M.Sc. CHEMISTRY

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

FOR STUDENTS ADMITTED FROM THE YEAR 2023-24 ONWARDS

27/1/24

27/01/24

27/1/24

M.C Completed

M.Sc. CHEMISTRY
ANALYTICAL CHEMISTRY SPECIALISATION

Syllabus for III and IV Semesters

[Under Restructured CBCS Scheme]

(for the batches admitted in academic year 2023-24 onwards under CBCS pattern)

Grand total marks and credits (all 4 semesters) 2400 marks – 80 credits

(Approved in the P.G. BOS meeting held on 27-01-2024)

Semester - III (Analytical Chemistry)

	Instruction Hrs/week	Internal assessment	Semester exam	Total marks	Credits
CH(AC)301T (Core)	3	50 marks	50 marks	100	3
CH(AC)302T (Core)	3	50 marks	50 marks	100	3
CH(AC)303T (Elective)	3	50 marks	50 marks	100	3
CH(AC)304T (Elective)	3	50 marks	50 marks	100	3
CH351P (AC LAB 1)	4		50 marks	50	2
CH352P (AC LAB 2)	4		50 marks	50	2
CH353P (AC LAB 3)	2		25 marks	25	1
CH354P (AC LAB 4)	2		25 marks	25	1
Seminar	2		50 Marks	50	2
Total	26			600	20

Semester - IV (Analytical Chemistry)

	Instruction Hrs/week	Internal assessment	Semester exam	Total marks	Credits
CH(AC)401T (Core)	3	50 marks	50 marks	100	3
CH(AC)402T (Core)	3	50 marks	50 marks	100	3
CH(AC)403T (Elective)	3	50 marks	50 marks	100	3
CH451P(AC LAB1)	4		50 marks	50	2
CH452P(AC LAB2)	4		50 marks	50	2
CH453P (AC LAB3)	2		25 marks	25	1
CH454P (Project)	12	50 marks	125 marks	175	6
Total	31			600	20

Grand total marks and credits (all 4 semesters) 2400 marks - 80 credits

M.Sc. SEMESTER III ANALYTICAL CHEMISTRY SPECIALISATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH (AC) 301T (CORE): ANALYTICAL TECHNIQUES
AC-01: Sampling & Data handling
AC-02: Thermal & Radiochemical methods of analysis
AC-03: Atomic Spectroscopy

PAPER II CH (AC) 302T (CORE): SPECTROSCOPIC METHODS OF ANALYSIS-I
AC-04: ^{13}C and 2D NMR
AC-05: Electron Spin Resonance Spectroscopy
AC-06: Mossbauer and Nuclear Quadrupole Resonance Spectroscopy

PAPER III CH (AC) 303T (ELECTIVE III A): MISCELLANEOUS METHODS OF ANALYSIS
AC(CB1)-07: Surface Analysis Methods
AC(CB1)-08: Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC(CB1)-09: Micromeritics, Dissolution and disintegration

PAPER III CH (AC) 303T (ELECTIVE III B): CLASSICAL, ELECTROANALYTICAL AND SPECTROSCOPIC METHODS OF ANALYSIS
AC(CB1)-07: Titrimetric and Gravimetric analysis.
AC(CB1)-08: Electroanalytical Methods
AC(CB1)-09: Optical Methods

PAPER IV CH (AC) 304T (ELECTIVE IV A): APPLIED ANALYSIS
AC(CB2)-10: Industrial Analysis
AC(CB2)-11: Food and Agricultural analysis
AC(CB2)-12: Analysis of Air and Water Pollutants and Sewage water treatment

PAPER-IV CH(IC) 304T (ELECTIVE IV B): NUCLEAR CHEMISTRY, ZEOLITES & SOLID STATE CHEMISTRY
AC(CB2)-10: Nuclear Chemistry
AC(CB2)-11: Zeolites and Molecular Sieves
AC(CB2)-12: Solid State Chemistry

LABORATORY COURSE
Paper V CH (AC) 351P: Titrimetry, Solvent extraction and Chromatography
Paper VI CH (AC) 352P: Spectrophotometry –I
Paper VII CH(AC) 353P: Water analysis
Paper VIII CH(AC) 354P: Spectrophotometry II

SEMINAR

M.Sc. SEMESTER IV
ANALYTICAL CHEMISTRY SPECIALISATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH (AC) 401T (CORE): SPECTROSCOPIC METHODS OF ANALYSIS-II
AC-13: Electronic spectroscopy,
AC-14: IR & Raman spectroscopy
AC-15: Fluorimetry, Phosphorimetry, **Nephelometry and Turbidimetry**

PAPER II CH (AC) 402T (CORE): SEPARATION METHODS AND MASS SPECTROMETRY
AC-16: Solvent extractions & Chromatography-I
AC-17: Chromatography -II
AC-18: Advanced Mass spectrometry

PAPER III CH (AC) 403T (ELECTIVE IIIA): LABORATORY MANAGEMENT AND QUALITY ASSURANCE
AC(CB1)-19: Laboratory Automation and Management, LIMS and Computer aided Analysis
AC(CB1) -20: Quality Control and Quality Assurance
AC(CB1)-21: Quality Standards, Management and Accreditation

PAPER III CH(AC) 403T (ELECTIVE III B): APPLIED ANALYSIS AND GREEN ANALYTICAL CHEMISTRY
AC(CB1)-19: Enzyme catalysis- Analytical applications
AC(CB1)-20: Forensic Chemical Analysis
AC(CB1)-21: Green Analytical Chemistry

LABORATORY COURSE
Paper IV CH (AC) 451P: Electro analytical techniques - I
Paper V CH (AC) 452P: Evaluation of Physical Parameters of Tablets, Spectroscopic Techniques and problems
Paper VI CH (AC) 453P: Electro analytical techniques - II

PROJECT CH (AC) 454P

M.Sc. ANALYTICAL CHEMISTRY SPECIALIZATION
SEMESTER-III

PAPER I CH (AC) 301T (CORE) ANALYTICAL TECHNIQUES

AC – 01: Sampling & Data handling
AC – 02: Thermal & Radiochemical methods of analysis
AC – 03: 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.

Errors and Evaluation:-Accuracy, precision, sensitivity, detection limits, significant figures, rounding off. Types of errors – determinate and indeterminate errors. Ways of expressing accuracy, absolute and relative errors. Significant figures and propagation of errors. Confidence limit, Test of significance – the F-test and T-test. The statistical Q-test for rejection of a result, statistics for small data sets. Linear least squares method. The correlation coefficient. Calculation for the above parameters.

AC – 02: Thermal and Radiochemical methods of Analysis — 15 Hrs

Thermal methods of analysis: Thermogravimetry, Differential Thermal Analysis and Differential Scanning Calorimetry, instrumentation. Methodology of TG, DTA and DSC. Application of TG to study of oxalates and chromates. Determination of Glass transition, Heat capacity determination, Characterization of polymer blends. Problems based on decomposition path way and % composition. Evolved gas analysis.

Thermometric titrimetry – theory, instrumentation, applications.

Radiochemical methods of analysis: Radioactive tracer techniques and its applications, isotope dilution analysis, neutron activation analysis, radiometric titrations: principle, theory, applications and problems.

AC – 03: Atomic Spectroscopy — 15 Hrs

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 applications in qualitative and quantitative analysis.

Atomic Emission Spectroscopy (AES): Principle of AES, Instrumentation, Interferences, evaluation methods, Application in quantitative analysis.

Inductively Coupled Plasma- Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Applications of ICP-AES.Comparison with AAS.

SUGGESTED BOOKS

1. Principles of Instrumental Analysis - Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers (1998).
2. Analytical Chemistry – Gary D. Christian, 6th ed., John Wiley and sons. Inc., New York (1994).
3. Instrumental methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors (1986).
4. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle,Prentice Hall, New Jersey, USA(1997).
5. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5th ed., Longmann, ELBS Publications (2000).
6. Principles and practice of Analytical Chemistry, F.W.Fifield & D Kealey, 5th Ed.Blackwell Science (2000).
7. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork (2003).
8. Analytical Chemistry An Introduction, Crouch, 7th Ed. Saunders College Publishing (2000).
9. Organic Analytical Chemistry theory and practice, Jag Mohan, Narosa Publications (2003).
10. Pharmaceutical analysis, Watson
11. Electronic Absorpption Spectroscopy and related techniques, D.N.Satyanarayana, University Press (2001).

PAPER II CH (AC) 302T (CORE): SPECTROSCOPIC METHODS OF ANALYSIS I

AC – 04: ^{13}C & 2D NMR Spectroscopy
AC – 05 : Electron Spin Resonance Spectroscopy
AC – 06 : Mossbauer and Nuclear Quadrupole Resonance Spectroscopy

AC – 04: ^{13}C & 2D NMR Spectroscopy — 15 Hrs

^{13}C NMR spectroscopy: Introduction, Types of 13Cnmr spectra: undecoupled, proton decoupled and off-resonance decoupled spectra. 13C 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}CJ) 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}CNMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (1H-1H COSY) , Hetero COSY (^{1}H,^{13}C COSY,HMQC), long range ^{1}H,^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy experiments and their applications.

AC – 05: Electron Spin Resonance Spectroscopy — 15 Hrs

Principle; Selection Rules; Instrumentation; Application of ESR to the study of simple free radicals - methyl ($CH_3^{\cdot}$), amine ($NH_2^{\cdot}$), diphenylpicrylhydrazyl, cyclopentadienyl ($C_5H_5^{\cdot}$), hydroxy methyl ($CH_2OH^{\cdot}$) radicals; Zero-Field Splitting (ZFS) and Kramer's degeneracy; Effective Spin ; ESR Spectra of d^1-d^9 Transition metal complexes with examples; Calculation of g values with simple examples; Interpretation of g in cubic, axial and rhombohedral geometries; Intensities of $g_{\parallel}$ and $g_{\perp}$peaks; Evidence for metal-Ligand bond covalency – Cu(II)-bis-salicylaldimine, Cu(II)-diethyldithiophosphinate, Vanadyldithiophosphinate, Cu(II)-tetraphenylporphyrin, Co(II)-phthalocyanine and $K_2[IrCl_6]$; Application of ESR in structure determination - $[(NH_3)_5\ Co\ O_2\ Co\ (NH_3)_5]^{5+}$; Calculation of 'g' and 'A' values from esr spectral data in i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}. ESR spectra of dinuclear Cu (II) complexes.

AC – 06:Mossbauer and Nuclear Quadrupole Resonance Spectroscopy — 15 Hrs

Mossbauer Spectroscopy: Principle; Experimental Considerations and Presentation of the Spectrum; Isomer Shifts; Quadrupole splitting and Magnetic hyperfine splitting; Selection Rules.

Applications:

Iron Compounds: Low-spin and High-spin Fe(II) and Fe(III) Complexes , π-bonding Effects in Iron complexes, Study of High-spin Low-spin Cross-over, Diamagnetic and Covalent Compounds, Structural aspects of Iron Carbonyls and Iron-Sulphur Proteins.

Tin Compounds: Tin Halides and Organotin Compounds.

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

SUGGESTED BOOKS

1. Nuclear Magnetic Resonance Basic principles, Atta-ur-Rahman, Springer-Verlog (2011)
2. Spectroscopy of organic compounds, P S Kalsi, 8th Edition, New Age International Publishers (2020)
3. Organic Spectroscopy, William Kemp, 3rd Edition, Visionias (2020)
4. Introduction to organic spectroscopy, Donald Pavia, 5th Edition, Cengage India Private Limited (2015)
5. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and S.Craddock, ELBS, Blackwell Scientific publications (1987).
6. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., (1977).
7. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing (1992).
8. Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, D.N. Satyanarayana, Dreamtech press, Wiley (2022).
9. Magneto Chemistry, Dutta & Shyamal, Oxford Chemistry Primers, Vol 62 (1993).
10. Instrumental Methods of Chemical Analysis, Gurdeep R Chatwal, Sham K. Anand, Himalaya Publishing House, (2019)
11. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, (1976).
12. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London (1971).
13. Principles of Instrumental Analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd. (1998)
14. Hand book of Instrumental Techniques for Analytical Chemistry, Frank Settle, Prentice Hall (1997).
15. Physical Methods in Advanced Inorganic Chemistry, Hill and Day, Interscience publishers (1968).

PAPER III CH (AC) 303T (ELECTIVE III A): MISCELLANEOUS METHODS OF ANALYSIS

AC(CB1)-07: Surface Analysis Methods
AC(CB1)-08: Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence
AC(CB1)-09: Micromeritics, Dissolution and disintegration

AC(CB1)-07: Surface Analysis Methods — 15 Hrs

Introduction, types of surface measurements.

Photon Probe Techniques: Photoelectron Spectroscopy: Principle and instrumentation, types of photoelectron spectroscopy – UPS & XPS. Binding energies, Koopman's theorem, Chemical shifts. Photoelectron spectra of simple molecules: N_2, O_2, and F_2. Vibrational structure of PES bands, potential energy curves, interpretation of vibrational spectral data for ionized (M^+) species, prediction of nature of molecular orbitals. ESCA in qualitative analysis.

Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle, Instrumentation, applications. Transmission Electron Microscopy (TEM) - Principle, Instrumentation, applications. Auger electron spectroscopy (AES) - Principle, Instrumentation, applications.

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

Scanning probe microscopy Techniques: Atomic Force Microscopy - Principle, Instrumentation, applications.

AC(CB1)-08: Diffraction Methods, X-Ray Absorption and X-Ray Fluorescence — 15 Hrs

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

Electron Diffraction by gases: Principle; Advantages; Radial distribution curves – Interpretation of results for $PBrF_2S$, PF_3S, PF_2HS; Limitations – $HClO_4$, Silylmonothioacetate and Germylmonothioacetate and $HgCl_2$ molecules.

Neutron Diffraction: Principle, Application in Hydrogen bonding studies, combined use of X – ray and Neutron diffraction studies, 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(CB1)-09: 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

1. Structural Methods in Inorganic Chemistry: E.A.V. Ebsworth, David W H Rankin, Stephen Cradock, Second edition,Blackwell Publishers, 1991.
2. Physical Methods in Chemistry - R.S. Drago, W.B. Saunders Co.(1977).
3. Instrumental Methods & Chemical Analysis – Galen Ewing, 5th ed., McGraw-Hill Publishing Company Ltd.,(1985).
4. Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York(1994).
5. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers (1998)
6. Solid state Chemistry and its Applications : Anthony R.West, Second edition, Wiley Publishers (2022).
7. Introduction to Solids: Leonid V. Azaroff, McGraw-Hill Education-Europe, 2017.
8. Atkin's Physical Chemistry : Peter Atkins and Julio de Paula, Tenth edition, Oxford Publications (2019).
9. Basic Course in Crystallography: J.A.K. Tareen, T.R.N. Kutty, University Press (2001).
10. Solid State Chemistry : D.K. Chakrabarthy, 2nd Edition, New Age Science (2010).
11. Principles and practice of Analytical Chemistry, F.W.Fifield & D Kealey, 5th Ed.Blackwell Science (2000).
12. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork (2003).

PAPER III CH (AC) 303T (ELECTIVE III B):
CLASSICAL, ELECTROANALYTICAL AND SPECTROSCOPIC METHODS OF ANALYSIS

AC(CB1)-07: Titrimetric and Gravimetric analysis.
AC(CB1)-08: Electroanalytical Methods
AC(CB1)-09: Optical Methods

AC(CB1)-07: Titrimetric and Gravimetric analysis. **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 H_3PO_4. 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 (Mg^{2+}&Ca^{2+}; Pb^{2+}&Ca^{2+}; Mn^{2+}&Mg^{2+}), 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(CB1)-08: Electroanalytical Methods **15 Hrs**

pH-metry: Accuracy of direct potentiometer measurements. The Glass pH electrode – Theory, construction, standard buffers, accuracy of pH measurements, measurements with the pH – meter, pH titration of unknown soda ash.

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.

AC(CB1)-19: Optical Methods **15 Hrs**

Refractometry: Theory, instrumentation, specific and molecular refraction, Abbe, Pulfrich and immersiton types, applications

Polarimetry: Theoritical considerations – Plane polarized light, optical activity, specific and molecular rotations. Iinstrumentation,, applications.

Optical rotator dispersion and Circular dichorism: Optical rotation, circular birefringence, circular dichroism and Cotton effect, Octet Rule, Experimental Techniques, Applications : quantitative analysis,determination of absolute configuration, conformational studies and equilibrium studies. Use of CD in the conformational studies of metal complexes, DNA and DNA-metal complexes.

SUGGESTED BOOKS

1. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5th ed.,Longmann, ELBS Publications (2000).
2. Principles and practice of Analytical Chemistry, F.W.Fifield & D Kealey, 5th Ed.Blackwell Science (2000).
3. Quantitative Chemical Analysis, Daniel C. Harris, 6th Ed. WH Freeman & Co. NewYork (2003).
4. Instrumental Methods & Chemical Analysis – Galen Ewing, 5th ed., McGraw-HillPublishing Company Ltd.,(1985).
5. Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York(1994).
6. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College
   Publishers (1998).
7. Instrumental methods of Analysis - Willard, 6th ed., CBS Publishers &distributors (1986).
8. Analytical Chemisstry Instrumental techniques, Maninder Singh, DominentPublishers, New Delhi (2002).

PAPER IV CH (AC) 304T (ELECTIVE IV A): APPLIED ANALYSIS

AC(CB2)-10: Industrial Analysis
AC(CB2)-11: Food and Agricultural analysis
AC(CB2)-12: Analysis of Air and Water Pollutants and Sewage water treatment

AC(CB2)-10: 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 Cement: Composition of Portland cement, estimation of Aluminium oxide and Ferrous oxide. Determination of Alumina in Cement by Polarography.

Analysis of Oils & Fats: Theory, Melting point of fats, Chemical Characteristics: Saponification value, Iodine value,
Thiocyanogen value, ketone or perfume rancidity. Analysis of fatty acid composition in oil by GLC, Oxidation levels of fats by TLC.

Soaps & Detergents: Composition of Soaps. Determination of low level Surfactants,determination of Germicides in soaps and detergents by photometric method, analysis of phosphates by paper chromatography, determination of detergent alkylates by Mass Spectrometry .

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.

Analysis of Pharmaceuticals : Determination of Calcium in Vitamin D and Calcium formulations (Complexometry), 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(CB2)-11: Food and Agricultural analysis — 15 Hrs

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 SO_2 & 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).

AC(CB2)-12: Analysis of Air and Water Pollutants and Sewage water treatment

15 Hrs

Water Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness

Treatment of Water for Municipal Supply: Characteristics of potable water/Domestic water, WHO standards and Indian Standards. Aeration, Sedimentation with coagulation, Filtration, Sterilization and Disinfection: Ozonization, Chlorination, Breakpoint chlorination and Dechlorination.

Desalination of Brackish Water: electrodialysis, and reverse osmosis (RO).

Mineral Water and Purified Water: Typical Manufacturing Process, Flow Sheet Diagram of Mineral Water Manufacturing Process.

Sewage Water Treatment: On-Site Sewage Treatment Systems and Off-Site Sewage Treatment Systems.

Analysis of air pollutants-SO_2 and H_2S by Spectrophotometry, NO-NO_x (Colorimetric technique- Saltzman method), CO & CO_2 (IR), Aromatic hydrocarbons in automobile exhaust (GC).

Analysis of Water Pollutants- Analysis of anions (CN^-, Cl^-, F^-, SO_4^{2-}, PO_4^{2-}.) and Toxic metals (Cd) by Spectrophotometry.

SUGGESTED BOOKS

1. Analytical Chemistry - Gary D. Christian, 6th Ed. John Wiley and sons. Inc, New York (1994).
2. Fundamentals of Analytical Chemistry, Skoog & West, 9th Ed, Cingage Learning (2022)
3. Pharmaceutical Drug Analysis, Ashtosh Kar, Second edition, New Age International Publishers (2020)
4. Vogel's Text Book of Quantitative Chemical Analysis, J Mendham, R C Denney, J D Barnes, M Thomas, B. Sivasankar, 6th Ed, Pearson Education Ltd (2009)
5. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd (1995).
6. Environmental Analytical Chemistry, F W Fifield, P J Haines, 2nd Ed, Wiley-Blackwell (2000).
7. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut (2014).
8. Handbook of Analysis and quality control for fruit and vegetable products, S Ranganna, Tata Mc Graw Hill Publishers Ltd. (1986).
9. Introduction to chemical analysis of foods, S Suzanna & Nielsen, CBS Publishers & Distributors.
10. Practical pharmaceutical Chemistry, a H Beckett and J B Stenlake, III Ed, Vol I and Vol II, CBS Publishers & Distributors (1997).
11. Pharmaceutical Analysis, David G Watson, Churchill Livingstone Harcourt Brace and Company Ltd, (1999).
12. A Textbook of Engineering Chemistry, Dr. Y. Bharathi Kumari and Dr. Jyotsna Cherukuri, VGS Publications, First Edison, India (2009).
13. Engineering Chemistry, Jain P C and Monica Jain, 15th Edition, Dhanpat Rai Publishing Company Ltd, New Delhi, India (2005).

14.Textbook of Engineering Chemistry, C Parameswara Murthy, C V Agarwal, Andra Naidu, BS Publications, Hyderabad, India.
15. Water Encyclopedia - Domestic, Municipal, and Industrial Water Supply and Waste Disposal, Jay H. Lehr and Jack Keeley, Wiley-Interscience, Published by John Wiley & Sons, Inc., Hoboken, New Jersey.
16. Handbook of Water and Wastewater Treatment Technologies, Nicholas P. Cheremisinoff, PublishedbyButterworth-Heinemann, 225Wildwood Avenue, Woburn, MA 01801-2041.
17. Purified water: https://en.wikipedia.org/wiki/Purified_water#Purification_methods.

PAPER-IV CH(IC) 304T (ELECTIVE IV B): NUCLEAR CHEMISTRY, ZEOLITES & SOLID STATE CHEMISTRY

AC(CB2)-10: Nuclear Chemistry
AC(CB2)-11: Zeolites and Molecular Sieves
AC(CB2)-12: Solid State Chemistry

AC(CB2)-10: Nuclear Chemistry — 15 Hrs

Nuclear Chemistry: Introduction, the atomic nucleus-elementary particles; classification of nuclides based of Z and N values; binding energy, nuclear stability-nuclear binding energy theory, meson theory of nuclear forces, nuclear shell structure theory, nuclear fluid theory; Isotopes- isotopic constitution of elements, whole number rule and packing fraction.

Radioactivity: α, β, γ rays, disintegration theory, modes of decay, group displacement law, radioactive decay kinetics, half-life period, average life period, radioactive equilibrium, radioactive disintegration series.

Nuclear transformation and artificial radioactivity-Artificial transmutation of elements, types of nuclear reactions, nuclear fission-atomic bomb, nuclear fusion – hydrogen bomb.

Applications of radio isotopes: Reaction mechanism, structure determination, surface area of a powder, isotope dilution analysis, neutron activation analysis, radiometric titrations, carbon dating. (Problems wherever necessary)

AC(CB2)-11: Zeolites and Molecular Sieves — 15 Hrs

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, examplels 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 żeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

AC(CB2)-12:Solid State Chemistry — 15 Hrs

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: 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.

