclic reactions by Frontier Molecular Orbital (FMO) approach. Solving problems based on FMO approach.
Conservation of orbital symmetry: (Correlation Diagrams) approach- for electrocyclic and cycloadditions & cycloreversions.

OC-03: Photochemistry (15 hours)
Photochemistry: Photochemistry of \(\pi-\pi^*\) transitions: Excited states of alkenes, cis-trans isomerisation, and photo stationary state. Photochemistry of 1,3-butadiene Electrocyclisation and sigmatropic rearrangements, di-\(\pi\) methane rearrangement. Intermolecular reactions, photocycloadditions, photodimerisation of simple and conjugated olefins. Addition of olefins to \(\alpha, \beta\)-unsaturated carbonyl compounds. Excited states of aromatic compounds, Photoisimerisation of benzene.
Photochemistry of (n-π*) transitions: Excited states of carbonyl compounds, homolytic cleavage of α- bond, Norrish type I reactions in acyclic and cyclic ketones and strained cycloalkane diones.
Intramolecular abstraction of hydrogen: Norrish type II reactions in ketones, esters and 1,2 diketones, Addition to carbon-carbon multiple bonds, Paterno-Buchi reaction, Photochemistry of nitrites-Barton reaction

OC-04: $^{13}$C NMR spectroscopy (15 hours)
CW and PFT techniques. Types of $^{13}$C nmr spectra: undecoupled, proton-decoupled and offresonancedecoupled (ORD) spectra. $^{13}$C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear ($^{13}$C, $^{13}$C J) and heteronuclear ($^{13}$C, $^1$H J and $^{13}$C- $^2$H J ) coupling.
Applications of $^{13}$C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. $^{13}$C-NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

Recommended Books:
1. Some modern methods of organic synthesis by W Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic synthesis by O House
4. Organic synthesis by Michael B Smith
5. Molecular Reactions and Photo chemistry by Depuy and Chapman
6. Organic synthesis by Robert E Ireland
7. Organic Synthesis - The disconnection approach by S Warren
8. Organic Synthesis by C Willis and M Willis
9. Handbook of reagents for organic synthesis by Reich and Rigby, Vo I, IV
10. Problems on organic synthesis by Stuart Warren
11. Total synthesis of natural products: the Chiron approach by S.Hanessian
12. Organic chemistry Claydon and others 2005
13. Name Reactions by Jie Jack Li
14. Reagents in Organic synthesis by B.P.Mundy and others.
15. Tandem Organic Reactions by Tse-Lok Ho
16. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B Morrill
17. Organic Spectroscopy by William Kemp
18. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
19. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
20. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
22. Modern NMR techniques for chemistry research by Andrew B Derome
23. NMR in chemistry - A multinuclear introduction by William Kemp
24. Spectroscopic identification of organic compounds by P S Kalsi
25. Introduction to organic spectroscopy by Pavia
29. Photochemistry by C W S Wells
30. Organic Photochemistry by Turro
31. Molecular Photochemistry by Gilbert & Baggo
32. Organic Photochemistry by D Coyle
33. Optical rotatory dispersion by C Djerassi
34. Optical rotatory dispersion and circular dichroism by P Crabbe
35. Mechanism and Structure in Organic chemistry by S Mukherjee
37. Pericyclic Reactions by Mukherjee
38. Conservation of Orbital Symmetry by Woodward and Hoffmann
39. Organic Reactions and Orbital Symmetry, Gilchrist and Storr
40. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
41. The Nature of Chemistry — Units 17-19 - Aromaticity — Open University, U K. Publications
Paper III: FYIC 903 Physical Chemistry

PC-01: Applications of Schrödinger equation

PC – 01: Applications of Schrödinger equation (15 hours)
Atoms in external field, Zeeman and anomalous Zeeman effect.