SUGGESTED BOOKS

1. Essentials of nuclear chemistry, H.J.Arnikar, 5th Edition, New Age International Publishers (2022).
2. Text book of inorganic chemistry, P.L.Soni, Mohan Katyal, 20th Revised Edition, Sultan Chand & Sons (2022)
3. Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen ,Elseviver Pub. Amsterdam (2001).
4. Zeolites molecular sieves- Structure, chemistry and use, Breck.D.W, John Wiley & Sons N.Y. (1974).
5. Solid-State Chemistry an Introduction (2nd Edition) – Lasley Smart and Elaine Moore Chapman & Hall(1996)
6. Solid State Chemistry- D.K.Chakraborty (New Age International Pvt.Ltd. New Delhi, (2000)
7. Introduction to Soilds-L.V.Azaroff, Tata McGraw Hill Publication Ltd., New York (1960)
8. Principles of the Solid State-H.V.Keer , Wiley Eastern Ltd.New Delhi (1994).
9. Solid state Chemistry –N.B.Hannay , Prentice Hall, New Jersey (1967).
10. Chemisorption, B. M. W. Trapnell, Butterworths Scientific Publications, London(1955).
11. Adsorption on solids, VladimirPonec, Zlatko Knor, Slavoj Cerny, Butterworth & Co publishers (1974).
12. Catalysis: Principle and Applications, B. Viswanathan, S. Sivasanker, A. V. Ramaswamy, Narosa Publishing House(2002).

LABORATORY COURSE

Paper V CH (AC) 351P: Titrimetry, Solvent extraction and Chromatography
4 Hrs/Week

I. Titrimetry:

1. Soil Analysis: Determination of
   (i) Ca^{2+}, (ii) Mg^{2+}, (iii) CO_3^{2-} & HCO_3^-.
2. Cement Analysis:
   (i) Determination of Ca in Cement
3. Oil Analysis: Determination of
   (i) Saponification value and
   (ii) Iodine value of an oil sample

II Solvent extraction:

1. Determination of Pb using Dithiazone
2. Determination of Fe(II) using Oxine

III. Chromatography (Demonstration):

1. Separation of Co & Ni in Cellulose column
   (i) Column preparation and separation
   (ii) Analysis of eluents by titrimetry
2. Separation of amino acids in a mixture by TLC using Ninhydrin
3. Separation of and identification pigments in leaves by column chromatography
4. Separation of additives in Ink by GC.
5. Separation of synthetic corticosteroids in by HPLC.

Paper VI CH (AC) 352P: Spectrophotometry –I **4 Hrs/week**

I. Spectrophotometry:

1. Determination of Manganese in steel
2. Determination of Phosphorous in human serum
3. Determination of Nickel using DMG
4. Determination of pKa of an organic Indicator (Methyl Orange)
   (i) Evaluation of λ_{max} for HMR (λ_A) and MR− (λ_B)
   (ii) Verification of Beer's Law for HMR and MR− at both λ_{max} and determination of their relative amounts in the solution
5. Simultaneous determination of Cr and Mn in an admixture

(i) Determination of molar absorption coefficients and verification of additivity of absorbamces

(ii) Determination of Chromium and Manganese in a mixture
6. Determination of composition of Complex:
(i) Cu(II)-EDTA by Job's Method
(ii) Cu(II)-EDTA by Mole ratio Method
(iii) Fe(II)-o-Phen by Job's Method and
(iv) Fe(II)-o-Phen by Mole ratio Method

II. Atomic Absorption Spectroscopy
Determination of i) Fe, ii) Zn, iii) Cu, iv) Pb.

Paper VII CH(AC) 353P: Water analysis. **2 Hrs/week**

I Water analysis:

1. Determination of residual Chlorine in water by Iodometry
2. Determination of Dissolved Oxygen.
3. Determination of COD.
4. Determination of BOD.
5. Determination of fluoride ion
6. Determination of sulphate ion
7. Determination of hardness of water

Paper VIII CH(AC) 354P: Spectrophotometry I **2 Hrs/week**

I. Colorimetry:
1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of Paracetamol
4. Determination of Creatinine
5. Estimation of Ascorbic acid
6. Determination of protein by biurette method
7. Estimation of urea by diacetyl monoxime method

SUGGESTED BOOKS

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememan et.al., John Wiley & Sons (1984).
2. Analytical Chemistry by Gary D.Christian 6th Edition John Wiley & Sons Inc., New York (1994).
3. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rEdition Elbs Publication (1969).
4. Vogel's Text Book of Quantitative Inorganic Analysis Jeffery etal 4th edition Elbs Publications (1988).

5. Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd (2002).
6. Analytical Chemistry Theory and Practice by R.M. Verma 3rd Edn., CBS Publishers & Distributors (1994).
7. Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications (1997).
8. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 2nd edn. (1996)
9. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers (2001)
10. Separation methods, MN Sastri, 2nd edn, Himalaya Publishing House (1996)
11. Hand book of analysis and quality control for fruit and vegetable products. S. Ranganna, 2nd edn, Tata MCGraw-Hill Publishing Company (2002).
12. Gas Chromatography, Rajbir Singh, 1st edn, Mittal Publications (2002)

M.Sc. SEMESTER - IV
ANALYTICAL CHEMISTRY SPECIALIZATION

(For the batches admitted in academic year 2023-24 onwards under CBCS pattern)

PAPER I CH (AC) 401T (CORE): SPECTROSCOPIC METHODS OF ANALYSIS-II

AC-13: Electronic spectroscopy,
AC-14: IR & Raman spectroscopy
AC-15: Fluorimetry, Phosphorimetry, Nephelometry and Turbidimetry

AC – 13: Electronic spectroscopy — 15 Hrs

UV and visible spectroscopy: Beer Lamberts law, Real limitations to Beer's law, instrumentation for colorimetry and spectrophotometry – Numerical problems based on Beer'slaw, simultaneous & differential spectrophotometry. First derivative spectrophotometry. Classification of Electronic Spectra for Metal Complexes, Selection rules: Electric dipole transitions, Magnetic dipole transitions, Orbital selection rules, Spin selection rules, Relaxation in selection rules. Nature of electronic spectral bands: band widths, band intensities. Factors influencing band shapes: Jahn-Teller effect, Spectrochemical series, Nephelauxetic effect. Orgel diagrams for d^1-d^9 configurations in O_h and T_d geometries, Crystal field spectra of O_h and T_d metal complexes of 3d metals, Charge Transfer Spectra. Calculation of 10Dq values, Racah parameter (B') and Nephelauxetic ratio (β).

AC – 14: IR & Raman spectroscopy — 15 Hrs

IR Spectroscopy: Principle, instrumentation, sample handling, Fourier transform infrared spectroscopy- Principle, instrumentation & its advantages. IR in quantitative analysis. Applications of IR spectroscopy: structure analysis of organic compounds, inorganic molecules-sulphato, carbonato, nitrato & metal chelates - acetylacetanato complexes. Analysis of petroleum hydrocarbons, oil and grease contents by EPA method, Quantitative analysis of multi-component mixtures.

Raman Spectroscopy: Theory, Instrumentation, sample handling, Illumination diagnosis and structure analysis, polarization measurements, quantitative analysis, laser applications, Resonance Raman spectroscopy: Principle, theory and its applications.

AC –15: 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, spectroflourimeters and Phosphorimeters. Applications of fluorimetry- Determination of Inorganic cations, fluorimetric reagents. Fluorimetric determination of organic species – Thiamine, Aneurine Hydrochloride, Plolycyclic aromatic hydrocarbons. Phosphorimetry: Determination of Aspirin in blood serum. Chemiluminescence: Origin, measurements. Analytical applications - Atmospheric pollutants (Oxides of Nitrogen and Sulphur compounds, Ozone). Detection

in Gas chromatography, High performance liquid chromatography and Capillary electrophoresis. Detection of Enzyme reaction products. Immunoassay and Nucleic acid assays.

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

Suggested Books

1. Principles of Instrumental Analysis– Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers (1998).
2. Introduction to Ligand Fields – Figgis, Wiley Eastern Ltd (1966).
3. Inorganic Electronic Spectroscopy – A.B.P. Lever, Elsevier Publishing Company, London (1968).
4. Chemical Analysis – A. K. Srivatsava & Jain, 3rd ed., S. Chand & Company Ltd. (1977).
5. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle. Prentice hall, New Jersey, USA (1997).
6. Analytical Chemistry – Gary D. Christian, 6th ed, John Wiley and sons. Inc., New York (1994).
7. Analytical Chemistry – Skoog & West, 6th ed, W.B. Saunders (1998).
8. Infrared and Raman Spectra of Inorganic and Coordination Compounds, Kazuo Nakamoto, 5th ed., John Wiley & Sons (1995).
9. Vogel's Text book of Quantitative Analysis – J. Mendham et al, 6th ed., Pearson Education Ltd (2002).
10. Instrumental methods of Analysis - Willard, 6th ed., CBS Publishers & distributors (1986).
11. Analytical Chemistry Instrumental techniques, Maninder Singh, Dominent Publishers, New Delhi (2002).

PAPER II CH (AC) 402T (CORE): SEPARATION METHODS AND MASS SPECTROMETRY

AC-16: Solvent extractions & Chromatography-I
AC-17: Chromatography -II
AC-18: Advanced Mass spectrometry

AC-16: Solvent extractions & Chromatography-I **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. Applications to extractions of metal ions by chelating agent (Dithiazone, and cupferron) determination of alkaloids in crude drugs.

HPTLC: Principle, Technique, advantages over TLC

Gas Chromatography (GC) – Theory, Data acquisition and processing Applications, Monitoring of ethylene dibrombide (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.

AC –17: Chromatography - II **15 Hrs**

Supercritical fluid chromatography (SFC): Instrumentation of SFC, stationary and mobile phases used in SFC, Detectors, Advantages of SFC. Technique and applications of SFC.

Size Exclusion Chromatagraphy: Principle of Gel Chromatography, Filtration Chromatography, Instrumentation, retention behaviour, resolution, selection of gel type, applications. Ion Exclusion: Principle and applications.

Electrophoresis: Introduction, Definition

Paper Electrohoresis: 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

Ultra Performance Liquid Chromatography: Principle, Instrumentation

AC-18: Advanced Mass spectrometry **15 Hrs**

Introduction to Mass Spectrometry: Principle and Block diagram of mass spectrometer (MS)

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

Hyphenated Techniques: GC-MS Principle, Instrumentation, Interfaces- Direct coupling interface and Open split interface, Applications of GC-MS. **LC-MS-** Principle, Instrumentation – Interfaces- Moving belt interface, Particle beam interface, Thermospray interface, Electrospray interface, Atmospheric pressure chemical ionization interface, Applications of LC-MS. **ICP – MS** – Principle, Instrumentation, and Applications.

Tandem Mass Spectrometry (MS/MS or MS^2):,Principle, Instrumentation, Applications.

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

1. Separation Methods - M. N. Sastri, 1st ed., Himalaya Publishers (1991).
2. Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt CollegePublishers (1998).
3. Analytical Chemistry - Gary D.Christian, 6th ed, John Wiley and sons. Inc., New York, sixth edition (1994).
4. Mass spectrometry for Chemists and Biochemists, Robert A.W. Johnstone and Macolm.E. Rose, 2th ed Cambridge University Press (1996).
5. Structural methods in Inorganic chemistry - E.A.V. Ebsworth, et al ELBS Publications (1988)
6. Introduction to analytical Gas Chromatography, Raymond PW Scott,2nd Ed. MarcelDekker, Inc. New York (1988).
7. Techniques and practice of Chromatography, Raymond PW Scott, Marcel Dekker, Inc.New York (1995).
8. Liquid Chromatography-Mass Spectrometry Principles & Applications, WMA Neissen& JV Greef, Marcel Dekker, Inc. New York (1992).
9. Matrix-assisted laser desorption/ionization - https://en.wikipedia.org/wiki/Matrix-assisted_laser_desorption/ionization

PAPER III CH (AC) 403T (ELECTIVE IIIA): LABORATORY MANAGEMENT AND QUALITY ASSURANCE

AC(CB1)-19: Laboratory Automation and Management, LIMS and Computer aided Analysis
AC(CB1) -20: Quality Control and Quality Assurance
AC(CB1)-21: Quality Standards, Management and Accreditation

AC(CB1)-19: Laboratory Automation and Management, LIMS and Computer aided Analysis **15 Hrs**

Laboratory Automation: Introduction, classification of Analytical methods, Types of instrumental methods, Instruments for analysis. Planning for laboratory automation. An overview of automatic instruments & instrumentation. Flow Injection Analysis, Discrete Automatic systems.

Laboratory Management Introduction – Administration, Geographical location, Internal organization of the laboratory, Architectural issues, laboratory infrastructure of equipment and instrumentation. Relationship with the industrial exploratory, regulatory work and the analytical laboratory. Disciplines represented in the Laboratory. Educational requirements of the laboratory personnel. Regular academic research work, work load statistics and coordination between routine work and research cell. opportunities for training.

Good laboratory practices: Instrumental standardization, optimization of procedures. Quality Programme, Instrument and Organisation calibration, Customer Satisfaction.

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,

AC(CB1) -20: Quality Control and Quality Assurance **15 Hrs**

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 blind samples 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.,).

Documentation for quality assurance: Raw Data - Type of notebooks, control of note book distribution and data entry. General Reagents and volumetric reagents. Sampling – sampling methods, sample labeling, sample log-in/register. Sample analysis, reporting, recording and personal training. Filing quality assurance documentation. Data

Acquisition. Quality control data and calculations. Computer generated analytical reports. Security considerations.

Establishing a Quality Assurance program: Management commitment. Define the quality assurance program. Writing standard operating procedures. Topics for standard operating procedures. Consolidating the programme. Monitoring the program – monitoring quality assurance data, reporting quality assurance problems. Writing the quality assurance manuals.

AC(CB1)-21: Quality Standards, Management and Accreditation **15 Hrs**

Analytical Methods: Choosing the methods- standard methods, official methods, literature methods. Validation of new methods - comparison of analytical methods. 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.

Standard reference materials: Standards of Analysis, Analytical standards, reference materials, High purity substances, working and secondary standards.

Quality Management: Quality systems, the operational aspects required to deliver a quality system (Traceability, quality control, quality assurance, quality management and quality manual) calibration and test methods. Total Quality Management (TQM) – Essentials of TQM: Quality Planning, Quality control, Quality Audit, Quality surveillance, Quality assurance, Quality circles.

Laboratory Accreditation: International organization for standardization, National accreditation board for testing and calibration laboratories. Need for laboratory accreditation. International aspects of laboratory accreditation and in India. Criteria for laboratory accreditation. Benefits of laboratory accreditation. Introduction to ISO 9000, ISO 9000-2000 series of standards on quality management system, Introduction to ISO organization, Registration / certification, Structure of ISO 9000-2000 family of standards. Advantages of ISO 9000-2000. Requirements of ISO 9001-2000 Significance of ISO 9001, 9002, 9003 & 9004. Requirements of ISO9000/IS14001.

Suggested Books

1. Principles of Instrumental Analysis - Skoog. Holler, Nieman, 5th ed., Harcourt College Publishers (1998).
2. Model for Quality assurance in design/development production, installation and servicing, ISO 9001.
3. Journal of Validation technology, Vol.-III and IV (1997).
4. Instrumental Methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors (1986).
5. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed. Frank Settle, Prentice Hall, New Jersey, USA (1997).
6. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York (1986).
7. Quality in Totality – Parag Diwan, Deep & Deep Publications, 1st ed. (2000).

8. QA manual – DH Shah, Business Horizons, 1st ed. (2000).
9. Applying ISO-9000 Quality Management Systems, International Trade Centre Publishing, UNCTAD/WTO. Geneva, Switzerland, Indian Edition Printed by D.L.Shah Trust.
10. How to practice GLP, PP Sharma, Vandana Publications, New Delhi (2000),
11. Training manuals on ISO 9000 / 2000 PQM, Girdhar J Gyani, Raj Publishing House, (2001)
12. Quality Assurance in Analytical Chemistry, B.W. Wenclawiak, Springer India (2004).

PAPER III CH(AC) 403T (ELECTIVE III B): APPLIED ANALYSIS AND GREEN ANALYTICAL CHEMISTRY

AC(CB1)-19: Enzyme catalysis- Analytical applications
AC(CB1)-20: Forensic Chemical Analysis
AC(CB1)-21: Green Analytical Chemistry

AC(CB1)-19: Enzyme catalysis- Analytical applications — 15 Hrs

Basic principles, Catalysis – measurement of catalytic reactions, Non-specificity of catalysts, types of reactions catalyzed. Enzyme catalysis, enzyme kinetics, properties of enzymes, enzyme inhibitors and activators, enzyme specificity, Determination of enzymes and enzyme substrates. Example of enzymatic analysis: Dehydrogenase reactions, Substrate determinations: Glucose, Uric acid. Immobilized enzymes. Evaluation methods.

AC(CB1)-20: Forensic Chemical Analysis — 15 Hrs

Contact traces – Analysis of soil, fibre and paint evidence in forensic work.

Analysis of narcotic drugs and psychotropic substances (opiates, cannabinoids, barbiturates, benzodiazepines, amphetamimes 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(CB1)-21: Green Analytical Chemistry — 15 Hrs

Green Analytical Chemistry: Concepts and trends

"Greening" Sample Treatment: Reduced and solvent- free sample preparation methodologies, alternative solvents, energy saving procedures.

Green Instrumental Analysis: Assessment of analytical methods for "Greenness", greening flow injection analysis, chemical sensors, liquid green chromatography.

Suggested Books

1. Analytical Chemistry - Gary D. Christian, 6th ed. John Wiley and sons. Inc, New York (1994).
2. Kinetics methods of analysis – Marck & Rekniz Vol.25
3. Practical Pharmaceutical Chemistry, A.H. Beckett et al, 3rd ed. – Vol. 1 & Vol. 2 CBS Publishers & distributors (1986).
4. Green Analytical Chemistry: Theory & Practice, Miguel De La Guardia, Sergio Armenta, Elsevier (2010)
5. Green Analytical Chemistry, Mihkel Koel, Mihkel Kaljurand, RSC Publishing (2010)

LABORATORY COURSE

Paper IV CH (AC) 451P: Electro analytical techniques - I **4 Hrs/week**

I. POTENTIOMETRY:

1. Determination of Ferrous using $K_2Cr_2O_7$
2. Determination of iron in iron wire using KMnO4
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. Preparation of carbonate free base, Standardization of base
5. Determination of Dissociation constants of Histidine monohydrochloride
6. Determination of binary stability constants of Cu(II) – Histidine complex

III.POLAROGRAPHY:

1. Polarographic determination of Cu & Zn in brass

Paper V CH (AC) 452P: Evaluation of Physical Parameters of Tablets, Spectroscopic Techniques and problems **4 Hrs/week**

I. 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.

II. FLUORIMETRY

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

III. FLAME PHOTOMETRY:

1. Determination of i)Na, ii)K, iii)Ca, iv)Li

IV. STRUCTURAL ELUCIDATION - based on spectral data from UV-Vis, IR, NMR and Mass Spectrometry (Minimum of five problems)

Paper VI CH (AC) 453P: Electro analytical techniques - I **2 Hrs/week**

I. CONDUCTOMETRY:

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

SUGGESTED BOOKS

1. Chemistry Experiments for Instrumental Methods, Donald T Sawyer William R.Hememan etal John Wiley & Sons (1984).
2.Analytical Chemistry by Gary D.Christian 6th Edition , John Wiley&Sons Inc New York (1994).
3.A Text Book of Quantitative Inorganic Analysis by A.I. Vogel 3rd Edition Elbs Publication (1969).
4.Vogel's Text Book of Quantitative Inorganic Analysis Jeffery et.al 4th edition Elbs Publications (1988).
5.Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd (2002).
6.Analytical Chemistry Thoery and Practice by R.M. Verma 3rd Edn.CBS Publishers & Distrbutors (1994).
7.Comprehensive Experimental Chemistry by V.K. Ahluwalia etal New Age Publications (1997).
8.Laboratory hand Book of Instrumental Drug Analysis by B.G. Nagavi 2nd edn. (1996)
9. A Text Book of Quantitative Inorganic Analysis by A.I.Vogel 3rd Edition, ELBS Publication (1969).
10.Determination and use of Stability Constants – Martell and Motekaitis VCH Publishers INC (1988).
11.Metal Complexes in Aqueous Solutions A.E.Martell and R.D. Handcock, Plenum Press, New York (1996).
12.Experiments in Chemistry, D.V. Jahagirdar, 2nd edn, Himalaya Publishing House, (2003)
13.Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4thedn. CBS publishers (2001)

CH(IC) 454P: PROJECT **12 Hrs/Week**

Marks Distribution for Project Assessment

INTERNAL ASSESSMENT

Research Design Seminar	1 credit	25 marks
Progress Seminar	1 credit	25 marks

SEMESTER END ASSESSMENT

Dissertation	1 credit	50 marks
Final presentation	2 credits	50 marks
Viva Voce during final presentation	1 credit	25 marks

M.Sc. CHEMISTRY

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

FOR STUDENTS ADMITTED FROM THE YEAR 2023-24 ONWARDS

M.Sc. CHEMISTRY
INORGANIC CHEMISTRY SPECIALISATION

Syllabus for III and IV Semesters
[Under Restructured CBCS Scheme]
(for the batches admitted in academic year 2023-24 onwards under CBCS pattern)
Grand total marks and credits (all 4 semesters) 2400 marks – 80 credits

(Approved in the P.G. BOS meeting held on 27-01-24)

Semester - III (Inorganic Chemistry)

	Instructions Hrs / Week	Internal assessment	Semester exam	Total	Credits
CH(IC)301T (core)	3	50 marks	50 marks	100 marks	3
CH(IC)302T (core)	3	50 marks	50 marks	100 marks	3
CH(IC)303T(Elective)	3	50 marks	50 marks	100 marks	3
CH(IC)304T(Elective)	3	50 marks	50 marks	100 marks	3
CH351P (IC LAB 1)	4		50 marks	50 marks	2
CH352P (IC LAB 2)	4		50 marks	50 marks	2
CH353P (IC LAB 3)	2		25 marks	25 marks	1
CH354P (IC LAB 4)	2		25 marks	25 marks	1
Seminar	2		50 Marks	50 Marks	2
Total	26			**600 marks**	**20**

Semester - IV (Inorganic Chemistry))

	Instructions Hrs / Week	Internal assessment	Semester exam	Total	Credits
CH(IC)401T (core)	3	50 marks	50 marks	100 marks	3
CH(IC)402T (core)	3	50 marks	50 marks	100 marks	3
CH(IC)403T (Elective)	3	50 marks	50 marks	100 marks	3
CH451P (IC LAB 1)	4		50 marks	50 marks	2
CH452P (IC LAB 2)	4		50 marks	50 marks	2
CH453P (IC LAB 3)	2		25 marks	25 marks	1
CH454P (Project)	12	50 marks	125 marks	175 marks	6
Total	31			**600 marks**	**20**

Grand total marks and credits (all 4 semesters) 2400 marks - 80 credits

M.Sc. SEMESTER III
INORGANIC CHEMISTRY SPECIALISATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH(IC)301T (CORE): BONDING, GROUP THEORY AND ITS APPLICATIONS

IC - 07: Group Theory, Normal mode analysis and Spectral Activity
IC - 08: MOT of Metal Complexes
IC - 09: Electronic Spectroscopy of Metal Complexes

PAPER II CH(IC)302T (CORE): MOLECULAR SPECTROSCOPY OF INORGANIC COMPOUNDS

IC -10: NMR and NQR of Inorganic compounds
IC - 11: Applications of ESR to Metal Complexes
IC -12: Mossbauer and Photo Electron Spectroscopy.

PAPER III CH(IC) 303T (ELECTIVE IIIA) : ANALYTICAL TECHNIQUES-I

IC(CB1)-13: AAS, AES, ICP-AES and Flame Photometry
IC(CB1)-14: Diffraction Methods
IC(CB1)-15: Advanced Mass spectrometry

PAPER III CH(IC) 303T (ELECTIVE IIIB): SUPRAMOLECULAR, GREEN CHEMISTRY, NUCLEAR CHEMISTRY

IC(CB1)- 13: Supramolecular Chemistry
IC(CB1)- 14: Green Chemistry
IC(CB1)- 15: Nuclear Chemistry

PAPER IV CH (IC) 304T (ELECTIVE IVA): ANALYTICAL TECHNIQUES-II

IC(CB2) -16: Data Handling
IC(CB2)- 17: Thermal Methods
IC(CB2)- 18: Advanced Separation Techniques

PAPER IV CH (IC) 304T ELECTIVE IVB: APPLIED ANALYSIS

IC(CB2)-16: Clinical and Pharmaceutical Analysis
IC(CB2)-17: Food and Agricultural Analysis
IC(CB2)-18: Water Treatment and Analysis of Air/Water Pollutants

LABORATORY COURSES

PAPER V CH (IC) 351 P: Synthesis and Characterization of Metal Complexes
PAPER VI CH (IC) 352 P: Electro-analytical techniques-I
PAPER VII CH (IC) 353 P: Estimation of Metal and Ligands in Complexes
PAPER VIII CH (IC) 354 P: Electro-analytical techniques-II

SEMINAR

M.Sc. SEMESTER IV
INORGANIC CHEMISTRY SPECIALISATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH(IC) 401T (CORE): ORGANO METALLIC CHEMISTRY OF TRANSITION METAL COMPLEXES

IC -19: Mono, Di, Tri Tetra, Penta, Hexa hapto Complexes: Structure and Bonding.
IC- 20: Catalytic Role of OTMC-I
IC -21: Catalytic Role of OTMC-II

PAPER II CH(IC) 402T (CORE): BIOINORGANIC CHEMISTRY

IC-22: Transport of Oxygen, Electrons and Metal ions
IC-23: Metallo Enzymes of Iron, Zinc and Nickel
IC-24: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese

PAPER III CH(IC) 403T (ELECTIVE III A): MEDICINAL INORGANIC CHEMISTRY AND PHOTOCHEMISTRY

IC(CB1)-25: Metal ion interactions with nucleic acids and their Spectroscopic analysis
IC(CB1)-26: Metal complexes in Clinical Chemistry
IC(CB1)-27: Photochemistry of Metal Complexes

PAPER III CH(IC) 403T (ELECTIVE III B): INORGANIC MATERIAL CHEMISTRY

IC(CB1)-25: Solid State Chemistry
IC(CB1)-26: Nanotechnology
IC(CB1)-27: Liquid Crystals

LABORATORY COURSES

PAPER IV CH (IC) 451P: Conventional methods of analysis
Paper V CH (IC) 452P: Spectroscopic techniques-I
Paper VI CH (IC) 453P: Spectroscopic techniques-II

PROJECT CH (IC) 454P

M.Sc. INORGANIC CHEMISTRY SPECIALIZATION
SEMESTER-III

PAPER I CH(IC)301T (CORE): BONDING GROUP THEORY AND ITS APPLICATIONS

IC-07: Group Theory, Normal mode analysis and Spectral Activity
IC-08: MOT of Metal Complexes
IC-09: Electronic Spectroscopy of Metal Complexes

IC-07: Group Theory, Normal Mode Analysis and Spectral Activity — 15 Hrs

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} groups. Matrix representation of symmetry elements *E*, C_n, S_n, i and σ elements. Reducible and irreducible representations, properties of irreducible representations, construction of character tables for: C_{2v}, C_{2h} and C_{3v} groups. 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, cis-N_2F_2 , ClF_3), C_{3v}(eg. $NH_3, POCl_3$), C_{2h} (trans-N_2F_2), D_{3h} (BF_3), Td (SO_4^{2-}), Oh (SF_6). Internal coordinate method of analysis for C_{2v} (H_2O), C_{3v} (NH_3), C_{2h} (trans-N_2F_2).

Direct product – symmetry requirements for overtones, binary and ternary combination bands. Normal mode analysis-Structure Fitting, Effect of Coordination on Ligand Vibrations: ammine, aquo and carbonyl complexes. Assigning Denticity of Ligands (SO_4^{2-}, CO_3^{2-}).

IC-08: Molecular Orbital Theory of Metal Complexes — 15 Hrs

Limitations of crystal field theory, Adjustments to the crystal field theory to allow for covalence - The Adjusted Crystal Field Theory. Experimental evidences for metal ligand orbital overlap. Introduction to molecular orbital theory, in-phase and out-of-phase combination of atomic orbitals. Symmetry classification of metal orbitals in cubic and non-cubic environments: Octahedral, Tetrahedral, Square planar, Square pyramidal and Trigonal bipyramidal geometries – Concept of ligand group orbitals (LGOs), symmetry classification of ligand group orbitals in Octahedral, Tetrahedral, and Square planar geometries. Construction of molecular orbital energy level diagrams (MOED): Octahedral metal complexes with (i) Sigma (σ), (ii) sigma(σ) &Pi (π) and (iii) sigma (σ), Pi (π) and Pi* (π*) bonding contribution from the Ligands - Tetrahedral Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi (π), and Square Planar Metal Complexes with (i) Sigma (σ) and (ii) sigma(σ) &Pi (π) bonding contribution from the ligands - Molecular orbital electron configurations and calculation of Magnetic Moments.

IC-09: Electronic Spectroscopy of Metal Complexes — 15 Hrs

Classification of Electronic spectra for metal complexes, selection rules: Electric dipole transitions, Magnetic dipole transitions, orbital selection rules, spin selection rules, relaxation in selection rules. Nature of electronic spectral bands: Band widths, band

intensities. Factors influencing band shapes: Jahn-Teller effect, Spectrochemical series, Nephelauxetic effect. Orgel diagrams for d^1-d^9 configurations, Crystal field spectra of O_h and T_d metal complexes of 3d metals. Charge transfer spectra. Strong field configurations: The method of descending symmetry, Correlation diagrams for d^2 and d^8 configurations in O_h and T_d. Tanabe-Sugano diagrams for d^2 and d^8 Configurations. Calculation of 10Dq Values, Racah Parameter (B') and Nephelauxetic Ratio (β).

SUGGESTED BOOKS

1. Symmetry and Spectroscopy of Molecules, K. Veera Reddy, 2nd Edition, New Age International (P) Limited Publishers (2009)
2. Chemical Applications of Group Theory, F. A. Cotton, 3rd edition, Wiley NY (1990)
3. Symmetry and Group Theory In Chemistry, Mark Ladd, Harwood Publishers, London (2000)
4. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
5. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998)
6. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991)
7. Molecular Symmetry- Anintroduction to Group theory and its uses in chemistry, David S. Schoenland, Van Norstrand series, (1965).
8. Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier (1984).
9. Introduction to Ligand fields, B. N. Figgis, Interscience publishers, (1966)
10. Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds, K. Nakamoto, Wiley, (2009).
11. Infrared spectra of complex molecules, L.J.Bellamy. Chapman and Hall, 3rd edition, (1975).

PAPER II CH(IC)302T (CORE): MOLECULAR SPECTROSCOPY OF INORGANIC COMPOUNDS

IC-10: NMR and NQR of Inorganic compounds
IC-11: Applications of ESR to Metal Complexes
IC-12: Mossbauer and Photo Electron Spectroscopy

IC-10: NMR and NQR of Inorganic compounds — 15Hrs

Nuclear Magnetic resonance Spectroscopy: Principle, magnetic vs chemical equivalence - F_2POPF_2, $[H_2P_2O_7]^{2-}$. Virtual coupling and its importance in study of metal complexes - $[Pd\{P(CH_3)_3\}_2I_2]$. Spin dilute systems-satellites in Pt(II) complexes cis-$[Pt(PEt_3)_2Cl_2]$, $Sn(CH_3)_4$, $(CF_3)_2Hg$. NMR time scale and its use in studying stereo chemical non –rigidity - (PF_5, $[Rh(PR_3)_5]^+$.
^{1}H-NMR of [PtHCl(PEt$_3$)], $[Pt(NH_3)_3(CH_3)_3]$, BH_4^-, NH_4^+, [^{6}η-$C_7H_8Mo(CO)_3$], [^{7}η-$C_7H_7Mo(CO)_3]^+$, B_2H_6, $^{29}SiH_3SiH_3$.
^{19}F NMR of BF_4^- , H_2PF_3, $HPOF_2$, IF_5, $(CH_3)_2PF_3$.
^{31}P NMR of $[Mo(CO)_3(PPh_3)_3]$, [Rh (PPh_3)$_3$Cl], trans-$[PtCl_4(PEt_3)_2]$, $PF_2H(^{15}NH_2)_2$
^{13}C NMR of [^{4}η $C_8H_8Ru(CO)_3$], FeICp(CO)$_{12}$, [$^{13}C^{15}NCo(DH)_2$pyridine],
$^{13}C\{^1H\}$ NMR spectrum of σ-bonded C_6H_5 ligand.
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)
Nuclear Quadrupole Resonance Spectroscopy: Principle, nuclear quadrupole resonance experiment, Structural information from NQR spectra- $PFCl_4$, PCl_4Ph, $Ga_2Cl_7^-$ and $TeCl_4$ Interpretation of nuclear quadrupole coupling constants.

IC-11: Applications of ESR to Metal Complexes — 15 Hrs

Principle; Selection Rules; Instrumentation; Application of ESR to the study of simple free radicals - methyl ($CH_3^{\cdot}$), amine ($NH_2\cdot$), diphenylpicrylhydrazyl, cyclopentadienyl ($C_5H_5^{\cdot}$), hydroxy methyl ($CH_2OH\cdot$) radicals; Zero-Field Splitting (ZFS) and Kramer's degeneracy; Effective Spin ; ESR Spectra of d^1-d^9 Transition metal complexes with examples; Calculation of g values with simple examples; Interpretation of g in cubic, axial and rhombohedral geometries; Intensities of $g_{\parallel}$ and $g_{\perp}$peaks; Evidence for metal-ligand bond covalency – Cu(II)-bis-salicylaldimine, Cu(II)-diethyldithiophosphinate,Vanadyldithiophosphinate,Cu(II)-tetraphenylporphyrin, Co(II)-phthalocyanine and $K_2[IrCl_6]$; Application of ESR in structure determination - $[(NH_3)_5\ Co\ O_2\ Co\ (NH_3)_5]^{5+}$; Calculation of 'g' and 'A' values from esr spectral data in i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}. ESR spectra of dinuclear Cu (II) complexes.

IC-12: Mossbauer and Photoelectron Spectroscopy — 15 Hrs

Mossbauer Spectroscopy: Principle, Experimental considerations and presentation of the spectrum, Isomer shifts – Quadrupole splitting and magnetic hyperfine splitting, Selection rules.

Applications: (i) Iron compounds: Low-spin and high-spin Fe(II) and Fe(III) complexes - π-bonding effects in iron complexes, Study of high-spin low-spin cross-over, diamagnetic and covalent compounds, structural aspects of iron carbonyls and iron-sulphur proteins. (ii) Tin compounds: Tin halides and organo-tin compounds. (iii) 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^+.

Photoelectron Spectroscopy: Principle and instrumentation, types of photoelectron spectroscopy – UPS & XPS. Binding energies, Koopman's theorem, Chemical shifts. Photoelectron spectra of simple molecules: N_2, O_2, and F_2. Vibrational structure of PES bands, potential energy curves, interpretation of vibrational spectral data for ionized (M^+) species, prediction of nature of molecular orbitals. ESCA in qualitative analysis. Principles of Auger electron spectroscopy.

SUGGESTED BOOKS

1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, ELBS, Blackwell Scientific publications (1987).
2. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., (1977).
3. Physical Methods for Chemists, Russell S. Drago Second edition, Saunders College Publishing (1992).
4. Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, D.N. Satyanarayana, Dreamtech press, Wiley (2022).
5. Magneto Chemistry, Dutta & Shyamal, Oxford Chemistry Primers, Vol 62 (1993).
6. Instrumental Methods of Chemical Analysis, Gurdeep R Chatwal, Sham K. Anand, Himalaya Publishing House, (2019)
7. Principles of Mossbauer spectroscopy, T. C. Gibb, Chapman and Hall, London, (1976).
8. Mossbauer Spectroscopy, N. N. Greenwood and T. C. Gibb, Chapman and Hall, London, (1971).
9. Principles of Instrumental Analysis, Skoog, Holler and Nieman, Harcourt Asia PTE Ltd. (1998)
10. Hand book of Instrumental Techniques for Analytical Chemistry, Frank Settle, Prentice Hall (1997).
11. Physical Methods in Advanced Inorganic Chemistry, Hill and Day, Interscience publishers (1968).
12. International series of Monographs, Vol. 53: Photoelectron Spectroscopy, Edited by D Beckerand D. Betteridge (1972).

PAPER III CH(IC) 303T (ELECTIVE IIIA) : ANALYTICAL TECHNIQUES - I

IC(CB1)-13 AAS, AES, ICP-AES and Flame Photometry
IC(CB1)-14: Diffraction Methods
IC(CB1)-15: Advanced Mass spectrometry

IC(CB1)-13: AAS, AES, ICP-AES and Flame Photometry — 15 Hrs

Atomic Absorption Spectroscopy (AAS): Principles of AAS, Instrumentation – flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS, interferences in flame AAS–chemical and spectral. interferences in furnace AAS-Use of platform atomization, chemical modifiers and background correction, evaluation methods in AAS and application in qualitative and quantitative analysis- Estimation of micronutrients by AAS
Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation, evaluation methods, Application in quantitative analysis.
Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES): Limitations of AES, Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source, ICP-AES – Instrumentation. Application of ICP-AES, Comparison with AAS.
Flame Photometry: Principle, Theory, Instrumentation and Applications

IC(CB1)-14 : Diffraction Methods — 15 Hrs

X – ray Diffraction: X –rays and their generation – choice of radiation; Miller indices; Braggs equation; Experimental methods – Powder and single crystal methods; Indexing the reflections; Systematic absences; Electron density studies by X – rays – Platinum phthalocyanine complex, Advantages and limitations of X – ray Diffraction.
Electron Diffraction by gases: Principle; Advantages; Radial distribution curves – Interpretation of results for $PBrF_2S$, PF_3S, PF_2HS ; Limitations – $HClO_4$, Silylmonothioacetate and Germylmonothioacetate and $HgCl_2$ molecules.

Neutron Diffraction: Principle, Application in Hydrogen bonding studies, combined use of X – ray and Neutron diffraction studies, Advantages and limitations.

IC(CB1)-15: Advanced Mass spectrometry — 15 Hrs

Introduction to Mass Spectrometry: Principle and Block diagram of mass spectrometer (MS)
Mass Analyzers: Quadruple, Ion traps, Time of flight (TOF) mass analyzers
Hyphenated Techniques:
GC-MS Principle, Instrumentation, Interfaces- Direct coupling interface and Open split interface, Applications of GC-MS.
LC-MS- Principle, Instrumentation – Interfaces- Moving belt interface, Particle beam interface, Thermospray interface, Electrospray interface, Atmospheric pressure chemical ionization interface, Applications of LC-MS.
ICP – MS – Principle, Instrumentation, and Applications.
Tandem Mass Spectrometry (MS/MS or MS^2): Principle, Instrumentation, Applications.
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 BOOK

1.Analytical Chemistry, Gary Christian, VI Edition, John Wiley & Sons (2007)
2.Instrumental Methods of Chemical Analysis, H. Kaur. Pragati Prakashan (2012)
3.Vogel's Text Book of Quantitative Chemical Analysis, 6th Edition, Pearson Education Ltd. (2000)
4.Principles of Instrumental Analysis Douglas A. Skoog, F.James Holler, Timothy A. Nieman, Saunders College Publishers, (1998)
5.Hand book of Instrumental Techniques for Analytical Chemistry, Frank A. Settle, Prentice Hall, (1997)
6.Principles of Analytical Chemistry, M Valcarcel. Springer Berlin, Heidelberg, (2000)
7.Solid state Chemistry and its Applications: Anthony R. West, Second edition, Wiley Publishers, (2022).
8.Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, David W H Rankin, Stephen Cradock, 2nd Edition, Blackwell Publishers, (1991).
9.Introduction to Solids, Leonid V. Azaroff, McGraw-Hill Education-Europe, (2017).
10.Physical Chemistry, Peter Atkins and Julio de Paula, Tenth edition, Oxford University Press, (2019).
11.Basic Course in Crystallography, J.A.K. Tareen, T.R.N. Kutty, University Press, (2001).
12.Solid State Chemistry, D.K. Chakrabarthy, 2nd Edition, New Age Science, (2010).
13.Physical Methods in advanced Inorganic Chemistry, H.A.O. Hill, P.Day, Interscience Publishers, (1968)
14.Instrumental Methods of Analysis, Willard, Merrit, Dean, and Settle, Seventh Edition, CBS Publishers, (2004)
15.Mass spectrometry for Chemists and Biochemists, Malcolm E. Rose, Robert A. W. Johnstone, 2nd Edition, Cambridge University Press, (1996)
16.Physical methods for Chemists, Russell S. Drago, 2nd Edition, Saunders College Publishing, (1992)
17. Mass Spectrometry Basics, Christopher G Herbert, Robert A.W. Johnstone, 1st Edition, CRC Press, (2002)
18.Mass Spectrometry-A Textbook by Jürgen H. Gross, 3rd Edition, Springer-Verlag Berlin Heidelberg, (2018)
20.Matrix-assisted laser desorption/ionization - https://en.wikipedia.org/wiki/Matrix-assisted_laser_desorption/ionization

PAPER III CH(IC) 303T (ELECTIVE IIIB) : SUPRAMOLECULAR, GREEN CHEMISTRY, NUCLEAR CHEMISTRY

IC(CB1)-13: Supramolecular Chemistry
IC(CB1)-14: Green Chemistry
IC(CB1)-15: Nuclear Chemistry

IC(CB1)-13: Supramolecular Chemistry — 15 Hrs

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 thermodynamics 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 electrostatic 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(CB1)-14: Green Chemistry — 15 Hrs

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-metallocene catalysis.

IC(CB1)-15: Nuclear Chemistry — 15 Hrs

Nuclear Chemistry: Introduction, the atomic nucleus-elementary particles; classification of nuclides based on Z and N values; binding energy, nuclear stability-nuclear binding energy theory, meson theory of nuclear forces, nuclear shell structure theory, nuclear fluid theory; Isotopes- isotopic constitution of elements, whole number rule and packing fraction; **Radioactivity**-α, β, γ rays, disintegration theory, modes of decay, group displacement law, radioactive decay kinetics, half-life period, average life period, radioactive equilibrium, radioactive disintegration series.

Nuclear transformation and artificial radioactivity-Artificial transmutation of elements, types of nuclear reactions, nuclear fission-atomic bomb, nuclear fusion – hydrogen bomb. **Applications of radio isotopes**: Reaction mechanism, structure determination, surface area of a powder, isotope dilution analysis, neutron activation analysis, radiometric titrations, carbon dating. (Problems wherever necessary)

SUGGESTED BOOKS

1. Supramolecular Chemistry – Concepts and Perspectives, Jean-Marie Lehn, 1st Edition, Wiley-VCH Verlag GmbH, (1995)
2. Principles and methods in Supramolecular chemistry, Hans-Jorg Schneider and A. Yatsimirsky, John Wiley and Sons, (2000)
3. Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M. Khopkar, 2nd Edition, Narosa Publishing House, (2005)
4. Green Chemistry- An Introductory text, Mike Lancaster, 2nd Edition, RSC, (2010).
5. Essentials of nuclear chemistry, H.J.Arnikar, 5th Edition, New Age International Publishers (2022)
6. Text book of inorganic chemistry, P.L.Soni, Mohan Katyal, 20th Revised Edition, Sultan Chand & Sons (2022)

PAPER IV CH (IC) 304T (ELECTIVE IVA): ANALYTICAL TECHNIQUES - II

IC(CB2)-16: Data Handling
IC(CB2)-17: Thermal Methods
IC(CB2)-18: Advanced Separation Techniques

IC(CB2)-16: Data Handling — 15 Hrs

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, Absolute and relative uncertainty

Comparison of results – student's t-test (when the reference value is known, comparison of means of two methods, paired 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(CB2)-17: Thermal Methods — 15 Hrs

Thermogravimetric analysis (TGA): Principle, Instrumentation- working function of each co1nponent, Applications of TOA - study of oxalates, nitrates, chromates and sulphates, determination of carbon black in polythene.

Differential thermal analysis (DTA): Principle, Instrumentation, Methodology, Applications - Differential thermogram of sulphur, TG and DT A of manganese phosphine monohydrate.

Differential scanning calorimetry (DSC): Principle, Instrumentation - power compensated DSC instrument and Heat flow DSC instrument, Methodology, 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 TOA/MS and TGA/FTIR, High resolution TGA, Microthermal analysis.

IC(CB2)-18: Advanced Separation Techniques — 15 Hrs

Introduction, classification of chromatographic techniques

Separations by extractions: Solid phase extraction- Principle, methodology, applications. Flow injection analysis-Types, applications.

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, dithiazone, 8-hydroxy quinoline and cupferron.

Affinity chromatography – Principle, methodology, Instrumentation and applications.

Chiral chromatography – Principle, Instrumentation and applications.

Size Exclusion Chromatography (SEC) or Gel – filtration Chromatography – Principles, Instrumentation, factors affecting SEC, 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 and applications of SFC.

SUGGESTED BOOKS

1. Principles of Instrumental Analysis: Holler, Skoog and Ccrouch, 6th edition, Cengage Learning (2007).
2. Instrumental methods of chemical analysis B.K. Sharma, 1st Edition, Krishna Prakashan Media p Ltd (2011)
3. Instrumental Methods of analysis, Willard Mersritt, Dean and Settle, 7th edition, CBS Publishers (1986).
4. Analytical Chemistry – Gary D. Christian, 6th ed., John Wiley and sons. Inc., New York (1994).
5. Instrumental methods of Analysis - Willard, Merit, Dean, 6th ed., CBS Publishers & distributors, (1986).
6. Hand Book for Instrumental Techniques for Analytical Chemistry, Ed: Frank Settle, Prentice Hall, New Jersey, USA, (1997).
7. Vogel's Text book of Quantitative Analysis – GJ Jeffery, J Bassett et al, 5th ed., Longmann, ELBS Publications, (2000).