PC- 02: Chemical Kinetics – II

PC- 02: Chemical Kinetics – II (15 hours)

PC –03: Electrochemistry – II

PC –03: Electrochemistry – II (15 hours)
The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallelplate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

**PC – 04: Bonding in molecules** *(15 hours)*


Concept of hybridization – sp, sp$^2$, and sp$^3$ hybrid orbitals.

Semiempirical MO methods. The Hückel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. $\pi$-electron charges and bond orders. Simplification secular determinants of cyclopropenyl system, cyclobutadiene and benzene using molecular symmetry. Extension of the Hückel approach to molecules containing heteroatoms.

Orbital symmetry and reactivity: $\text{H}_2 + \text{F}_2 \rightarrow 2\text{HF}$ reaction. $2\text{NO} \rightarrow \text{N}_2 + \text{O}_2$ reaction.

**Reference Books**

1. Quantum Chemistry, Ira N. Levine, Prentice Hall
5. Quantum Chemistry by R. K. Prasad
8. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan
12. Rates and Equilibriums of Organic Reactions, J. E. Leffler & E. Grunwald, Dover publications
13. Reaction Dynamics, edited by N. Sathyamurthy, Narosa Publishing House
17. Atkin’s Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
Paper IV: FYIC 904 GENERAL CHEMISTRY
(ANALYTICAL TECHNIQUES, SPECTROSCOPY and GREEN CHEMISTRY)

GC-01: Atomic Spectroscopy
GC-02: CD, ORD and 2D NMR techniques
GC-03: Diffraction Methods
GC-04: Green Chemistry

GC-01: Atomic Spectroscopy (15 hours)

**Atomic Absorption Spectroscopy (AAS):** Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences – chemical and spectral, evaluation methods in AAS and application in qualitative and quantitative analysis.

**Atomic Emission Spectroscopy (AES):** Principles of AES, Instrumentation, Interferences, evaluation methods, Application in quantitative analysis.


GC – 02: CD, ORD and 2D NMR techniques (15 hours)

**Optical Rotatory Dispersion (ORD) and CD Spectroscopy:** Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Helicity rule, Exciton chirality method-Exciton coupling between identical chromophores. Benzene sector and chirality rule. Application of the rules to the study of absolute configuration and conformations of organic molecules.

**2D-NMR techniques:** Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY ($^1$H - $^1$H COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY ($^1$H, $^{13}$C COSY, HMOC), long range $^1$H, $^{13}$C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

GC-03: Diffraction Methods (15 hours)


**Electron Diffraction by Gases:** Principles - Radial Distribution Curves - Interpretation of Results for PBrF$_2$S, PF$_3$S, PF$_3$HS, HClO$_4$, Silyl monothioacetate and Germyl monothioacetate and HgClI$_2$ molecules - Advantages and Limitations.

GC-04 : Green Chemistry  (15 hours)


1. Solvent free reactions-principle, scope, utility of solvent free condition reactions.


2. Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, epoxidation, Dihydroxylation (Syn- & Anti-)

3. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects.

a) Microwave Solvent free reactions (Solid state Reactions) - Deacetylation, deprotection, saponification of esters, alkylation of reactive methylene compounds, synthesis of nitriles from aldehydes, reductions.

b) Microwave assisted reactions in water — Hoffmann elimination, hydrolysis, oxidation, saponification reactions.

c) Microwave assisted reactions in organic solvents — Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels- Alder reaction, decarboxylation.

d) Microwave assisted reactions under PTC conditions:

4. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.

5. Organocatalysis: Aldol reactions, Acyl transfer reactions, nucleophilic N-heterocyclic carbenes in asymmetric organocatalysis, setter reaction and Baker’s Yeast.