PAPER IV CH (IC) 304T ELECTIVE IVB: APPLIED ANALYSIS

IC(CB2)-19: Clinical and Pharmaceutical Analysis
IC(CB2)-20: Food and Agricultural Analysis
IC(CB2)-21: Water Treatment and Analysis of Air/Water Pollutants

IC(CB2)-19:Clinical and Pharmaceutical Analysis — 15 Hrs

Clinical Analysis: Determination of the following by titrimetry: (1) Serum Calcium (2) Serum/Plasma Bicarbonate (3) Inorganic Phosphate.
Determination of serum Sodium and Potassium by Flamephotometry.
Determination of the following by spectrophotometry (1) Blood Glucose (2) Total serum Cholesterol (3) Total serum Protein (4) Blood Urea in Serum (5) Blood Creatinine

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 indipivefrin eye drops (GC), Assay of hydrocortisone cream. (HPLC). Impurity profiling of Propranolol (GC-MS), famotidine (LC-MS).

IC(CB2)-20: Food and Agricultural analysis — 15 Hrs

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 butylated hydroxy 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 and Fe
Analysis of Fertilizers – Moisture determination by Karl Fischer titration methods. Determination of Ammonical nitrogen and Ammonical nitrate nitrogen. Determination of total phosphates as P_2O_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(CB2)-21: Water Treatment and Analysis of Air/Water Pollutants — 15 Hrs

Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness.
Treatment of Water for Municipal Supply: Characteristics of potable water/Domestic water, WHO standards, and Indian Standards. Aeration, Sedimentation with coagulation, Filtration, Sterilization and Disinfection: Ozonation, Chlorination, Breakpoint chlorination and Dechlorination
Desalination of Brackish Water: electrodialysis, and reverse osmosis (RO).

Mineral Water and Purified Water: Typical Manufacturing Process, Flow Sheet Diagram of Mineral Water Manufacturing Process,

Sewage Water Treatment: On-Site Sewage Treatment Systems and Off-Site Sewage Treatment Systems.

Analysis of air pollutants- SO_2 and H_2S by Spectrophotometry, NO-NOx (Colorimetric technique- Saltzman method), CO & CO_2 (IR), Aromatic hydrocarbons in automobile exhaust (GC)

Analysis of Water Pollutants- Analysis of anions (CN^-, Cl^-, F^-, SO_4^{2-}, PO_4^{2-}.) and Toxic metals (Cd) by Spectrophotometry

SUGGESTED BOOKS

1. Medical Laboratory Technology, Mukherjee, Tata McGraw Hill Education, (1988)
2. Medical Laboratory Technology, Ramnik Sood, Medical Publishers Pvt. Ltd. (1999)
3. Biochemical Methods, S. Sadasivam, A. Manickam, 2nd edition., New Age International (P) Ltd. (1997)
4. Practical Pharmaceutical Chemistry, A.H. Beckett, 3rd edition, Vol. 1 & Vol. 2 CBS Publishers & Distributors, (1986).
5. Pharmaceutical Analysis, P. Primoo. CBS Publishers, New Delhi, (1999).
6. Text book of Pharmaceutical Analysis, Kenneth. A. Connors, John Wiley & Sons, (1999).
7. Pharmaceutical Chemistry: Instrumental Techniques, Lesile. G. Chatten, 2nd Edition, CBS Publisher, (2008)
8. Pharmaceutical Drug Analysis, Asuthoshkar, NEW AGE International Pvt Ltd, (2020).
9. Handbook of analysis and quality control for fruit and vegetables products, S. Ranganna, 2nd edition, Tata McGraw-Hill Publishing Ltd. (1986)
10. Introduction to the Chemical Analysis of Foods, S. Suzanne Neilsen, CBS Publishers, New Delhi, (2002).
11. A Text book of Soil Chemical Analysis, P.R. Hesse, CBS Publishers, (1998).
12. Methods of Analysis of Soils Plants Waters Fertilisers and Organic Manures, HLS Tandon, 2nd edition, FDCO publications, (1999).
13. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, 6th Edition, Pearson Education Ltd. (2009)
14. Environmental Pollution Analysis, S M Khopkar, Wiley Eastern Ltd. (1993).
15. Environmental Analytical Chemistry, F W Fifield, P J Haines, 1st Edition, Blackie Academic Professional (1995).
16. Environmental Chemistry, B K Sharma, Goel Publishing House, Meerut (1996).
17. A Textbook of Engineering Chemistry, Dr. Y. Bharathi Kumari and Dr. Jyotsna Cherukuri, VGS Publications, First Edison, India (2009).
18. "Engineering Chemistry", Jain P C and Monica Jain, 15th Edition, Dhanpat Rai Publishing Company Ltd, New Delhi, India (2005).
19. Textbook of Engineering Chemistry, C Parameswara Murthy, C V Agarwal, Andra Naidu, 1st Edition, BS Publications, Hyderabad (2008).
20. Water Encyclopedia - Domestic, Municipal, and Industrial Water Supply and Waste Disposal, Jay H. Lehr and Jack Keeley, Wiley-Interscience, Volume 1, Published by John Wiley & Sons, Inc., Hoboken, New Jersey (2005).
21. Handbook of Water and Wastewater Treatment Technologies, Nicholas P. Cheremisinoff, Published by Butterworth-Heinemann (2002).

LABORATORY COURSES (III Semester)

PAPER V CH (IC) 351P: Synthesis and Characterization of Metal Complexes
4 hrs/week

Laboratory preparation and characterization of *3d* transition metal complexes of *tetrahedral*, *square planar* and *octahedral* geometries.

1. $VO(acac)_2$
2. $CoCl_2(Py)_2$
3. $Na[Cr(NH_3)_2(SCN)_4]$
4. Prussian Blue
5. Turnbull's Blue
6. $K_3[Cr(C_2O_4)_3]$ $3H_2O$
7. Solid phase synthesis of trans-bis(glycinato)copper (II)
8. $Fe(acac)_3$
9. Cis and trans $[CoCl_2(en)_2]Cl$
10. Potassium bis(peroxo)oxo(1,10-phenanthroline) vanadium(V) trihydrate
11. Tetra-butylammoniumhexamolybdate (VI)
12. MnO_2nano particles
13. Calculate percent yield, Solubility, TLC, Recrystallization of all complexes
14. Record and interpret the IR spectra and UV
15. SEM analysis of MnO_2nano particles

SUGGESTED BOOKS

1. Practical Inorganic Chemistry, G. Marr and B. W. Rockett Van Nostrand Reinhold, 1972.
2. Practical Inorganic Chemistry by G. Pass H. Sutchiffe,2nd edn., Chapman and Hall,1974.
3. Experimental Inorganic/Physical Chemistry – An Investigative integrated approach toPractical Project work, Mounir A. Malati, Woodhead publishing ltd (1999).
4.Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books international (2006)

PAPER VI CH (IC) 352P: Electro-Analytical Techniques-I

4 hrs/week

I. Potentiometry

Potentiometric Titrations and Calculation of End Point Potentials for the following systems:

i) $Fe^{2+}$and VO^{2+} Mixture vs. Ce^{4+}
ii) Assay of sulphanilamide
iii) Determination of Silver
iv) Mixture of halide anions (Cl^- and I^-) 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) Histidine monohydrochloride (H_2L)
3. Determination of binary constants of
i) Cu(II)-en
ii) Ni(II)-His and
iii)Ni(II)-Gly Systems
4.Determination of stability constant of ternary (Gly-Ni(II)-His) system - Calculation of Log K.

III. 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

SUGGESTED BOOKS

1. A Text Book of Quantitative Inorganic Analysis by A. I. Vogel, 3rd Edition Elbs Publication (1969).
2. Vogel's Text Book of Quantitative Inorganic Analysis, G.H. Jeffery et al. 4th Edition ELBS Publications, Longman group, UK (1997).
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th Edition. Pearson Education Ltd (2002).
4. Determination and use of Stability Constants – Martell and Motekaitis, 2nd Edition VCH Publishers INC (1992).
5. Metal Complexes in Aqueous Solutions A.E. Martell and R.D. Handcock, 1st Edition, Springer Science, Plenum Press, New York (1996).
6. Analytical Chemistry by Gary D. Christian 6th Edition, John Wiley & Sons Inc, New York (1994).

PAPER VII CH (IC) 353P: Estimation of Metal and Ligand in Complexes

2 hrs/week

1.Estimation of copper by iodometry in trans-bis(glycinato)copper (II)complex.
2.Estimation of oxalate by permanganometry in potassium tris oxalato chromate (III) trihydrate complex.
3.Estimation of chromium by iodometry in potassium tris oxalato chromate (III)trihydrate complex.
4.Estimation of vanadium by iodometry in Potassium bis(peroxo)oxo (1,10-phenanthroline) vanadium(V) trihydrate complex
5. Estimation of peroxide by permanganometry in Potassium bis(peroxo)oxo (1,10-phenanthroline) vanadium(V) trihydrate complex
6.Estimation of molybdenum by gravimetry in Tetra-butylammonium hexa molybdate complex.

SUGGESTED BOOKS

1.Practical Inorganic Chemistry by G. Pass H. Sutchiffe,2nd edn., Chapman and Hall,1974.
2.Text book of Quantitative Inorganic Analysis, 3rd edition, A.I. Vogel, ELBS (1969)
3.Vogel's text book of Quantitative Inorganic analysis, 4th edition, Jeffery et.al., ELBS (1988).
4.Vogel's text book of Quantitative Inorganic Analysis, 6th edition, J. Mendham et.al., Pearson education ltd (2002).
5.Experimental Inorganic/Physical Chemistry – An Investigative integrated approach toPractical Project work, Mounir A. Malati, Woodhead publishing ltd (1999).
6.Advanced experimental Inorganic chemistry, Ayodhya Singh, Campus books international (2006)

PAPER VIII CH (IC) 354P: Electro-analytical techniques-II — 2 Hrs/week

I Conductometry:

1. Determination of the Composition of Cu(II)-Oxine Complex
2. Determination of the Composition of Cu(II)-EDTA Complex
3. Interaction of Pyrophosphate with
   (i) Mg^{2+}, (ii) Ca^{2+} and (iii) Cu^{2+}
4. Determination of Aspirin with KOH

II Polarography

1. Determination of $E_{½}$ 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

SUGGESTED BOOKS

1. A Text Book of Quantitative Inorganic Analysis by A.I.Vogel, 3rd Edition, Elbs Publication (1969).
2. Vogel's Text Book of Quantitative Inorganic Analysis Jeffery et. al., 4th Edition ELBS Publications (1991).
3. Vogel's Text Book of Quantitative Chemical Analysis, 6th Edition. Pearson Education Ltd (2002).
4. Analytical Chemistry by Gary Christian, 6th Edition, John Wiley & Sons Inc New York (1994).
5. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake 4th Edition. CBS publishers (2001).

M.Sc. SEMESTER - IV
INORGANIC CHEMISTRY SPECIALIZATION

(For the batches admitted in academic year 2023-24 onwards under CBCS pattern)

PAPER I CH(IC) 401T (CORE): ORGANO METALLIC CHEMISTRY OF TRANSITION METAL COMPLEXES

IC-19: Mono, Di, Tri Tetra, Penta, Hexa hapto Complexes: Structure and Bonding.
IC-20: Catalytic Role of OTMC-I
IC-21: Catalytic Role of OTMC-II

IC-19: Mono, Di, Tri Tetra, Penta, Hexa hapto Complexes: Structure and Bonding. 15 Hrs

Nomenclature and Classification based on the number of Coordinated Carbons (hapticity) and number of electrons donated by the Ligand. 16 and 18 electron rules. Electron counting covalent and ionic models. η^1 – Complexes: Bonding of Ligand to Metal: α and β Interaction and agostic interaction, Ortho-effect. Bonding in Metal – Carbene and Carbyne Complexes. η^2 –Complexes: Structure and Bonding in η^2 Complexes-Zeises salt – Trans Effect – Rotation of Olefin around Metal-Olefin Bond. η3 - Complexes: Metal-Allyl Complexes –Structure and Bonding in η3 Allyl Complexes – Fluxionality. η4 Complexes: Structure and Bonding in η4 Complexes –Butadiene Complexes. η5 – Complexes: Structure and Bonding in Ferrocene– Reactions of Ferrocene – Mechanism of Electrophilic substitution – Friedel Crafts acylation, alkylation, nitration, halogenation and Metallation Reactions. η^6 Complexes: Dibenzene chromium –structure and Bonding in Bis(arene) metal Complexes.

IC-20: Catalytic Role of OTMC-I 15 Hrs

Oxidative addition: Stereochemistry and Mechanism of Oxidative Addition, Reductive Elimination Insertion Reactions –(1,1-insertion &1,2-insertion),β-hydride elimination, Hydrogenation of Olefins, Transfer Hydrogenation, Hydrosilation of Olefins,Isomerisation of Olefins, Ziegler –Natta Polymerization of Olefins , Oligomerization of Butadiene, Alkene Metathesis, Dupont-1,4-hexadiene synthesis, Oxidation of Olefins to Carbonyl Compounds, Cyclohexanol, Cyclohexanone, p-Xylene.

IC-21: Catalytic Role of OTMC- II 15 Hrs

Reactions of Carbon monoxide and Hydrogen: Hydroformylation, Carbonylation, Syngas-Water gas shift Reaction (WGS), Reactions of Syngas. Applications of Metal Clusters in Catalysis: Hydroformylation of Ethylene using $[HRu_3(CO)_{11}]^-$, Hydrogenation of Olefins, Use of $[Fe_6C(CO)_{16}]^{2-}$as a model for Fischer – Tropsch process. Recent Developments in Homogeneous Catalysis: Phase Transfer Catalysis (PTC) – Homogeneous Transition Metal Catalysed Reactions under Phase Transfer Conditions: Hydrogenation. Bio-Catalysis: Enzyme Analogue Catalysis: Introduction, Examples of Enzymatic Conversions, Reduction of >C=O and >C=C< bonds, Templates: Introduction, Metal Cations as Templates, Covalent molecules as Templates, External and Internal Templates, Homogeneous Catalysts and their Heterogenization and Immobilization by Aqueous Catalysis.

SUGGESTED BOOKS

1.Organometallics: A Concise Introduction, Ch Elschenbroich and A Salzer, 2 nd Edition, Wiley VCH(1992)

2.Organotransition Metal Chemistry Fundamental Concepts and Applications, Akio Yamamoto, 1stEdition, Wiley-Interscience (1991)

3.Homogeneous Catalysis by Metal Complexes, M M Taqui Khan and A E Martel, 1 st Edition, New York,Academic Press (1974)

4. Applied Homogeneous Catalysis with Organometallic Compounds: A Comprehensive Handbook inThree Volumes, B Cornils, and Wolfgang A. Herrmann, 2 nd Edition, Wiley VCH (2008)

5. Organometallic Compounds, Volume 2, G E Coates, M C H Green, K Wade, Methuen Publisher (1967)

6. Advanced Inorganic Chemistry, Cotton, Wilkinson, Murillo, and Bochmann, 6 th Edition, Wiley VCH(2007)

7. Symmetry and Spectroscopy of Molecules, K Veera Reddy, 2 nd Edition, Newage publishers (2020)

8. Homogeneous catalysis, G W Parshall and S D Ittel, 2 nd Edition, Wiley–Interscience (1994)

9. Basic Organometallic Chemistry, Anil Elias, and B D Gupta, 2 nd Edition, Universities Press (2013)

PAPER II CH(IC) 402T (CORE): BIOINORGANIC CHEMISTRY

IC-22: Transport of Oxygen, Electrons and Metal ions
IC-23: Metallo-Enzymes of Iron, Zinc and Nickel
IC-24: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese

IC-22: Transport of Oxygen, Electrons and Metal ions — 15 Hrs

Transport of Oxygen: Hemocyanin (Hc) and Hemerythrin(Hr) – Introduction, Structure of active sites with and without oxygen.
Transport of Electrons: Iron-Sulphur Proteins- Rubredoxins and Ferredoxins (2Fe,3Fe, 4Fe, 8Fe Proteins), High Potential Iron-Sulphur Proteins, Structural and Spectral features of Iron-Sulphur Proteins; Electron-transport by Cytochromes, Azurin and Plastocyanin; Acotinase-Fe-S enzyme.
Transport and Storage of Metal Ions: Iron-Transport by Transferrin and Siderophores; Ferritin in Iron Storage; Transport of Na^+ and K^+ across cell membranes by Na^+- K^+ ATPase; Transport of calcium across Sarcoplasmic Reticulum by Ca^{2+}-ATPase.

IC-23: Metallo-Enzymes of Iron, Zinc and Nickel — 15 Hrs

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, Carboxy Peptidase, Alcohol Dehydrogenase - Role of Zinc.
Nickel Enzymes: Urease, Hydrogenase and Factor F430: Reactions catalyzed, mechanistic aspects.

IC-24: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese — 15 Hrs

Cobalt Enzymes: Cobalt in Vitamin B_{12} - Structural Features of Vitamin B_{12} with reference to coordination of Cobalt - Different Oxidation States of Cobalt - Various forms of Vitamin B_{12} and Active Enzyme forms - Types of Reactions Catalyzed by i) Methyl Cobalamin ii) Deoxyadenosyl Cobalamin - 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, Xanthine oxidase and Sulfite oxidase.
Manganese Enzymes: Biological Roles and Mechanistic Aspects of Arginase, and Water – oxidase.

SUGGESTED BOOKS

1. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University Science Books, California USA (1994).
2. Principles of Bioinorganic Chemistry, S.J. Lippard and M. Berg, University Science Book s, California (1994).
3. Biological Chemistry of Elements, J.J.R. Franstodasilva and R.J.P. Williams, Oxford University Press (1991).

4. Metal Ions in Biological Systems (Series), Ed. H. Sigel Marcel Dekkar, New York.
5. Inorganic Biochemistry, J.A. Cowan, VCH publishers (1993).
6. Advances in Inorganic Biochemistry, edited by G.L. Eichorn & Luigi G.Marzilli, Elsevier (1984).
7. Bioinorganic Chemistry, Vol-I edited by G.L. Eichorn.
8. Bioinorganic Chemistry, K.Hussain Reddy, Second edition, New Age International publishers (2001).
9. Interactions of metal ions with nucleotides and nucleic acids and their constituents Helmut Sigel Chem. Soc. Rev., 1993, 22, 255-267.
10. Biochemistry, Geoffrey L. Zubay, Dubuque C. Brown publisher (1995).
11. Biochemistry, Mary K. Campbell, Shawn O. Farrell, Owen M. McDougal, Ninth Edition, Cengage Learning India Pvt.Ltd.(2022)

PAPER III CH(IC) 403T (ELECTIVE III A): MEDICINAL INORGANIC CHEMISTRY AND PHOTOCHEMISTRY

IC(CB1)-25: Metal ion interactions with nucleic acids and their Spectroscopic analysis
IC(CB1)-26: Metal complexes in Clinical Chemistry
IC(CB1)-27: Photochemistry of Metal Complexes

IC(CB1)- 25: Metal ion interactions with nucleic acids and their Spectroscopic analysis — 15 Hrs

Nucleic bases, nucleosides and nucleotides. Proton binding sites and metal binding sites of nucleic acid constituents-Purine and Pyrimidine bases, nucleosides and nucleotides; Covalent structure of polynucleotides, secondary structure of DNA: The double helix anti and syn conformations of nucleotides; B, A, & Z forms of DNA; Tertiary structure of DNA, Supercoiled DNA (Form-I), Nicked DNA (Form II) and Linear DNA (Form-III). General factors that influence metal ion binding sites in solution. Stability of phosphate- metal ion complexes. Metal ion interactions – Intra-molecular equilibrium constant KI, percentage of closed isomers - Outer Sphere and Inner Sphere isomers of M-ATP Complexes. Influence of Metal Ions on Stability of Nucleic Acids (T_M).
Introduction to DNA binding studies; UV-Vis absorption spectroscopy and metal complex DNA binding studies; Applications of fluorescence quenching in metal complex DNA binding studies; calculation of binding constants. Equilibrium dialysis-Competition dialysis to assess base and sequence specificity, Partition analysis, Viscosity studies; DNA cleavage activity with ligand/metal complexes-Analysis by Gel electrophoresis.

IC(CB1)-26: Metal complexes in Clinical Chemistry — 15 Hrs

Theory and mode of action of therapeutic chelating agents, Single ligand Chelation Therapy– Aminopolycarboxylic acids, desferrioxamine, penicillamine, triethylenetetramine. Mixed ligand chelation therapy, metallothionens in detoxification. Role of metal ions in the action of antibiotics: bleomycin, adriamycin and tetracyclines. Cisplatin [$cisPt(NH_3)_2Cl_2$] mode of action, non-classical platinum antitumour agents. Gold-containing drugs used in therapy of rheumatoid arthritis, a therapeutic agent for Menkes disease: Copper-histidine, anti-viral chemotherapy and metal peptide interaction.

IC(CB1)-27: Photochemistry of Metal Complexes — 15 Hrs

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 $Cr(CO)_6$, $Mn_2(CO)_{10}$ and $Fe(CO)_5$.
Structured phosphorescence 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.

SUGGESTED BOOKS

1. Bioinorganic Chemistry. Inorganic elements in the Chemistry of life, Wolfgang Kaim & Brigette Schwederdki; 2nd Edition, Wiley (2013).
2. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, University Science Books, California USA (1994).
3. Handbook of Metal-Ligand interactions in Biological fluid Bioinorganic medicine, Guy Berthon Vol 1 and 2 – 1st Edn.Marcel Dekker, NY (1995).
4. Concepts of Inorganic Photochemistry, A.W. Adamson and P. D. Fleschaner, Wiley, (1975).
5. Inorganic Photochemistry, Journal of Chemical Education, Vol 60. No 10, (1983).
6. Photochemistry of Coordination compounds V. Balzani and Carassiti, Academic press, London (1970).
7. Elements of inorganic Photochemistry G.J. Ferrendi, Wiley, (1988)
8. Drug -Nucleic Acid Interactions, Volume 340 Jonathan B. Chaires, Michael J. Waring Academic Press, (2001).
9. Mechanistic Bioinorganic Chemistry Edited by byH.Holden Thorp and Vincent L. Pecoraro, Chemical Society, Washington DC (1995).
10. Metal Complex -DNA Interactions, Editor(s): Nick Hadjiliadis, EinarSletten, Blackwell Publishing Ltd.(2009)
11. Gel Electrophoresis - Principles and basics edited by Sameh Magdeldin ISBN 978 - 958 -51-0458-2, 76 pages, Publisher: InTech, (2012)

PAPER III CH(IC) 403T (ELECTIVE III B): INORGANIC MATERIAL CHEMISTRY

IC(CB1)-25: Solid State Chemistry
IC(CB1)-26: Nanotechnology
IC(CB1)-27: Liquid Crystals

IC(CB1)-25: Solid State Chemistry — 15 Hrs

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(CB1)-26: Nanotechnology — 15 Hrs

Metal Nanoclusters –Introduction, Magic numbers, theoretical modeling of nanoparticles, geometric structure, electronic structure, reactivity, fluctuations, magnetic clusters, bulk to nano transition.
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: **Micelles 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 Nano Particles, Methylmethacrylate Nanoparticles. Sol -Gel process for the fabrication of Glassy and Ceramic materials.

IC(CB1)-27: Liquid Crystals **15 Hrs**

Introduction, Types of Mesophases, Characterization of Liquid Crystals, Physical Properties of Liquid Crystals, Structure of Liquid Crystal forming compounds, Classification of Liquid Crystals-Thermotropic Liquid Crystals and Lyotropic Liquid Crystals, Chemical Properties of Liquid Crystals, Applications with special reference to Display systems, Applications and Importance of Lyotropic Liquid Crystals, Future of Liquid Crystals.

SUGGESTED BOOKS

1. Solid-State Chemistry an Introduction () – Lasley Smart and Elaine Moore, 2nd Edition Chapman & Hall, (1996)
2. Solid State Chemistry, D.K. Chakraborty, New Age International Pvt.Ltd. New Delhi, (2000)
3. Introduction to Solids, L.V. Azaroff, 2nd Edition, Tata McGraw Hill Publication Ltd. New York (1977)
4. Principles of the Solid State, H.V. Keer; Wiley Eastern Ltd. New Delhi, (1994)
5. Solid state Chemistry, N.B. Hannay, Prentice Hall, New Jersey, (1967)
6. Introduction to nanotechnology by Charles P. Poole Jr, Frank J. Owens, Wiley Student Edition (2006).
7. Hand Book of Nanophase Materials, Chapter1, A.N. Gold Stein ed, Marcel Decker, New York, (1997)
8. Clusters of Transition Atoms, Morse, Chem. Rev 86, 1049 (1986).
9. Hand Book of Nanostructured materials, Vol. 5, Chapter 6, P.M. Ajayan, H.S Nalwa, ed, Academic Press, San Diego, (2000)
10. Hand Book of Nanophase and Nanostructured materials, volume I: Synthesis, Zhong Lin Wang, Yi Liu, Ze Zhang, Kluwer Academic/Plenum Publishers, (2002)
11. Liquid Crystals, Nature's delicate phase of matter", Peter J Collings, Princeton University Press, (2002)
12. Liquid Crystals: Fundamentals, Shri Singh, 1st Edition, World Scientific Publishing Company; (2002)

LABORATORY COURSES (IV Semester)

PAPER IV CH (IC) 451P: Conventional methods of analysis **4 Hrs/Week**

Titrimetry:

Soil samples (5-6 samples)

1. Determination of CO_3^{2-}
2. Determination of HCO_3^-
3. Determination of Ca^{2+}
4. Determination of Mg^{2+}

Oil samples (5-6 samples & comparative study)

5. Determination of saponification value
6. Iodine number
7. Acid value
8. Ester value

Water analysis: (5-6 samples)

9. Determination of Dissolved Oxygen
10. Determination of COD
11. Determination of residual Chlorine in water by Iodometry

Separation Methods

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

SUGGESTED BOOKS

1.Chemistry Experiments for Instrumental Methods, Donald T Sawyer, William R. Hememan, John Wiley & Sons, (1984)

2.Analytical Chemistry by Gary D. Christian 6thEdition, John Wiley & Sons Inc. New York, (1994)

3.A Text Book of Quantitative Inorganic Analysis, A.I. Vogel, 3rdEdition, ELBS Publication, (1969)

4.Vogel's Text Book of Quantitative Inorganic Analysis, Jeffery et. al 4th edition, ELBS Publication, (1988).

5.Vogel's Text Book of Quantitative Chemical Analysis, 6th edition. Pearson Education Ltd. (2002)

6.Analytical Chemistry Theory and Practice by R.M. Verma 3rd Edn. CBS Publishers & Distrbutors (1994).

7.Comprehensive Experimental Chemistry by V.K. Ahluwalia et.al, New Age Publications (1997)

8. Laboratory hand Book of Instrumental Drug Analysis.by B.G. Nagavi 4ndedn. Vallabh Prakashan Publishers, (2012)

Paper-V CH (IC) 452P: Spectroscopic techniques-I **4 hrs/week**

I Spectrophotometry

1. Estimation of manganese in steel using KIO_4 as oxidant.
2. Estimation of chromium using 1,5-diphenylcarbazide
3. Simultaneous determination of Chromium and Manganese
   (i) Determination of molar absorption coefficients and verification of additivity of absorbamces
   (ii) Determination of Chromium and Manganese in a mixture
4. Determination of pKa of an indicator
   (i) Evaluation of λ_{max} for HMR (λ_A) and MR^- (λ_B)
   (ii) Verification of Beer's Law for HMR and MR^- at both λ_{max} and determination of their relative amounts in the solution
5. Estimation of Nickel using dimethylglyoxime
6. Determination of composition of Complex:
   (i) Cu(II)-EDTA by Job's Method
   (ii) Cu(II)-EDTA by Mole ratio Method
   (iii) Fe(II)-o-Phen by Job's Method and
   (iv) Fe(II)-o-Phen by Mole ratio Method

II Fluorimetry

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

III Atomic Absorption Spectroscopy

1. Determination of i) Fe and ii) Mg

SUGGESTED BOOKS

1. Text Book of Quantitative Inorganic Analysis, Jaffery et.al, 4th Edition, ELBS Publication, (1991)
2. A Text Book of Quantitative Inorganic Analysis, A.I. Vogel, 3rd Edition, ELBS Publication, (1969)
3. Quantitative Analysis, Day and Underwood Prentice Hall, 6th Edition, Pearson Education India, (2015)
4. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake, 4th Edition,. CBS Publishers, (2001)

Paper-VI CH (IC) 453P: Spectroscopic techniques-II **2 hrs/week**

I Colorimetry

1. Determination of blood sugar
2. Determination of blood cholesterol
3. Determination of creatinine
4. Determination of paracetamol
5. Determination of fluoride ion
6. Determination of sulphate ion

II Flame photometry

1. Determination of Na
2. Determination of K

SUGGESTED BOOKS

1. Medical Laboratory Technology, A Procedure Manual for Routine Diagnostic Tests-Volume III, Kanai L Mukherjee, Tata McGraw-Hills publishing company, (1995)
2. Text Book of Quantitative Inorganic Analysis, Jaffery et.al, 4th Edition, ELBS Publication, (1991)
3. Quantitative Analysis, Day and Underwood Prentice Hall, 6th Edition, Pearson Education India, (2015)
4. Analytical Chemistry Theory and Practice, R.M. Verma, 3rd Edition, CBS Publishers & Distributors, (1994)
5. Practical Pharmaceutical Chemistry, A.H. Beckett and J.B. Stenlake, 4th Edition, CBS Publishers, (2001)

CH(IC) 454P: PROJECT **12 Hrs/Week**

Marks Distribution for Project Assessment

INTERNAL ASSESSMENT

Research Design Seminar	1 credit	25 marks
Progress Seminar	1 credit	25 marks

SEMESTER END ASSESSMENT

Dissertation	1 credit	50 marks
Final presentation	2 credits	50 marks
Viva Voce during final presentation	1 credit	25 marks

M.Sc. CHEMISTRY

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

FOR STUDENTS ADMITTED FROM THE YEAR 2023-24 ONWARDS

MC

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters
[Under Restructured CBCS Scheme]
(for the batches admitted in academic year 2023-24 onwards under CBCS pattern)
Grand total marks and credits (all 4 semesters) 2400 marks – 80 credits

(Approved in the P.G. BOS meeting held on 27-01-24)

Semester - III (Organic Chemistry)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(OC)301T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)302T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)303T (Elective)	3	50 marks	50 marks	100 marks	3
CH(OC)304T (Elective)	3	50 marks	50 marks	100 marks	3
CH351P (OC LAB1)	4		50 marks	50 marks	2
CH352P (OC LAB2)	4		50 marks	50 marks	2
CH353P (OC LAB3)	2		25 marks	25 marks	1
CH354P (OC LAB4)	2		25 marks	25 marks	1
Seminar	2		50 Marks	50 Marks	2
Total				600 marks	20

Semester - IV (Physical Chemistry)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(OC)401T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)402T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)403T (Elective)	3	50 marks	50 marks	100 marks	3
CH451P (OC LAB1)	4		50 marks	50 marks	2
CH452P (OC LAB2)	4		50 marks	50 marks	2
CH453P (OC LAB3)	2		25 marks	25 marks	1
CH454P (Project)	12	50 marks	125 marks	175 marks	6
Total				600 marks	20

Grand total marks and credits (all 4 semesters) 2400 marks - 80 credits

M.Sc. SEMESTER - III
ORGANIC CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH (OC) 301T(CORE): SYNTHETIC REAGENTS, ^{13}C AND 2D NMR
OC-07: Synthetic Reagents-I
OC-08: Synthetic Reagents-II
OC-09: ^{13}C NMR and 2D NMR spectroscopy

PAPER II CH (OC) 302T(CORE): MODERN ORGANIC SYNTHESIS
OC-10: Asymmetric synthesis
OC-11: Synthetic strategies
OC-12: New Synthetic reactions

PAPER III CH (OC) 303T (ELECTIVE IIIA): BIOORGANIC CHEMISTRY AND CONFORMATIONAL ANALYSIS (CYCLIC SYSTEMS) & ORD
OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes
OC(CB1)-14: Proteins, Enzymes and Lipids
OC(CB1)-15: Conformational analysis-II (Cyclic Systems) & ORD

PAPER III CH (OC) 303T (ELECTIVE IIIB): PROCESS CHEMISTRY AND DEVELOPMENT
OC(CB1)-13: Process chemistry and Principles
OC(CB1)-14: Process Development /Optimization
OC(CB1)-15: Process Development /Optimization

PAPER IV CH (OC) 304T (ELECTIVE IVA: GREEN CHEMISTRY AND NEW TECHNIQUES
OC (CB2) -16: Principles of Green chemistry and Green Synthesis
OC (CB2) -17: Organic nanomaterials and Supramolecular chemistry
OC (CB2) -18: New techniques and concepts in organic synthesis

PAPER IV CH (OC) 304T (ELECTIVE IVB): PESTICIDES
OC (CB2) - 16: Introduction to pesticides
OC (CB2) - 17: Synthetic insecticides
OC (CB2) - 18: Natural insecticides & herbicides

LABORATORY COURSES
Paper-V CH (OC) 351P: Synthesis of organic molecules
Paper-VI CH (OC) 352P: Separation and identification of organic compounds
Paper-VII CH (OC) 353P: Isolation of natural products and Thin layer chromatography
Paper-VIII CH (OC) 354P: Separation of three component mixtures by chemical methods and Column chromatography

SEMINAR

M.Sc. SEMESTER - IV
ORGANIC CHEMISTRY SPECIALIZATION
(for the batches admitted in the academic year 2023-24 and later under CBCS pattern)

PAPER-1 CH (OC) 401T(CORE): DRUG DESIGN AND DRUG DISCOVERY
OC-19: Principles of Drug design and drug discovery
OC-20: Lead modification and SAR Studies
OC 21: QSAR studies and computer aided drug design

PAPER-II CH (OC) 402T(CORE): ADVANCED HETEROCYCLIC CHEMISTRY
OC-22: Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms
OC-23: Six membered heterocyclics with two heteroatoms and Five membered heterocyclics with more than two heteroatoms
OC-24: Six membered heterocyclics with more than two heteroatoms and Larger ring heterocyclics

PAPER-III CH (OC) 403 T(ELECTIVE IIIA):DRUG SYNTHESIS AND MECHANISM OF ACTION
OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes
OC(CB1)-26: Drugs acting on genetic material and immune system
OC(CB1)-27: Drugs acting on receptors and ion channels

PAPER III CH (OC) 403 T(ELECTIVE IIIB): ADVANCED NATURAL PRODUCTS
OC(CB1)-25: Biosynthesis of natural products
OC(CB1)-26: Structure determination of natural products
OC(CB1)-27: Total stereo selective synthesis of natural products.

LABORATORY COURSES
Paper-IV CH (OC) 451P: Spectroscopic identification of organic compounds
Paper-V CH (OC) 452P: Synthesis of following drugs
Paper-VI CH (OC) 453P: Practice of chemistry software prgrammes

PROJECT CH(OC)454P

M.Sc. SEMESTER - III
ORGANIC CHEMISTRY Specialization
(for the batches admitted in academic year 2023-24 and later under CBCS pattern)

PAPER I

CH (OC) 301T(CORE): SYNTHETIC REAGENTS, ^{13}C AND 2D NMR

OC-07: Synthetic Reagents-I
OC-08: Synthetic Reagents-II
OC-09: ^{13}C NMR and 2D NMR spectroscopy

OC-07: Synthetic Reagents-I — 15 Hrs

i) Protecting groups:
a) Protection of alcohols by silyl ether(TBDMS,TBPS) and ester formation
b) Protection of 1,2-diols by acetal, ketal and carbonate formation
c) Protection of amines by t-butyloxycarbonyl, fmoc groups.
d) Protection of carbonyls by thiol acetal (Umpolung) groups.
e) Protection of carboxylic acids 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, 2) Horner-Wordsworth-Emmons reaction.
iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.
v) C-H Activation: Introduction, Rh catalysed C-H activation.

OC–08: 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: Crv oxidants Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation.
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.

OC–09: ^{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), Hetero COSY (^{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.

BOOKS SUGGESTED:

1. 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
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
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, 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
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
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
26. Stereo selectivity in organic synthesis by R S Ward.
27. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
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(CORE): MODERN ORGANIC SYNTHESIS

OC-10: Asymmetric synthesis
OC-11: Synthetic strategies
OC-12: New Synthetic reactions

OC-10: 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 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 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. Asymmetric Diels-Alder reaction.
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.

OC-11: Synthetic Strategies **15 Hrs**

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. .
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.

OC-12: New Synthetic reactions **15 Hrs**

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling,
Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia- Lythgoe olefination and Peterson's stereoselective olefination.
3. Multicomponent Reactions: Ugi, Passerini, Biginelli and Bergman 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.

BOOKS SUGGESTED:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moschcr
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
13. Name reactions by Jie Jacj Li

PAPER III CH (OC) 303T (ELECTIVE IIIA): BIOORGANIC CHEMISTRY AND CONFORMATIONAL ANALYSIS (CYCLIC SYSTEMS) & ORD

OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes
OC(CB1)-14: Proteins, Enzymes and Lipids
OC(CB1)-15: Conformational analysis-II (Cyclic systems) & ORD

OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes — 15Hrs

Carbohydrates: Introduction to the importance of Carbohydrates. Types of naturally occuring sugars. Deoxy sugars, aminosugars, branched chain sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. Synthesis of amino, halo and thio sugars. Conformational structures of sucrose. Structure and biological functions of starch, cellulose, glycogen and chitin.
Nucleic acids: Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA.
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 nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH)

OC(CB1)-14: Proteins, Enzymes and Lipids — 15 Hrs

Proteins: Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods.
Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three point contact models. Enzyme selectivity –chemo, regio, diastereo and enantio selectivity – illustration with suitable examples. Factors affecting enzyme catalysis.
Lipids: Introduction and classification of lipids. Stereochemical notation in lipids. Chemical synthesis and biosynthesis of phospholipids and glycolipids.

OC(CB1)-15: Conformational analysis-II (Cyclic systems) & ORD — 15 Hrs

Conformational analysis-II (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, SN2 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

method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

BOOKS SUGGESTED:

1. Organic Chemistry Vol.I and Vol.II by I.L.Finar
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. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon
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.Ahluwalia
11. Biotransformations in Organic Chemistry by K Faber.
12. Principles of biochemistry by Horton & others.
13. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian & others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg. 22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri 23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. wilen
16. Stereochemistry: Conformation & Mechanism by P S Kalsi
17. The third dimension in organic chemistry, by Alan Bassendale
18. Stereo selectivity in organic synthesis by R S Ward.
19. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
20. Optical rotatory dispersion by C Djerassi
21. Optical rotatory dispersion and circular dichroism by P Crabbe
22. Mechanism and Structure in Organic chemistry by S Mukherjee

PAPER III CH (OC) 303T (ELECTIVE IIIB): PROCESS CHEMISTRY AND DEVELOPMENT.

OC(CB1)-13: Process chemistry and Principles
OC(CB1)-14: Process Development /Optimization - I
OC(CB1)-15: Process Development /Optimization - II

OC(CB1)-13: Process Chemistry and Principles **15 Hrs**

Introduction to Pharmaceutical Industry, Product life cycle and its different functions in product life cycle management, Research &Development, Production/Manufacturing, Quality Control, Quality Assurance, Intellectual Property, Regulatory Affairs.
Route selection: SELECT (Safety, Environmental, Legal, Economics, Control, Throughput) Safe route, Environment friendly route, Legal (more insights into Intellectual Property on patent infringment related topic), Economic and commercially viable route, Control & Scalable route, Feasibility of selected route/s for optimum throughput (Depends on number of routes proposed for development), Structure confirmation of product at each stage by IR, NMR, Mass, Conclusion of feasibility study

OC(CB1)-14: Process Development / Optimization - I **15 Hrs**

Process Chemistry: Introduction & importance of process optimization in product development, Starting material/s : Definition, Reagent/s: Definition, different types of reagents; Catalysts, stoichiometry calculations, Solvent/s: Definition, different types of solvents and their compatibility. **Process Safety Engineering:** Reaction condition/s: Definition, different reaction conditions, exothermic &endotherimic conditions (DSC / TSU, Reaction calorimetry and gas evolution study) endothermic conditions. **Analytical:** Reaction monitoring technique/s or In-process controls: Definition, different types of monitoring techniques: TLC, HPLC and GC, Impurity identification and their structure elucidation: UV, IR,Mass, NMR. Fixing Specifications in each stage: Definition, significance of fixing specifications, Different detectors (UV, RI, ELSD, CAD).

OC(CB1)-15: Process Development / Optimization - II **15 Hrs**

Reaction Parameters: Reaction Kinetics (Homogeneous, Heterogeneous reactions, Mixing, Temperature, Time and Critical Process parameter identification). **Work up & product isolation:** Definition, different types of work ups: Quenching, extraction and distillation/concentration & isolation. **Purification:** Definition, different types of purifications: Washing, precipitation, crystallization. **Filtration study. Drying:** Different types of drying methods, ATD (Air tray dryer), VTD (Vacuum tray dryer), RCVD (Rotatory cone vacuum dryer), FBD (Fluid Bed Dryer), Lyophilization, Spray Drying. **What-if and Stability study:** Definitions & its requirement in scale up, Finalizing the Critical Process parameters based on the Optimization and what if study. Risk mitigations by considering Critical Material Attributes and critical process parameter. **Report writing**

SUGGESTED BOOKS

1. Practical Process Research & Development-Neal Anderson (Chapter-2)
2. Process Chemistry in Pharmaceutical Industry by Kumar Gadamasetti, Vol I & II, CRC Press,

3. The chemistry of process development in fine chemical & pharmaceutical chemistry. C. Someswara Rao. Asian Books Private Limited New Delhi.
4. Analytical Chemistry by D. Kealey& P. J, Haines
5. Chemical Analysis, Modern Instrumentation Methods and Techniques by Francis Rouessac and AnnickRouessac, University of Le Mans, France
6. Pharmaceutical Drug Analysis by AshutoshKar published by New Age International (P) Limited, Publishers.
7. HPLC and UHPLC for Practicing Scientists by Michael W. Dong,
8. Process Chemistry in Pharmaceutical Industry by Kumar Gadamasetti, Vol I & II, CRC press
9. The chemistry of process development in fine chemical & pharmaceutical chemistry. C. Someswara Rao. Asian Books Private Limited New Delhi.
10. Analytical Chemistry by D. Kealey& P. J, Haines
11. Chemical Analysis, Modern Instrumentation Methods and Techniques by Francis Rouessac and AnnickRouessac , University of Le Mans, France
12. Pharmaceutical Drug Analysis by AshutoshKar published by New age international (P) Limited, Publishers.
13 HPLC and UHPLC for Practicing Scientists by Michael W. Dong
14 Fundamentals of Medicinal Chemistry by Thomas
15. Practical Process Research & Development by Neal G Anderson
16. P. J. Dunn, The importance of Green Chemistry in Process Research and Development, Chem. Soc. Rev., 2012, 41, 1452-1461.
17. Pharmaceutical Quality by Design: A Practical Approach by Walkiria S. Schlindwein, Mark Gibson
18. Strategies for Organic Drug Synthesis and Design by Daniel Lednicer, Wiley
19. Pharmaceutical Process Chemistry, Editor(s):Prof.Dr. Takayuki Shioiri, Dr.Kunisuke Izawa, Dr. Toshiro Konoike, Wiley
20. The Art of Process Chemistry, Editor(s): Dr. Nobuyoshi Yasuda, Wiley
22. New Horizons of Process Chemistry: Scalable Reactions and Technologies, Editors: Tomioka, Kiyoshi, Shioiri, Takayuki, Sajiki, Hironao, Springer
23. Pharmaceutical Process Development: Current Chemical and Engineering Challenges edited by John Blacker & Michael T Williams-RSC publishing
24) Chemical Analysis, Modern Instrumentation Methods and Techniques by Francis Rouessac and AnnickRouessac , University of Le Mans, France
25) Pharmaceutical Drug Analysis by AshutoshKar published by New age international (P) Limited, Publishers.
26) HPLC and UHPLC for Practicing Scientists by Michael W. Dong
27) Analytical Chemistry by D. Kealey& P. J, Haines
28) Pharmaceutical Quality by Design: A Practical Approach by Walkiria S. Schlindwein, Mark Gibson

PAPER IV CH (OC) 304T (ELECTIVE IVA): GREEN CHEMISTRY, NANOMATERIALS AND NEW TECHNIQUES IN ORGANIC SYNTHESIS

OC (CB2) -16: Principles of Green chemistry and Green Synthesis
OC (CB2) -17: Organic nanomaterials and Supramolecular chemistry
OC (CB2) -18: New techniques and concepts in organic synthesis

OC (CB2) -16: Principles of Green Chemistry and Green Synthesis **15 Hrs**

Introduction of Green Chemistry. Principles of Green Chemistry. Introduction to alternative approaches. Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations i) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction. ii) Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes. iii) Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasoundCannizaro reaction, Reformatsky reaction and Strecker synthesis. iv) Organic Synthesis in Green Solvents: introduction Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and diydroxylation reactions. v) Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction. vi) 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 (CB2) -17: Organic Nanomaterials and Supramolecular Chemistry **15 Hrs**

Organic Nanomaterials:

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation.
Molecular Devices: Photochemical devices, Liquid crystals.
New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Types of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs) and Graphenes.

Supramolecular Chemistry :
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 anology, Structures and applications of Cryptands,Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.r
Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, properties and applications.

OC (CB2) -18: New techniques and concepts in organic synthesis **15 Hrs**

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.
Solid phase oligodeoxynucleotide synthesis: Phospho triester, phosphite triester and phosphoramidite pathway

Oligosaccharide synthesis: Glycosidation: cylic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.
Phase Transfer catalysis: Onium and crwon ethers as PTC.
Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-Diels Alder reaction.
Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.
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.
Determination of absolute configuration: Mosher's method.