SUGGESTED BOOKS

15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
20. Organic Spectroscopy by William Kemp
21. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
22. Carbon-13 NMR for organic chemists by G C Levy and O L Nelson
23. Optical rotatory dispersion and circular dichroism by P Crabbe
24. Optical rotatory dispersion by C Djerassi
25. Modern NMR techniques for chemistry research by Andrew B Derome
Laboratory Courses

PAPER 905 Inorganic Chemistry Practicals: 6 hrs/week

Instrumental Methods of Analysis

I Potentiometry:
   i. Determination of Fe$^{2+}$ in Iron wire using K$_2$Cr$_2$O$_7$ and KMnO$_4$
   ii. Determination of Ferrous and Vanadyl in a mixture by Ceric Ammonium Nitrate.
   iii. Assay of sulphanilamide in sample.

II pHmetry:
   i. Determination of CO$_3^{2-}$ and HCO$_3^-$ in a mixture
   ii. Determination of the dissociation constants of Glycine (HL)
   iii. Determination of binary constants of Ni(II) – Gly Systems

III Conductometry:
   i. Determination of the Composition of Cu(II)-Oxine Complex
   ii. Determination of the Composition of Cu(II)-EDTA Complex

IV Spectrophotometry
   i. Estimation of manganese in steel
   ii. Estimation of chromium.
   iii. Determination of composition of Complex by Job’s Method and Mole ratio Method in Cu(II)-EDTA

V Colorimetry
   i. Determination of blood sugar
   ii. Determination of blood cholesterol
   iii. Determination of Paracetamol

VI Fluorimetry
   i. Determination of Riboflavin
   ii. Determination of Quinine Sulphate.

VII Flame photometry
   i. Determination of Na
   ii. Determination of K

VII Atomic Absorption Spectroscopy (Demonstration): Determination of Mg and Pb.
Suggested Books
1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William
Paper-906 ORGANIC CHEMISTRY Practicals: 6 hrs/week

Spectroscopic identification of organic compounds, Chromatography and Isolation of Natural Products

1. Identification of unknown organic compounds by interpretation of IR, UV, 1H -NMR, 13C NMR and mass spectral data. A minimum of 10 representative examples should be studied.
2. Separation by column chromatography: Separation of a mixture of ortho and paranitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.
3. Isolation of the following natural products:
   - Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction),
   - Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

Recommended books:
1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beekett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster
Spectrophotometry:
1. Estimation of Cu(II) using EDTA
2. Estimation of Fe(III) using thiocyanate
3. Estimation of Mn(II) by spectrophotometry using periodate
4. Spectrophotometric titration of Cu(II) vs EDTA
5. Spectrophotometric titration of Fe(II) vs 1,10-phenanthroline
6. Determination of composition and Gibbs energy of formation of Fe(III) – salicylic acid complex
7. Simultaneous determination of dichromate and permanganate in a mixture

Potentiometry:
1. Titration of strong acid (HCl) vs strong base (NaOH)
2. Titration of weak acid vs strong base (NaOH) & calculation of dissociation constants
   - **Weak acids:** Acetic acid, Chloro acetic acid, Dichloro acetic acid, Trichloro acetic acid, Propinoic acid and butyric acid
3. Titration of a mixture of strong (HCl) and weak acids vs strong base (NaOH)
   - **Weak acids:** Acetic acid, Chloro acetic acid, Dichloro acetic acid, Trichloro acetic acid, Propinoic acid and butyric acid
4. Dibasic acid (Oxalic acid) vs strong base (NaOH) & determination of $pK_{a1}$ and $pK_{a2}$
5. Redox titrations:
   a) Fe(II) vs Ce(IV) and calculation of formal redox potential of Fe(II)/Fe(III)
   b) Fe(II) vs MnO$_4^-$
   c) Fe(II) and V (v) vs Ce (IV)
   d) I$^-$ vs MnO$_4^-$
6. Precipitation titrations
   a) Mixture of halides (KCl & KI) vs AgNO$_3$
   b) Mixture of KSCN & KI vs AgNO$_3$
7. Fe (III) vs EDTA (Complexometric titration)
Suggested Books

1. Senior Practical Physical Chemistry, B.D. Khosla, V.C Garg.

2. Experimental Physical Chemistry, Athawale, V.D., New Age International
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