BOOKS SUGGESTED:

1. P.T. Anastes & J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).
3. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers
6. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
9. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
10. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications
11. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
12. Stereochemistry of organic compounds - Principles & Applications by D Nasipuri
13. Nanochemistry by G.B. Sergeev; Elsevier
14. Nanochemistry: A chemical approach to nano materials , G.A. Ozin & A.C. Arsenault; RSC publishers.
15. Stereo differentiating reactions by Izumi
16. Some modern methods of organic synthesis by W Carruthers
17. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
18. Organic synthesis by Michael B Smith
19. Organic Synthesis by C Willis and M Wil lis
20. Problems on organic synthesis by Stuart Warren
21. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
22.The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
33. Name reactions by Jie Jacj Li

PAPER IV CH (OC) 304T (ELECTIVE IVB): PESTICIDES

OC (CB2) - 16: Introduction to pesticides
OC (CB2) - 17: Synthetic insecticides
OC (CB2) - 18: Natural insecticides & herbicides

OC(CB2) - 16: Introduction to pesticides — 15 Hrs

i) Defination, Classification and importance of pesticides
ii) Pest control: Different methods -chemical insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents..
a) Biological pheremones: Definition and classification, synthesis of Disparlure, Exobrevicomin. Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants.
b) Insect juvenile hormones: JH-A, JH-B,Synthesis of juvabione. Structural formula and importance of methopren.
c) Moulting harmones-structural formulae and mode of action of ecdysones
d) Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agricultiure. Structural formula and importance of Blasticidin-S, Kasugamycin, Avermectin-B. Invermectin, piercidins and phytoalexins.
iii) Environmental pollution from pesticides. iv) Integrated pest management.
v) Pesticide formulations: Dusts, Granules, Wettable powders, Emmulsions and Aerosols.
vi) Formulation and residue analysis of organochlorine, organophophorous and carbamate insecticides.

OC(CB2) -17: Synthetic Insecticides — 15 Hrs

A. Synthetic origin:
i) Organochlorine insecticides- synthesis and mode of action of methoxychlor, perthan and Endosulfan.
ii) Organophosphorous insecticides synthesis and mode action of Phosphoric acid derivatives. Dichlorophos, parathion and TEPP
iii) Carbamate insecticides- synthesis and mode of action of carbamyl and Baygon
B. Natural origin:
i) Insecticides of palnt origin-synthesis and importance of pyrethrins (I and II), Rotenone. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol Antifeedants).
ii) Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin and Fenvalerate.
iii) Concept of Bioinsecticides - Bacillus thiuringiensis.
iv) Concept of pro-insecticides-structure and mode of action of pro-pheremones and pre-pro-insecticides.

OC(CB2) -18: Natural insecticides & herbicides — 15 Hrs

i) Fungicides: Synthesis application and mode of action of the following classes: (a) Quinones-chloranil and Benquinox b) perchloromethylmercaptan derivative-captan, folpet Mesulfan c) Benzimidazoles-carbendazim and Thiabandazole
ii) Rodenticides: a) Anticoagulents-synthesis and application of warfarin. Dicoumarol and

Bromodiolen. b) Acute poisons- application of pindone, Ratindan, Sodium Fluoroacetate Barium fluoroacetate, Antu, Tetramine, pindone and castrix. No. of Congress reduce.
ii) Herbicides : Synthesis, applications and mode of action of the following a) Aryloxyalkyl carboxylic acid derivative: 2,4-D. MCPA, 2.4.5-1 and 2,4,5-TP b) Carbamates- propham and chloropham, c) Urea derivatives Monouron and diuron, d) Aliphatic acids- Dalapon. ICA. e) Aromatic acids -2,3,6-TBA Dicamba and Amiben.

BOOKS SUGGESTED:

1) Naturally occurring insecticides: M.Jacobson and D.G.Crosby.
2) Insecticides for future:Jacobson
3) Insect juvenile harmone 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.Kaufnan
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) Pespticides managements and insecticide resistance: Watson and brown
22) Organo phosphorous pesticides M.eto

LABORATORY COURSES

Paper- V CH (OC) 351P: Synthesis of Organic Molecules **4 Hrs/Week**

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 ($NaBH_4$ reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

Paper-VI CH (OC) 352P: Separation and Identification of Organic Compounds **4 Hrs/Week**

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 hydroxi de 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.

Paper-VII CH (OC) 353P: Isolation of Natural Products and Thin Layer Chromatography **2 Hrs/Week**

A. 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.

B. Identification of Components in the extracts by TLC

Paper-VIII CH (OC) 354P: Separation of Three Component Mixtures by Chemical Methods and Column Chromatography: **2 Hrs/Week**

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

Column Chromatography: Separation of four mixtures of two components each using silica gel as adsorbent and a suitably polar eluent. The column chromatography should be monitored by TLC.

BOOKS SUGGESTED:

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

SEMINAR **2 Hrs/ week**

M.Sc. SEMESTER - IV
ORGANIC CHEMISTRY SPECIALIZATION
(For the batches admitted in academic year 2023-24 onwards under CBCS pattern)

PAPER I CH (OC) 401T (CORE): DRUG DESIGN AND DRUG DISCOVERY

OC-19: Principles of Drug Design and Drug Discovery
OC-20: Lead Modification and SAR Studies
OC-21: QSAR Studies and Computer Aided Drug Design

OC -19: 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 purturbation 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. Drug discovery without lead serendipity Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

OC-20: 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-21: QSAR Studies and Computer Aided Drug Design — 15 Hrs

QSAR: Introduction, physicochemical properties pKa, electronic effects and Hammett constants(6), lipophilicity constant(x), 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.

BOOKS SUGGESTED :

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
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J. Arienes
9. Principles of Medicinal Chemistty VolI & 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 Harikishan singh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
16.Strategies for organic drug synthesis and design By Daniel Ledneicer.
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotechnology By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol.1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery. Edited by Povi Krogsgaard - Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal-Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342-6363.
http://www.pfizer.com/news/featured stories/featured stories martin edwards.jsp

PAPER II CH (OC) 402T(CORE): ADVANCED HETEROCYCLIC CHEMISTRY

OC-22: Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms
OC-23: Six membered heterocyclics with two heteroatoms and Five membered heterocyclics with more than two heteroatoms
OC-24: Six membered heterocyclics with more than two heteroatoms and Larger ring heterocyclics

OC-22: Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms — 15 Hrs

Heterocyclic compounds: Introduction, Nomenclature Synthesis and reactivity of indole, quinone, isoqunoline and acridine.
Nonaromatic heterocyclics: Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines,Azetidines, Oxetanes and Thietanes.
Five membered heterocyclics with two heteroatoms: Synthesis, reactivity, aromatic character and importance of the following Heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole.

OC-23: Six membered heterocyclics with two heteroatoms and Five membered heterocyclics with more than two heteroatoms — 15 Hrs

Six membered heterocyclics with two heteroatoms: Synthesis, reactivity, aromatic character and importance of the following Heterocycles:Pyridazine, Pyrimidine, Pyrazine, Oxazine, Thiazine.
Five membered heterocyclics with more than two heteroatoms: Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoles, 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.

OC-24: Six membered heterocyclics with more than two heteroatoms and Larger ring heterocyclics — 15 Hrs

Six membered heterocyclics with more than two heteroatoms: 1,2,3-triazine, 1,2,4-triazine, 1,3,5-trianne, tetrazines. Synthesis and importance of purines and pteridines. Syntheis of Caffeine. theobromine and theophylline.
Larger ring heterocyclics: Synthesis, structure, stability and reactivity of Azepines, Oxepines, Thiepines. Synthesis of diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepines, Azocines and Azonine.

BOOKS SUGGESTED:

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
4. Principles of Modern Heterocyclie Chemistry, A.Paquette

5. Heterocyclic Chemistry, J,A.Joule & Smith
6. Handbook of Heterocyclic Chemistry, A.R.Katritzky
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

PAPER-III CH (OC) 403 T(ELECTIVE IIIA): DRUG SYNTHESIS AND MECHANISM OF ACTION

OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes
OC(CB1)-26: Drugs acting on genetic material and immune system
OC(CB1)-27: Drugs acting on receptors and ion channels

OC(CB1)-25: 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

b)Drugs acting on cell wall: Structure of bacterial cell wall, β-Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to pencillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β-Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactum

c)Drugs acting on specific enzymes: H+/K+ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

OC(CB1)-26: Drugs acting on genetic material and Chiral drugs **15Hrs**

Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amscarine, Nitracrine, Quinacrine and Chloroquine.

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.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.

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

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.

OC(CB1)-27: 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:

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.
b)Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline
c)Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
d)Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists-synthesis and pharmacological activity of Serotonin and Metoclopramide.
e)Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.
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 Ca2+, Na+ and Cl- channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

BOOKS SUGGESTED:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B.Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye etal.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam etal
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
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 (OC) 403 T(ELECTIVE IIIB): ADVANCED NATURAL PRODUCTS

OC(CB1)-25: Biosynthesis of natural products
OC(CB1)-26: Structure determination of natural products
OC(CB1)-27: Total stereo selective synthesis of natural products.

OC(CB1)-25: Biosynthesis of Natural Products — 15 Hrs

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β-amyrin) and carotenoids, steroids – cholesterol.

OC(CB1)-26: Structure Determination of Natural Products — 15Hrs

a) **By Chemical Methods:** Determination of structure and stereochemistry of reserpine, abietic acid and rotenone.

b) **By Spectral Methods:**

i) IR, UV, ^{1}H NMR, ^{13}C NMR, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples: flavones, flavanones, coumarins, quinolines.

ii) DEPT and NOE of Geraniol; INEPT of **menthol.**

iii) Heteronuclear 2D-J resolved spectrum of **stricticine**, HETEROCOSY of **strictanol.**

OC(CB1)-27: Total Stereo Selective Synthesis of Natural Products — 15Hrs

Takasago synthesis of Menthol, Hoffmann-LaRoche synthesis of Biotin, Corey's synthesis of Prostaglandins (E2, F2α) and Paeoniflorin, Sharpless synthesis of L-hexoses, Danishefsky synthesis of Indolizomycin, Nicolaou's synthesis of Taxol, Meyer s synthesis of Dynemicin A.

BOOKS SUGGESTED:

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

27/11/24

13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed.R O C Norman and J M Coxen
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

Laboratory courses

Paper-IV CH (OC) 451P: Spectroscopic Identification of Organic Compounds **4 Hrs/Week**
Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR, and mass spectral data (five examples with 2D-NMR). A minimum of 25 representative examples should be studied.

Paper-V CH (OC) 452P: Synthesis of following Drugs **4 Hrs/Week**
Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, FIuorescien, 4-Aminobenzene sulfonamide, antipyrine and phenothiazine, 2,4,5-tri phenyl imidazole, 4-chloro benzhydryl piperazine

Paper-VII CH (OC) 453P: Practice of Chemistry Software Programmes **2 Hrs/Week**
Chem Draw, analysis of IR and NMR using ACD/Id NMR processor. EXCEL: Drawing graphs, Molecular docking.

SUGGESTED 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

PROJECT CH (OC) 454P **12 Hrs/ week**

IV Semester Project Assessment for 175 Marks

Marks Distribution for Project Assessment

INTERNAL ASSESSMENT

Research Design Seminar	1 credit	25 marks
Progress Seminar	1 credit	25 marks

SEMESTER END ASSESSMENT

Dissertation	1 credit	50 marks
Final presentation	2 credits	50 marks
Viva Voce during final presentation	1 credit	25 marks

M.Sc. CHEMISTRY

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

FOR STUDENTS ADMITTED FROM THE YEAR 2023-24 ONWARDS

M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters
[Under Restructured CBCS Scheme]
(for the batches admitted in academic year 2023-24 onwards under CBCS pattern)
Grand total marks and credits (all 4 semesters) 2400 marks – 80 credits

(Approved in the P.G. BOS meeting held on 27-01-2024)

Semester - III (Physical Chemistry)

	Instruction Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)301T (Core)	3	50 marks	50 marks	100 marks	3
CH(PC)302T (Core)	3	50 marks	50 marks	100 marks	3
CH(PC)303T (Elective)	3	50 marks	50 marks	100 marks	3
CH(PC)304T (Elective)	3	50 marks	50 marks	100 marks	3
CH351P (PC LAB1)	4		50 marks	50 marks	2
CH352P (PC LAB2)	4		50 marks	50 marks	2
CH353P (PC LAB3)	2		25 marks	25 marks	1
CH354P (PC LAB4)	2		25 marks	25 marks	1
Seminar	2		50 Marks	50 Marks	2
Total	26			600 marks	20

Semester - IV (Physical Chemistry)

	Instruction Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PC)401T (Core)	3	50 marks	50 marks	100 marks	3
CH(PC)402T (Core)	3	50 marks	50 marks	100 marks	3
CH(PC)403T (Elective)	3	50 marks	50 marks	100 marks	3
CH451P (PC LAB1)	4		50 marks	50 marks	2
CH452P (PC LAB2)	4		50 marks	50 marks	2
CH453P (PC LAB3)	2		25 marks	25 marks	1
CH454P (Project)	12	50 marks	125 marks	175 marks	6
Total	31			600 marks	20

Grand total marks and credits (all 4 semesters) 2400 marks - 80 credits

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2023 -24 & later under CBCS pattern)

PAPER CH (PC) 301T (CORE): QUANTUM CHEMISTRY AND GROUP THEORY
PC - 07: Applications of Schrödinger equation
PC - 08: Angular momentum & approximate methods
PC - 09: Group theory

PAPER II CH (PC) 302T (CORE): SPECTROSCOPY
PC - 10: NMR, NQR and Mossbauer Spectroscopy
PC - 11: X-ray Spectroscopy & Diffraction techniques
PC - 12: Photoelectron and ESR spectroscopy

PAPER III CH (PC) 303T (ELECTIVE IIIA): ELECTROCHEMISTRY AND TYPES OF MATERIALS
PC(CB1)-13: Electrochemistry-II
PC(CB1)-14: Applied Electrochemistry
PC(CB1)-15: Types of Materials

Paper-III CH (PC) 303T (ELECTIVE IIIB): BIOPOLYMER CHEMISTRY
PC(CB1)-13: Bioenergetics and physical properties of biopolymers
PC(CB1)-14: Biological membranes and binding of ligands by biopolymers
PC(CB1)-15: DNA, genes and cloning

PAPER-IV CH (PC) 304T (ELECTIVE IVA): POLYMER CHEMISTRY
PC(CB2)-16: Polymerization and Kinetics of polymerization
PC(CB2)-17: Structure, Properties and Processing of polymers
PC(CB2)-18: Functional polymers

Paper IV CH (PC) 304T (ELECTIVE IVB): ENVIRONMENTAL CHEMISTRY
PC(CB2)-16: Pollution in Atmosphere
PC(CB2)-17: Pollution in Hydrosphere
PC(CB2)-18: Heavy Metal and Radiochemical Pollution.

LABORATORY COURSES

Paper-V CH (PC) 351 P: Chemical Kinetics - I
Paper-VI CH (PC) 352 P: Conductometry
Paper-VII CH (PC) 353 P: Estimations and Nanomaterial Synthesis & Characterization
Paper-VIII CH (PC) 354 P: Potentiometry and Graphical Analysis of Data & Molecular Visualization using Software tool

SEMINAR

M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(for the batches admitted in the academic year 2023 and later under CBCS pattern)

PAPER I CH (PC) 401T (CORE): THERMODYNAMICS AND CHEMICAL KINETICS
PC- 19: Statistical Thermodynamics
PC- 20: Non-equilibrium Thermodynamics
PC- 21: Chemical Kinetics-II

PAPER II CH (PC) 402T (CORE): SUPRAMOLECULAR CHEMISTRY, PHOTO CHEMISTRY AND COMPUTATIONAL CHEMISTRY
PC-22: Supramolecular Chemistry
PC-23: Photochemistry-II
PC-24: Computational Chemistry

PAPER-III CH (PC) 403 T(ELECTIVE IIIA) : CATALYSIS
PC(CB1)-25: Homogeneous catalysis
PC(CB1)-26: Micellar catalysis, Phase transfer and Photo catalysis
PC(CB1)-27: Heterogeneous catalysis

PAPER III CH (PC) 403 T(ELECTIVE IIIB) : DYNAMICS OF CHEMICAL REACTIONS
PC(CB1)-25: MO and VB theory of reactivity
PC(CB1)-26: Kinetic, isotopic, structural, solvent, steric and conformational effects
PC(CB1)-27: Nucleophilic, electrophilic and free radical reactivity

PAPER III CH (PC) – 403T (ELECTIVE IIIC): MOLECULAR MODELING AND IT'S APPLICATIONS
PC(CB1)-25: Molecular Modeling
PC(CB1)-26: Drug Design Methods I – Ligand Based
PC(CB1)-27: Drug Design Methods II - structure based

PAPER III CH (PC) 403T(ELECTIVE IIID): ENGINEERING CHEMISTRY
PC(CB1) -25: Water and Waste Water Treatment
PC(CB1) -26: Corrosion and Its Control
PC(CB1) -27: Energy Sources

PAPER III CH(PC) 403T(ELECTIVE IIIE): SUGAR CHEMISTRY AND SUGAR TECHNOLOGY
PC(CB1) -25: Sugar Chemistry
PC(CB1) -26: Sugar and Sugar byproducts
PC(CB1) -27: Methodology used in Sugar Analysis

LABORATORY COURSES
Paper IV CH (PC) 451P: Chemical Kinetics -II
Paper V CH (PC) 452P: Spectrophotometry
Paper VI CH (PC) 453P: pHmetry

PROJECT CH(PC)454P

M.Sc. SEMESTER - III
PHYSICAL CHEMISTRY Specialization
(for the batches admitted in academic year 2023 and later under CBCS pattern)

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

PC - 07: Applications of Schrödinger equation
PC - 08: Angular momentum and approximate methods
PC - 09: Group theory

PC–07: Applications of Schrödinger equation — 15 Hrs

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunnelling – examples - α-particle emission, inversion of NH_3, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

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

PC–08: 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.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Born-Oppenheimer approximation. Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Introduction to extended Huckel Theory.

Approximate methods- The variation method. Construction of variation function by the method of linear combinations. Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom. Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations. (no derivation). The Fock operator. Core hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions.

PC–09: 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_{2h}(trans-1,2-dichloroethene), C_{2v} (H_2O) and C_{3v} (NH_3) groups.

Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

BOOKS SUGGESTED:

1. Quantum Chemistry, Ira N. Levine, 6th Edition. Prentice Hall of India (2009)
2. Introduction to Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, 4th Edition, (1979)
3. Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill, 2nd Edition (1990)
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Oxford Univ. Press (2005)
5. Physical Chemistry-A Molecular approach, D.A. McQuarrie and J.D. Simon, Viva Pvt Ltd (1997)
6. Coulson's Valence, R. McWeeny, Oxford: ELBS and Oxford University Press(1979)
7. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley (1985)
8. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, ELBS(1969)
9. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons, 3rd Edition(1991)
10. Symmetry and Group Theory in Chemistry, Mark Ladd, Harwood Publishers, London (1998).
11. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, 2nd Edition, Plenum Press, NY (1995)
12. Molecular Symmetry and Group Theory, Robert L. Carter, John Wiley & Sons (1998)
13. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991)
14. Symmetry and Spectroscopy of Molecules by K Veera Reddy, New Age Int. Publishers(2007)

PAPER II CH (PC) 302T (CORE) : SPECTROSCOPY

PC - 10 : NMR, NQR and Mossbauer Spectroscopy
PC - 11 : X-ray Spectroscopy and Diffraction techniques
PC - 12 : Photoelectron and ESR spectroscopy

PC-10: NMR, NQR and Mossbauer Spectroscopy — 15 Hrs

Principle of NMR, Derivation of $h\nu = g\beta H$. Larmor processional frequency- spin-spin splitting (AX) - Quantitative treatment (proof for J= distance between two successive NMR spectral lines) – Instrumentation - CW instrument and FT instrument.

2D NMR Spectroscopy: Principles of 2DNMR-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 (NOE)- 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-11: 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.

X-ray diffraction: Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PC-12: PES and ESR Spectroscopy — 15 Hrs

Photoelectron Spectroscopy

Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS. Binding Energies, Koopman's Theorem, Chemical Shifts.

Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M+) species, Prediction of Nature of Molecular Orbitals.

ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance

Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'.

Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy and quadrupolar interactions.
Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bis-salcylaldimine, Bis-acetylacetanatovanadyl (II) and hexachloroiridium(IV) complexes

BOOKS SUGGESTED:

1. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons,4th Edition (2004)
2. Fundamentals of Molecular Spectroscopy, Banwell & McCash, McGraw Hill (1994)
3. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (1962)
4. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill(1988)
5. Basic principles of Spectroscopy, R. Chang, McGraw Hill (1971)
6. Molecular Spectroscopy by G Arhuldas, PHI Learning Private Ltd. New Delhi (2007)
7. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley-VCH publishers (2013)
8. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood (1990)
9. NMR basic principles - Atta-ur-Rahman, Springer (1986)
10. Two dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun & R. M. K. Carlson, Wiley-VCH(1994)
11. X-ray diffraction procedures for polycrystalline and amorphous materials, H. P. Klug & L. E. Alexander, John Wiley(1974)
12. Physical Chemistry, Ira N. Levine, McGraw Hill (2009)
13. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press (2018)
14. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press(1977)
15. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing(1992)
16. International series of Monographs, Vol. 53: Photoelectron Spectroscopy, Edited by D. Becker and D. Betteridge (1972)
17. Structural methods in inorganic chemistry, E.A.V. Ebsworth, Blackwell Scientific Publications, Oxford (1987)
18. Solid state chemistry and applications. A. R. West, John Wiley & Sons (1984)

PAPER III CH(PC) 303T(ELECTIVE IIIA): ELECTROCHEMISTRY AND TYPES OF MATERIALS

PC(CB1) - 13: Electrochemistry – II
PC(CB1) - 14: Applied Electrochemistry
PC(CB1) - 15: Types of materials

PC(CB1)-13: Electrochemistry – II — 15 Hrs

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunnelling Phenomenon.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion. Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion. Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

PC(CB1)-14: Applied Electrochemistry — 15 Hrs

Batteries: Battery parameters. Energy density power density and Ragone plot. Measures of battery performance. Primary and secondary batteries. Zn/MnO_2, lead-acid and Ni-Cd batteries and Lithium cells; Lithium-thionyl chloride cell and lithium-ion battery.

Fuel cells: General Chemistry of Fuel cells. Types of fuel cells: H_2/O_2 and methanol/O_2 fuel cells. Use of porous electrodes in fuel cells. Advantages, limitations and efficiency of fuel cells.

Photovoltaic cells: Semiconductor based photo-electrochemical cells. Electrochemical energy from solar energy.

Anodic oxidation of metals. Characteristics of anodic oxide films. Industrial application of anodic oxide films.

Electroplating: Technical importance. Mechanism of electroplating. Alkaline and acid plating of copper, nickel.

Electro-organic synthesis: Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon. Reduction of nitro compounds.

PC(CB1)-15: Types of 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 fiber reinforced composites.

Preparative methods of solid materials - Ceramic method (Solid State method), co-precipitation as a precursor to solid state reaction, solutions and Hydrothermal technique-gels (Zeolite synthesis).

Techniques of single crystal growth – growth from solutions: solvothermal technique-ex: α-Al_2O_3 – growth from melts: Czochrolaski and Kyropoulous methods– growth from vapor: vapor phase transport ex: $NiCrO_4$.

Nanostructured materials: Quantum structures & confinement: Quantum wells, wires and dots-examples & applications; Carbon Nanostructures-Graphite, Graphene, Fullerenes, alkali fullerides and their superconductivity property and Carbon nanotubes-electrical and mechanical properties & applications; Nano composites.

Non-linear optical (NLO) behavior– basic concepts, second and third harmonic generation, examples of organic, inorganic and polymer NLO materials.

BOOKS SUGGESTED:

1. Modern Electrochemistry Fundamentals of Electrodics Vol. 2A, J.O.M. Bockris, A.K.N. Reddy and M.G. -Aldeco, Plenum Publishers(2001)
2. Modern Electrochemistry Electrodics in Chemistry, Engineering, Biology, and Environmental Science Vol. 2B, J. O. M. Bockris and A. K. N. Reddy, Plenum Publishers(2001)
3. Industrial Electrochemistry, D. Pletcher, Chapman & Hall(1990)
4. An Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi(1942)
5. Electrochemistry – B K Sharma, Krishmas educational publishers (1960)
6. Fundamental principles of Modern Electroplating, Lowenheim, John Wiley(1963)
7. The physics and chemistry of solids. Stephen Elliot, John Wiley & Sons (1998)
8. Solid state chemistry and applications. A. R. West, John Wiley & Sons (2022)
9. New directions in solid state chemistry. CNR Rao and Gopalakrishnan, Cambridge University Press (1997)
10. Principles of the Solid State, H. V. Keer, New Age International(1993)
11. Material Science and Engineering – An Introduction, W. D. Callister, Jr., Wiley & Sons (1985)
12. Materials Science & Engineering – A First Course, V. Raghavan, Prentice Hall (2015)
13. Nanostructured Materials and Nanotechnology, edited by Hari Singh Nalwa, Acad. Press(1999)
14. Self-Assembled Nanostructures, Jin Zhang, Zhong-lin Wang, Jun Liu, Shaowei Chen & Gan-Yu-Liu, Kluwer Academic/Plenum (2006)
15. Introduction to Nanotechnology, Charles P. Poole Jr, F. J. Owens, Wiley India Pvt. Ltd. (2003)
16. Textbook of Nanoscience and Nanotechnology by B. S. Murty, P. Shankar, Baldev Raj, B.B.Rath and James Murday, Universities Press (2013).
17. Principles of Nanoscience and Nanotechnology, M.A.Shah and Tokeer Ahmad, Narosa Publishing House (2010)

Paper III CH(PC) 303T(ELECTVE IIIB) : BIOPOLYMER CHEMISTRY

PC(CB1) - 13: Bioenergetics & physical properties of biopolymers
PC(CB1) - 14: Biological membranes & binding of ligands by biopolymers
PC(CB1) - 15: DNA, genes and cloning

PC(CB1)-13: Bioenergetics and physical properties of biopolymers — 15 Hrs

Bioenergetics: The standard state in biological processes. ATP – the currency of energy. Gibbs energy change in ATP hydrolysis, comparison with other phosphates.

Principles of coupled reactions. Glycolysis and coupled reactions involving ATP. Biological oxidation-reduction reactions – transfer of H^+ ions and electrons. Synthesis of ATP in the mitochondria. The chemiosmotic theory. Gibbs energy change accompanying the proton movement.

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

Sedimentation: Sedimentation velocity. Sedimentation coefficient. The Sverdberg equation. Sedimentation equilibrium analysis. Ultra centrifugation Molecular weights. Light scattering method.
Electrophoresis: principle involved. Gel electrophoresis. Electrophoretic mobility. Applications.

PC(CB1)-14: Biological membranes and binding of ligands by biopolymers — 15 Hrs

Structure and function of cell membrane. Membrane equilibria and thermodynamics of membrane equilibria. Dialysis equilibrium. Osmotic pressure. Membrane potentials. Transport across membranes. Passive transport, facilitated transport and active transport.

Sodium-potassium pump. Selective ion transport and membrane potential. The Goldman equation (derivation not required). Nerve cells. The transfer of information in the body. The action potential and the mechanism of action potential propagation. Signal transducing mechanism involving gated ion channels in the plasma membrane.

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(CB1)-15: 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

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.

Satellite DNAs – micro and mini satellites. Sequence polymorphisms – RFLPs. Principles of DNA finger printing technology.

BOOKS SUGGESTED:

1. Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company (1980)
2. Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall (1998)
3. Physical Biochemistry: Principles and Applications, David Sheehan, John Wiley (2013)
4. Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books (2000)
5. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan(2021)
6. Biochemistry, L. Stryer, W. H. Freeman and Company,8th Edition(2021)
7. Concepts in Biochemistry, Rodney Boyer, Books/Cole Publishing Company(2005)
8. Modern Electrochemistry 2B, Bockris & Reddy, Kluwer Academic/ Plenum(2001)

Paper IV CH(PC) 304T(ELECTVE IVA): POLYMER CHEMISTRY

PC(CB2) - 16: Polymerization and Kinetics of polymerization
PC(CB2) - 17: Structure properties and processing of polymers
PC(CB2) - 18: Functional polymers

PC(CB2) - 16: 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.

Copolymerization reactions. Reactivity ratios and conditions required for the formation of copolymer. Alfrey and Price Q-e scheme for monomer and radical reactivity.

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

PC(CB2) - 17: Structure, properties and processing of polymers **15 Hrs**

Polymer solutions: The process of polymer dissolution. Thermodynamics of polymer dissolution. Entropy, heat and free energy of mixing of polymer solutions. Conformations of dissolved polymer chains. The freely jointed chain. Short-range and long-range interactions. The Flory-Huggins theory of polymer solutions. Dilute polymer solutions. Flory-Krigbaum theory.

Mechanical properties of polymers: The elastic state. Rubber-like elasticity and viscoelasticity. Newtonian and non-Newtonian behaviour. Maxwell and Voigt-Kelvin models of viscoelastic behaviour.

The crystal structure of polymers. Morphology of crystalline polymers. Crystallization and melting. Determination of Tm. Thermodynamics of crystalline melting. Heats and entropies of fusion. Degree of crystallinity. Factors affecting the crystallization.

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.

Processing of Polymers: Polymer Additives - Fillers, plasticizers, lubricants, catalysts, stabilizers, colorants, antioxidants, flame retardants. Processing techniques of polymers - One dimensional Coating, Molding and Casting of Polymers

PC(CB2) - 18: Functional polymers **15 Hrs**

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, polyacetic acid and polyvinylalcohol.

Polymers in Membrane separation. Filtration – micro, ultra and nanofiltration. Separation of gases – permeselectivity and gas permeability of representative polymers. Liquid separation – dialysis, electro osmosis and reverse osmosis.

Fire retarding polymers, photonic polymers.
Polymers in biomedical applications – artificial organs and controlled drug delivery.
Biosensors – Importance of sensors, Molecular imprinting polymers and their applications.

Books suggested:

1. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons (1984)
2. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern (1986)
3. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall (2003)
4. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and professional (1991)
5. Materials scince and engineering an introduction by William D Callister, Jr. Wiley Publishers(1997)
6. Polymer Chemistry, B. Vollmert, Springer publishers(1973)
7. Physical Chemistry of Polymers, A. Tagers, Mir Publishers(1972)
8. A text book of polymers, Vol. I,II,III, M.S. Bhatnagar, S. Chand publishers(2004)
9. Brian R. Eggins, Chemical Sensors and Biosensors, Analytical Techniques in the Sciences (ANTS), 2nd Edition, Wiley (2002).
10. Gabor Harsanyi, Sensors in Biomedical Applications - Fundamentals, Technology and Applications, CRC Press (2000).

Paper IV CH (PC) 304T(ELECTIVE IVB): ENVIRONMENTAL CHEMISTRY

PC(CB2) - 16: Pollution in Atmosphere
PC(CB2) - 17: Pollution in Hydrosphere
PC(CB2) - 18: Heavy Metal and Radiochemical Pollution.

PC(CB2) - 16: Pollution in Atmosphere — 15 Hrs

Typical Composition of Unpolluted Dry Air - Major Air Pollutants: Carbon Monoxide, Nitrogen Oxides, Sulphur Oxides, Particulate Matter, Hydrocarbons, Chlorofluorocarbons.

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

Nitrogen Oxides (NO_x): Reactions Leading to Formation of NO_x, Sources and Sinks, Concentration Profile, Harmful Effects of NO_x on Human Beings, Plants, Materials and Control of NO_x Emissions.

Sulphur Oxides (SO_x): Reactions Leading to Formation of SO_x, Sources of SO_x. Harmful Effects on Human Beings, Plants and Materials - Control of SO_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(CB2) -17: Pollution in Hydrosphere — 15 Hrs

Types of Water Pollutants and their Effects - Sources of Water Pollution: Domestic, Industrial, Agricultural, Soil,

Thermal and Radioactive Wastes - Types of Persistent Pollutants - Biomagnification of Persistent Pollutants, Effects of Biomagnified Pollutants on Human Beings (DDT) – Tripolyphosphates: Their Role in Eutrophication of Water Bodies - Ecological Consequences of Eutrophication,

Bacteriological Contamination of Water - Dissolved Oxygen in Natural Waters - Depletion of Dissolved Oxygen - Biological Oxygen Demand and Chemical Oxygen Demand as Indicators of Extent of Water Pollution - Nitrates, Nitrites, Nitrosoamines in Water: Their Toxic Effects On Human Beings - Treatment of Drinking Water Supplies.

PC(CB2) -18: Heavy Metal and Radiochemical Pollution — 15 Hrs

Essential and Toxic Elements in Nature - Mechanism of Metal Ion Toxicity - Effects on Non-Metalloenzymes, Metalloenzymes, Cell Membranes, Nucleic Acids - Concepts of Speciation, Biomethylation and Biomagnification.

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.

Organic Compounds - Harmful Effects of Radioactive Pollutants on Living Organisms - Permissible Limits of Radiation - Control and Disposal of Radioactive Wastes - Chernobyl Disaster.

Books Suggested:

1. Environmental Chemistry, John. W. Moore and Elizabeth Moore Academic press New York (1976)
2. Principles of Environmental Chemistry, Stanley E. Manahan 2nd Edition(2000)
3. Environmental Chemistry, 4th ed. A.K. De. New Age International Publishers (2000)
4. Environmental Pollution Analysis, S.M. Khopkar Wiley Eastern Ltd. (1995)
5. Environmental Chemistry, Colin Baird W.H. Freeman and Company New York (1995)
6. Text Book of Environmental Chemistry, Ayodhya Singh, Campus Books International publishers(2008)
7. Chemistry of the Environment, II Edn. Thomas G. Spiro William M. Stigliani
8. Fundamental Concepts of Environmental Chemistry, G.S. Sodhi Narosa Publishing House(2009)

LABORATORY COURSES

Paper-V CH (PC) 351 P: (Chemical Kinetics - I) **4 Hrs/week**

- 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^+]

Paper-VI CH (PC) 352 P: Conductometry **4 Hrs/ week**

Conductometry:

- Conductometric titrations:
  1. Mixture of strong acid, weak acid and $CuSO_4$ vs strong base
  2. Mixture of halides (chloride + iodide) vs $AgNO_3$
  3. Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and trichloroacetic acid and their mixtures vs strong base
  4. Precipitation titration: K_2SO_4 vs $BaCl_2$
- 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

Paper-VII CH (PC) 353 P: Estimations and Nanomaterial Synthesis and Characterization
2 hrs/ week

I. Estimations

1. Determination of Aspirin with KOH conductometrically.
2. Determination of assay of sulphanilamide-potentiometrically
3. Assay of paracetamol colorimetrically.

II. Synthesis of nanomaterials

4. Synthesis of TiO_2/ZnO (Sol-gel method)
5. Characterisation of ZnO, MgO, TiO_2, ZrO_2, γ-Al_2O_3 and zeolite($M_{2/n}O.Al_2O_3.xSiO_2$) by a) XRD b) SEM - EDAX c) TEM d) UV-DRS e) FT-IR f) XPS g) BET-SA

Paper-VIII CH (PC) 354 P: Potentiometry and Graphical Analysis of Data & Molecular Visualization using Software Tool **2 Hrs/ week**

♦ 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)
5. Mixture of halides vs $AgNO_3$ or Mixture of KI and KSCN vs $AgNO_3$

♦ Graphical Analysis of Data

6. The data obtained in all the experiments are to be analyzed by the students by usual graphical methods and with software tools like MS EXCEL and/or ORIGIN

♦Molecular visualization and/or energy calculations using Chem draw software tool

7. a) cyclohexane b) amino acids (acidic and basic) c) naphthalene and/or anthracene

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2 (1989)
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati(2007)
3. Experimental Physical Chemistry: V. Athawale and P. Mathur(2001)
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan (2015)
5. Practical in Physical Chemistry: P.S. Sindhu (2006)
6. Advanced Practical Physical chemistry: J.B.Yadav (2016)

SEMINAR **2 Hrs/ week**

M.Sc. SEMESTER - IV
PHYSICAL CHEMISTRY SPECIALIZATION
(For the batches admitted in academic year 2023 onwards under CBCS pattern)

PAPER I CH(PC)401 (CORE): THERMODYNAMICS AND CHEMICAL KINETICS

PC-19 : Statistical Thermodynamics
PC-20 : Non-equilibrium Thermodynamics
PC-21 : Chemical Kinetics-II

PC -19: Statistical Thermodynamics — 15 Hrs

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles.

The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory.
The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

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-20: Non-equilibrium Thermodynamics — 15 Hrs

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.

Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle of minimum entropy production.

Irreversible thermodynamics as applied to biological systems - examples.

Application to thermoelectric circuits. Seebeck and Peltier effect.

PC-21: 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) and kinetic equations for chemical relaxation.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses.

Specificity of enzyme-catalyzed reactions. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved. Enzyme irreversible and reversible inhibition. Discussion of equations involved.

BOOKS SUGGESTED:

1. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley (1974)
2. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley (1962)
3. Statistical Thermodynamics, M. C. Gupta, New Age International (2021)
4. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press (2022)
5. Molecular Thermodynamics, D. A. McQuarrie & J. D. Simon, University Science Books(1999)
6. Introduction to Non-equilibrium Physical Chemistry by R.P. Rastogi, Elsevier (2007)
7. Advanced physical chemistry by Gurtu and Gurtu, Pragati Edition(2021)
8. Physical chemistry by Puri and Sharma, Vishal Publishing Co.(2021)
9. Chemical Kinetics, K. J. Laidler, McGraw Hill (1987)
10. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & sons (1981)
11. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan(1993)
12. Chemical Kinetics and Reaction Mechanisms, J. H. Espenson, McGraw Hill(1981)
13. Physical Organic Chemistry, N. S. Isaacs, ELBS(1987)
14. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press (1985)
15. Lehninger Principles of Biochemistry, D. L. Nelson & M. M. Cox, MacMillan (2017)
16. Biochemistry by Jeremy M. Berg, Lubert Stryer, John Tymoczko and Gregory Gatto, W. H. Freeman and Company(2021)

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

PC-22: Supramolecular Chemistry
PC-23: Photochemistry
PC-24: Computational Chemistry

PC-22: Supramolecular Chemistry — 15 Hrs

Concepts: Molecules, super molecules and supramolecules. Nature of Supramolecular interactions. Molecular recognition – factors involved. Ionophores. Molecular receptors – design principles.

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-23: Photochemistry – II — 15 Hrs

Formation of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization.

E-type and P-type delayed fluorescence. Evaluation of triplet energy splitting ΔE_{ST}. 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-24: Computational Chemistry — 15 Hrs

Computational treatment of many electron systems:

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations.(no derivation). The Fock operator. Core hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions. Orbital energies and total energy. Helium atom example. Koopman's theorem. Hund's rules and theoretical basis of the Aufbau principle. Electron correlation energy.

The Hartree-Fock method for molecules. Restricted and unrestricted HF calculations. The Roothan equations. The Fock matrix. The Roothan matrix elements. GTOs and different types of basis sets. Minimal basis set. Model HF calculations on H_2. Discussion of results of HF calculations on simple molecules – H_2O and NH_3. Introduction to configuration interaction.

Density functional theory (DFT). Hohenberg-Kohn theorem. Kohn-Sham (KS) formulation of DFT. KS equations and KS orbitals. Brief explanation of exchange-correlation energy and exchange- correlation potential.

Books suggested:

1) J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York (2022)
2) Piet W. N. M. van Leeuwen, Supramolecular Catalysis, Wiley-VCH Verlag GmbH & Co.(2021)
3) Principles and methods in supramolecular chemistry, Hans-Jorg Schneider and A.Yatsimirsky, John Wiley and Sons(2000)
4) Analytical Chemistry of Macrocyclic and Supramolecular Compounds, S.M.Khopkar, Narosa Publishing House (2002)
5) Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Science (1991)
6) Quantum Chemistry, I. N. Levine, Prentice Hall(1991)
7) Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, Oxford University Press(1968)
8) Introduction to Computational Chemistry, F. Jensen, John Wiley & Sons (2012)
9) Elementary Quantum Chemistry, F. L. Pilar, McGraw Hill (1968)
10) Modern Quantum Chemistry, A. Szabo and N. S. Ostlund, Dover publishers(1982)
11) Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications(2011)
12) Physical Chemistry, D. A. McQuarrie and J. D. Simon, Viva Books Ltd.(2008)
13) Physical Chemistry, P. W. Atkins, Oxford University Press (2010)
14) Approximate Molecular Orbital Theory, J. A. Popple and D. L. Beveridge, McGraw Hill(1970)
15) Biophysical Chemistry, Cantor & Schimmel, W. H. Freeman and Company (1980)
16) Principles of Physical Biochemistry, Kensal E van Holde, W. Curtis Johnson & P. Shing Ho, Prentice Hall (2006)
17) Physical Biochemistry: Principles and Applications, David Sheehan, John Wiley(2009)
18) Physical Chemistry for the Chemical and Biological Sciences, Raymond Chang, University Science Books(2000)

PAPER III CH(PC) 403T(ELECTIVE IIIA): CATALYSIS

PC(CB1) -25: Homogeneous catalysis
PC(CB1) -26: Micellar catalysis, Phase transfer catalysis & Photo catalysis
PC(CB1) -27: Heterogeneous catalysis

PC(CB1)-25: 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.
Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function (Ho), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and its applications. Bunnett – Olson's criteria of acid-base catalyzed reactions with examples.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions. Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

PC(CB1)-26: Micellar catalysis, Phase transfer and Photo catalysis — 15 Hrs

Micelles: Classification of surface active agents. Micellization and micellar interactions. Structure of micelles – spherical and laminar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants.

Reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

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., quaternary ammonium salts and crown ethers.

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.

PC(CB1)-27: Heterogeneous catalysis **15 Hrs**

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

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. Adsorption isotherms - Langmiur Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts-Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM & AFM, XPS, AES, techniques.

Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

BOOKS SUGGESTED:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing (1974)
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill (1980)
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House (2002)
4. Catalysis, J. C. Kuriacose, Macmillan (2009)
5. Colloidal and surface chemistry , M. Satake, Y. Hayashi, Y.Mido, S.A.Iqbal and M.S.sethi(1996)
6. "Physical Organic Chemistry" by L.P.Hammett, chapter 9, McGraw Hill (1940)
7. Chemical Review, **57**, 1935(1957), M.A. Paul and F.A. Long
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Academic Press(1994)
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim(1983)
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer(1977)
11. Hand book of phase transfer catalysis edited by Y. Sasson and R. Neumann, Chapman & Hall(1997)
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Acad. Press(1975)
13. Reaction Kinetics in Micelles, E. H. Codes (Ed.), Plenum(1973)
14. Micelles – Theoretical and Applied Aspects, V. Moroi, plenum(1992)
15. Physical Chemistry of surfaces, A.W. Adamson and A.P. Gast, Wiley (1997)
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprensive Organometallic Chemistry
17. Principles and Practice of Heterogeneous Catalysis, J. M.Thomas and W.J.Thomas, VCH(1997)
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet (2012)
19. Modern methods of Organic Synthesis: Ahluwalia(2004)
20. Fundamental Concepts In Heterogeneous Catalysis by Jens K. Norskov , Felix Studt , Frank Abild-Pedersen, Thomas Bligaard, John Wiley & Sons Inc.(2014)

PAPER III CH(PC) 403 T(ELECTIVE IIIB) : DYNAMICS OF CHEMICAL REACTIONS

PC(CB1) -25: MO and VB theory of reactivity
PC(CB1) -26: Kinetic, isotopic, structural, solvent, steric and conformatlonal effects
PC(CB1) -27: Nucleophilic, electrophilic and free radical reactivity

PC(CB1)-25: Molecular Orbital (MO) and Valence Bond (VB) theory of reactivity 15 Hrs

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semiemperical methods and ab inito and density functional methods. Scope and limitations of several computational programmes. Quantitative MO theory-Huckel molecular orbital (HMO) method as applied to ethane energy levels. Orbital symmetry, orbital interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity. Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model nature of activation barrier in chemical reactions. Principle of reactivity Mechanistic significance of entropy, enthalpy and Gibbs free energy. Arrhenius equation, transition state theory. Uses of activation parameters.

PC(CB1)-26: Kinetic, isotopic, structural, solvent, steric and conformational effects 15 Hrs

Theory of isotope effects, Primary and secondary kinetic isotope effects. Heavy isotope effects. Tunneling effect Solvent effects. Structural effects on reactivity: Linear free energy relationship (LFER.). The Hammett equation, substituent constants, theories of substituent effects. interpretation of σ-values. Reaction constant ρ. Deviations from Hammett equation. Dual—parameter correlations, inductive substituent constant The Taft model, σ1, σR scales. Solvation and solvent effects: Qualitative understanding of solvent- solute effects on reactivity Thermodynamic measure of solvation. Effects of solvation on reaction and equilibrium. Various empirical indexes of solvation based on physical properties, solvent- sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

PC(CB1)-27: Nucleophilic, Electrophilic and Free Radical Reactivity 15 Hrs

Bases, nucleophiles, Electrophiles and Catalysts. Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales, Nucleofugality. The α-effect- Ambivalent nucleophiles. Acid-base catalysis. Specific and general catalysis. Bronsted catalysis. nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding micellar catalysts. Nucleophilic and electrophilic Reactivity: Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects, kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. Nucleophilicity and S2 reactivity based on curve-crossing model. Relationship between polar and electron transfer

reactions. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetics of SE2-Ar reaction, Structural effects on rates and selectivity. Curve crossing approach to electrophilic reactivity; Radical and pericyclic reactivity. (a)Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors affecting barrier heights in additions, regioselectivity in radical reactions. Reactivity, specificity and peri selectivity in pericyclic reactions.

BOOKS SUGGESTED:

1. Molecular mechanics. By U. Bukert and N. L. Allinger, ACS Monograph 177 (1982)
2. Organic Chemistry book of Orbitals. L. Salem and W. L. Jorgenson (1973)
3. Mechanism and theory in Organic Chemistry, T.M. Lowry, K. C. Richardson, Harper and Row (1987)
4. Introduction to theoretical Organic Chemistry and molecular modeling by W. B. Smith, VCH, Weinhein (1996)
5. Physical Organic chemistry, N.S. Isaacs (1987)
6. Supramolecular Chemistry - concepts and perspectives by J M Lehn (1995)
7. The Physical basis of Organic Chemistry by H. Maskill (1985).
8. Physical Organic Chemistry by Jack HineLaboratory course (1962)

PAPER III CH(PC) 403T(ELECTIVE IIIC): MOLECULAR MODELING AND IT'S APPLICATIONS

PC(CB1)-25: Molecular Modeling
PC(CB1)-26: Drug Design Methods I - Ligand Based
PC(CB1)-27: Drug Design Methods II - Structure Based

PC(CB1)-25: Molecular Modeling — 15 Hrs

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.

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(CB1)-26: Drug Design Methods I - Ligand Based — 15 Hrs

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, Ver loop Steric factor - Molecular Descriptor analysis: Craig plot, Topliss scheme, Bio isosteres - 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(CB1)-27: Drug Design Methods II - Structure Based. — 15 Hrs

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm, Incremental construction - Molecular Interactions, Scoring

functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

BOOKS SUGGESTED:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications(1996)
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press(1995)
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications(2010).
4. Recent advances in Bioinformatics by I. A. Khan and A Khanum Ukaaz publications (2003)
5. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH (1997)
6. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition(2007)
7. Bioinformatics – A Primer by P. Narayanan, New Age International, (PC) Ltd. (2005)
8. Introduction to Bioinformatics by Arthur M. Lesk, Oxford Univ. Press (Indian Edn) (2002)
9. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; (2007)
10. An Introduction to Medicinal Chemistry by G L Patrick, Oxford University Press(2001)
11. Bioinformatics: Methods and Applications: Genomics, Proteomics and Drug Discovery. S.C. Rastog, Namita Mendiratta, Parag Rastogi, PHI Larning Pvt. Ltd; (2006)
12. Pharmacy Practice Vol. I and II by Remington, Pharmaceutical Press(2012)
13. Burger's Medicinal Chemistry and Drug Discovery, 5th Edn., Wiley-Interscience, New York(1995)
14. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- Larsen Tommy liljefors and ULF Madsen(2002)

PAPER III CH(PC) 403T(ELECYIVE IIID): ENGINEERING CHEMISTRY

PC(CB1) - 25: Water and Waste Water Treatment
PC(CB1) - 26: Corrosion and Its Control
PC(CB1) - 27: Energy Sources

PC(CB1) - 25: Water and waste water treatment **15 Hrs**

Review of Hardness: causes, measurement of hardness, units- types of hardness, estimation of temporary and permanent hardness, numerical problems. Boiler troubles- scales and sludge formation, caustic embrittlement, priming and foaming. Methods for boiler water treatment: Soda-lime process, zeolite process, ion exchange process. Treating saline water: distillation, electrodialysis, reverse osmosis. Municipal water supply: sedimentation, filtration, sterilization. Waste water treatment: physical, chemical and biological treatment. Sewage water , COD and BOD , numerical problems

PC(CB1) - 26: Corrosion and its control: **15 Hrs**

Magnitude of the problem, theories of corrosion, Chemical and electrochemical corrosion, corrosion reactions, factors affecting corrosion- nature of metal, purity of metal, electrochemical series, over voltage, nature of oxide film, nature of corrosion product, nature of environment, effect of temperature, effect of pH, effect of oxidant, humidity. Corrosion control methods- design and material selection, cathodic protection, sacrificial anode, impressed current cathode.
Surface coating methods: Surface preparation, metallic coatings, application of metal coatings: hot dipping, galvanizing, tinning, cladding, electroplating, chemical conversion coatings. Organic surface coatings-paints, constituents of paints and their functions, methods of application of paints, failure of paint films, varnishes, enamels, lacquers.

PC(CB1) - 27: Energy Sources: **15 Hrs**

Conventional energy resources: Chemical fuels, classification, (solids, liquids, gaseous) . Solid fuels: coal, analysis of coal, proximate and ultimate analysis and their significance. Liquid fuels: petroleum, refining of petroleum, cracking, reforming. Synthetic petrol - Bergius and Fischer-Tropsch's process, knocking, anti-knocking agents, octane number. Diesel fuel: Cetane number. Other liquid fuels: LPG, biodiesel, kerosene, fuel oil, benzol, tar, power alcohol. Gaseous fuels: natural gas, coal gas, producer gas, oil gas, water gas, biogas, Combustion: Calorific value and its determination, bomb calorimeter. HCV and LCV values of fuels, problems. analysis of flue gas by Orsats method. Rocket fuels, solid propellants, liquid propellants, monopropellants, bipropellants.

Non-conventional energy resources: Nuclear fuels- nuclear reactor, nuclear fission, nuclear fusion, sources of nuclear fuels, disposal of radioactive wastes, reprocessing of nuclear fuels. solar, hydro, wind, tidal energies. Bio fuels, H_2 as a non-polluting fuel.

BOOKS SUGGESTED:

1. Text book of Engineering Chemistry by C.P. Murthy, C.V. Agarwal & A. Naidu: B.S. Publications, Hyderabad (2019).
2. Text book of Engineering Chemistry by S.S. Dara: S. Chand & Co. New Delhi (2008).
3. Engineering Chemistry by B. Siva Shanker: Mc-Graw Hill publishing Company Limited, New Delhi (2015)

4. Engineering Chemistry by J.C. Kuriocose &J. RajaramTata McGraw Hill Co. NewDelhi (2004)
5. Engineering Chemistry by P.C. Jain & Monica Jain, Dhanpatrai publishing company (2016)
6. Applied Chemistry – A text book of engineering and Technology – Springer (2012)
7. Text book of Engineering Chemistry by Shasi Chawla: Dhanpatrai Publishing company, New Delhi (2017)
8. Engineering Chemistry by R. Gopalan, D. Venkatappayya & D.V. Sulochana Nagarajan – Vikas Publishers (2005)
9. A Text Book of Engineering Chemistry by Shashi Chawla, Dhanpat Rai & Co.(2017)

PAPER III CH(PC) 403T(ELECYIVE IIIE):
SUGAR CHEMISTRY AND SUGAR TECHNOLOGY

PC(CB1) - 25: Sugar Chemistry
PC(CB1) - 26: Sugar & Sugar byproducts
PC(CB1) - 27: Methodology used in Sugar Analysis

PC(CB1) -25: Sugar Chemistry: **15 Hrs**

Carbohydrate nomenclature. Fischer, Haworth and conformational structures of mono and oligo saccharides. Chemical reactivity of sugars. Reducing and non-reducing sugars. Chiral nature of sugars. R-S nomenclature, Fischer D-L nomenclature of sugars. Sugar enantiomers, diastereo isomers, epimers and enomers. Acyclic structure of sugars, determination of relative and absolute configuration of sugars. Cyclic forms of sugars. Conformational analysis of sugars. Hassel- Otter effect. Delta-two effect. Anomeric effect. Calculation of conformational free energies. Optical rotation, specific rotation and molecular rotation of sugars. General epimer rule. Relationship between rotation and conformation.

PC(CB1) -26: Sugar & Sugar byproducts: **15 Hrs**

Structure determination of sucrose, synthesis of sucrose, biosynthesis of sucrose, chemical nature of sucrose. Oligo saccharide synthesis. Oligo saccharide optical rotating power (Hudson and Klyn rules). ^{13}C NMR spectroscopic data of glucose, fructose and sucrose. Uses of sugar chirons in organic synthesis. Sugar byproducts. Bagasse, molasses and press mud. Bagasse- characteristics and uses. Production of biogas, fiberboard and furfural. Press mud- extraction of cane wax, press mud and manure. Molasses- fermentation of molasses. Production of alcohol and rectified spirit.

PC(CB1) - 27: Methodology used in Sugar Analysis: **15 Hrs**

Sampling techniques. Determination of moisture in bagasse, molasses and cane sugar. Methods of estimation of total soluble solids in sugar and sugar house products. Optical methods of sugar analysis, sugar scales and normal weight. Estimation of reducing sugars and sugar present in cane juice by Eynon & Lane, Luff & Schoorl and Benedict's methods. Determination of sugars by Invertase method, Jackson- Gellis, Munsen- Walker's Cu_2O and De Whalley's' volumetric method. Determination of Ash by Carbonate- Ash and Cuitometeric (Conductometric) methods. Determination of various other constituents present in raw sugars. Estimation and chemical composition of cane and its juice.

BOOKS SUGGESTED:

1. Cane Sugar Hand Book, Maede & Chen, John Wiely & Sons (1993)
2. Determination of Food Carbohydrates, D. A. T. Southgate, Applied Science Publishers, London(1991)
3. Text Book of Sugar Chemistry and Sugar Technology, Mathur(1975)
4. Text Book of Sugar Byproducts, Morris Patrov
5. A Hand Book of Qualitative and Quantitative Organic Analysis, H. J. Clark, Orient Longman (2021)
6. Text Book of Biochemistry, Lehninger (2017)
7. Analysis of Sugars, Pleus
8. Text Book of Sugar Technology, Hugot (1986)
9. Instrumental Methods in Sugar Industry, Eckman

10. Principles of Instrumental Analysis, Skoog and West(1992)
11. Technical Methods of Analysis, Griffith, McGraw Hill
12. Advanced Sugar Chemistry, R. S. Shellaxberges (1982)
13. Sugar, John Yulkin, Jack Edelman, Liesel Hough(1971)
14. International Uniform Methods for Sugar Analysis, H. C. S. De Whelly

LABORATORY COURSES

Paper-IV CH (PC) 451P: Chemical Kinetics – II **4 Hrs/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-butyl chloride by conductometry**
  1. Effect of solvent's dielectric constant
  2. Polarizability (methanol/water mixture) on the rate of solvolysis
- **Study of oxidation of primary alcohols by dichromate by spectrophotometry**:
  1. Application of Taft equation

The data obtained in all the experiments are to be analyzed by the students both by usual graphical methods and regression techniques (linear/nonlinear) with software tools like MS EXCEL or ORIGIN

Paper-V CH (PC) 452P: Spectrophotometry **4 Hrs/week**

Colorimetry/Spectrophotometry

- Estimation of Cu(II) using EDTA
- Estimation of Fe(III) using thiocyanate
- Estimation of Fe(II) using 1,10-phenanthrolin
- Spectrophotometric titrations: Cu(II) vs EDTA and 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
- Estimation of Mn(II) by spectrophotometry using periodate.
- Determination of pKa of methyl red indicator
- Simultaneous determination of dichromate and permanganate in a mixture

Paper-VI CH (PC) 453P: pHmetry **2 Hrs/ week**

- 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 anddioxane
- Determination of pKa and pKb of glycine (calculation using a computer program)
- Determination of stability constant of a metal complex

Suggested books:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2 (1989)
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati(2007)
3. Experimental Physical Chemistry: V. Athawale and P. Mathur(2001)
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan (2015)
5. Practical in Physical Chemistry: P.S. Sindhu (2006)
6. Advanced Practical Physical chemistry: J.B.Yadav (2016)

PROJECT CH (PC) 454P **12 Hrs/ week**

IV Semester Project Assessment for 175 Marks

Marks Distribution for Project Assessment

INTERNAL ASSESSMENT

Research Design Seminar	1 credit	25 marks
Progress Seminar	1 credit	25 marks

SEMESTER END ASSESSMENT

Dissertation	1 credit	50 marks
Final presentation	2 credits	50 marks
Viva Voce during final presentation	1 credit	25 marks

M.Sc. CHEMISTRY

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

FOR STUDENTS ADMITTED FROM THE YEAR
2023-2024 ONWARDS

27/1/24

27/1/24

27/1/24

M.Sc. CHEMISTRY
(PHYSICAL ORGANIC CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters
[Under Restructured CBCS Scheme]
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)
Grand total marks and credits (all 4 semesters) 2400 marks –80 credits

(Approved in the P.G.BOS meeting held on 27-01-2024)

Semester - III (Physical Organic Chemistry)

	Instruction Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PO)301T (core)	3	50 marks	50 marks	100 marks	3
CH(PO)302T (core)	3	50 marks	50 marks	100 marks	3
CH(PO)303T (Elective)	3	50 marks	50 marks	100 marks	3
CH(PO)304T (Elective)	3	50 marks	50 marks	100 marks	3
CH(PO)351P	4		50 marks	50 marks	2
CH(PO)352P	4		50 marks	50 marks	2
CH(PO)353P	2		25 marks	25 marks	1
CH(PO)354P	2		25 marks	25 marks	1
Seminar	2		50 Marks	50 Marks	2
Total	26			600 marks	20

(*Core= compulsory papers common to all students admitted to M.Sc. Chemistry, OU)

Semester - IV (Physical Organic Chemistry)

	Instruction Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(PO)401T (core)	3	50 marks	50 marks	100 marks	3
CH(PO)402T (core)	3	50 marks	50 marks	100 marks	3
CH(PO)403T (Elective)	3	50 marks	50 marks	100 marks	3
CH(PO)451P	4		50 marks	50 marks	2
CH(PO)452P	4		50 marks	50 marks	2
CH(PO)453P	2		25 marks	25 marks	1
CH(PO)454P (Project)	12	50 marks	125 marks	175 marks	6
Total	31			600 marks	20

Grand total marks and credits (all 4 semesters) 2400 marks - 80 credits

M.Sc. SEMESTER - III
PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH(PO) 301T (CORE): QUANTUM CHEMISTRY AND GROUP THEORY
PO - 01: Applications of Schrödinger equation
PO - 02: Angular momentum & approximate methods
PO - 03: Group theory

Paper II CH (PO) 302T (CORE): MODERN ORGANIC SYNTHESIS
PO- 04: Synthetic Reagents – I
PO- 05: Synthetic Reagents – II
PO- 06: Synthetic Strategies

Paper-III-CH(PO)303T(ELECTIVE IIIA): SPECTROSCOPY, CHEMICAL KINETICS AND PHOTOCHEMISTRY
PO(CB1)-07:X-RaySpectroscopy & Diffraction techniques
PO(CB1)-08: Chemical Kinetics– II
PO(CB1)-09: Photochemistry – II

PAPER –III CH (PO) 303T(ELECTIVE IIIB): CATALYSIS
PO(CB1)-07: Homogeneous catalysis
PO(CB1)-08: Micellar catalysis, Phase transfer & Photo catalysis
PO(CB1)-09: Heterogeneous catalysis

Paper IV CH(PO) 304T(ELECTIVE IVA): NEW SYNTHETIC REACTIONS, CONFORMATIONAL ANALYSIS AND ^{13}C NMR SPECTROSCOPY

PO(CB2)-10: New Synthetic Reactions
PO(CB2)-11: Conformational Analysis II (Cyclic Systems)
PO(CB2)-12: ^{13}C NMR Spectroscopy

Paper IV CH(PO) 304T(ELECTIVE IVB): BIOORGANIC AND GREEN CHEMISTRY, NANOMATERIALS AND SUPRAMOLECULAR CHEMISTRY
PO(CB2)-10: Carbohydrates and Proteins
PO(CB2)-11: Principles of Green Chemistry and Synthesis
PO(CB2)-12: Organic Nanomaterials and Supramolecular Chemistry

LABORATORY COURSES

Paper V CH(PO) 351P: Chemical Kinetics

Paper VICH(PO) 352P: Synthesis of Organic compounds

Paper VIICH (PO) 353P : Potentiometry and Graphical Analysis of Data & Molecular Visualization using Software tools

PAPER VIII CH (PO) 354P : Separation and Identification of Organic Compounds

SEMINAR

M.Sc. SEMESTER - IV
PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH(PO) 401T (CORE): THERMODYNAMICS AND ELECTROCHEMISTRY
PO-13: Non-equilibrium Thermodynamics
PO-14: Statistical Thermodynamics
PO-15: Electrochemistry- II

Paper II CH(PO) 402T (CORE): HETEROCYCLIC CHEMISTRY, NEW TECHNIQUES IN ORGANIC CHEMISTRY AND ASYMMETRIC SYNTHESIS
PO-16: Five and six membered heterocycles with two hetero atoms
PO-17: New techniques and concepts in organic synthesis
PO-18: Asymmetric Synthesis

Paper III CH (PO) 403T(ELECTIVE IIIA): ADVANCED SPECTROSCOPY
PO(CB1) - 19: Photoelectron Spectroscopy (PES) and Electron spin Resonance Spectroscopy (ESR)
PO(CB1) - 20: NMR, NQR and Mössbauer Spectroscopy
PO(CB1) - 21: 2D NMR and ORD spectroscopy

Paper IV CH(PO) 403T(ELECTIVE IIIB): TOTAL STEREOSELECTIVE SYNTHESIS OF NATURAL PRODUCTS, BIOMOLECULES AND PHYSICAL PRINCIPLES OF SPECTROSCOPY and VIBRATIONAL SPECTROSCOPY
PO(CB1) - 19: Total Stereoselective Synthesis of Natural Products
PO(CB1) - 20: Biomolecules
PO(CB1) - 21: Physical principles of spectroscopy and Vibrational spectroscopy

LABORATORY COURSES

Paper-IV (Lab)-CH(PO) 451P: Instrumentation

Paper V (Lab)-CH(PO) 452P: Spectroscopic Identification of Organic Compounds

Paper-VI(Elective) -CH (PO) 453P : pH metry, Separation of mixtures and Chromatography

PROJECT CH (PO) 454P

M.Sc. SEMESTER - III
PHYSICAL ORGANIC CHEMISTRY Specialization
(for the batches admitted in academic year 2023and later under CBCS pattern)

PAPER I CH (PO) 301T(CORE): QUANTUM CHEMISTRY AND GROUP THEORY

PO - 01: Applications of Schrödinger equation
PO - 02: Angular momentum and approximate methods
PO - 03: Group theory

PO–01: Applications of Schrödinger equation — 15 Hrs

Systems with discontinuity in the potential field. A simple potential barrier. A potential barrier with a finite thickness. Quantum mechanical tunneling – examples - α-particle emission, inversion of NH_3, hydrogen transfer reactions.

The harmonic oscillator – detailed treatment. Wave functions and energies. Vibration of a diatomic molecule – harmonic oscillator model.

The rigid rotator – detailed treatment. Wave functions and energies. Spherical harmonics. Rigid rotator as model for a rotating diatomic molecule.

The hydrogen atom – detailed treatment. Angular and radial functions. Atomic orbitals. Measurability of the ground-state energy of hydrogen atom. Orthonormal nature of hydrogen-like wave functions. Probability calculations.

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

PO–02: 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.

Electron spin. Spin operators. Pauli principle and the Pauli exclusion principle.

Born-Oppenheimer approximation. Concept of hybridization – sp, sp^2, and sp^3 hybrid orbitals.

Semiempirical MO methods. The Huckel theory of conjugated systems. HMO calculations on ethylene, allyl system, butadiene, cyclopropenyl system and benzene. π–electron charges and bond orders. Introduction to extended Huckle Theory.

Approximate methods- The variation method. Construction of variation function by the method of linear combinations. Perturbation theory (first order and nondegenerate). Wave function and energy corrections. Application of perturbation theory to the helium atom. Time- dependent perturbation theory. Interaction of radiation and matter. Allowed and forbidden transitions.

Multi-electron atoms. The antisymmetry principle and the Slater determinant. The Hartree-Fock method. The Hartree-Fock equations (no derivation). The Fock operator. Core Hamiltonian. Coulomb operator and exchange operator. Slater-type orbitals (STOs) as basis functions.

PO–03: 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_{2h}(trans-1,2-dichloroethene), C_{2v} (H_2O) and C_{3v} (NH_3) groups.

Quantum mechanics and group theory. Wave functions as bases for irreducible representations. The direct product – vanishing of integrals. Projection operators. Symmetries of vibrations. IR and Raman activity.

BOOKS SUGGESTED:

1. Quantum Chemistry, Ira N. Levine, Seventh Edition, Pearson (2014).
2. Introductory Quantum Chemistry, A. K. Chandra, Tata McGraw-Hill (1994).
3. Elementary Quantum Chemistry, F. L. Pilar, Second Edition, McGraw Hill (2001).
4. Molecular Quantum Mechanics, P. W. Atkins & R. S. Friedman, Fifth Edition, Oxford University Press (2010).
5. Physical Chemistry-A Molecular approach, D.A. McQuarrie & J.D. Simon, First Edition, Viva Pvt. Ltd (2019).
6. Coulson's Valence, R. McWeeny, Third Edition, Oxford University Press (1980).
7. The Chemical Bond, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, John Wiley (2014).
8. Valency Theory, J. N. Murrel, S. F. A. Kettle & J. M. Tedder, Second Edition, Wiley (1969).
9. Chemical Applications of Group Theory, F. A. Cotton, Third Edition, John Wiley & Sons (1991).
10. Symmetry and Group Theory in Chemistry, Mark Ladd, Harwood Publishers, London (2000).
11. Symmetry Through the Eyes of a Chemist, I. Hargittai and M. Hargittai, Second Edition, Plenum Press, NY (1995).
12. Molecular Symmetry and Group Theory, Robert L. Carter, Second Edition, John Wiley & Sons (2001).
13. Group Theory for Chemists, G. Davidson, Macmillan Physical Science Series (1991).
14. Symmetry And Spectroscopy Of Molecules by K Veera Reddy, Second Edition, New Age International Publishers (2020).

PAPER II CH (PO) 302T(CORE):
MODERN ORGANIC SYNTHESIS

PO- 04: Synthetic Reagents I
PO- 05: Synthetic Reagents II
PO- 06: Synthetic Strategies

PO–04: Synthetic Reagents – I — 15 Hrs

i) Protecting groups:
a) Protection of alcohols by ether, silyl ether (TMS, TES, TIPS, TBDMS and TBDPS) and ester formation.
b) Protection of 1,2-diols by acetal, ketal and carbonate formation.
c) Protection of amines by benzyloxy carbonyl, *t*butyloxy carbonyl, 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, 2) Horner-Wordsworth-Emmons reaction.
b) Titanium- Carbene mediated olefination: Tebbe reagent.
iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.
v) C-H Activation: Introduction, Rh catalyzed C-H activation.

PO–05: 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^{+6} oxidants (Jones reagent, PCC, PDC), IBX, DMP, CAN, TEMPO, TPAP, Swern's 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.

PO–06: Synthetic Strategies — 15 Hrs

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis.

Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations.

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-difunctionalized, 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.

BOOKS SUGGESTED:

1. Some Modern Methods of Organic Synthesis by W. Carruthers, I. Coldham, Cambridge University Press (2004)
2. Guidebook to Organic Synthesis, Mackie, Raymond K, New York: Wiley (1990)
3. Organic Synthesis, Fourth Edition, Micheal B. Smith, Academic Press by Elsevier Inc. (2010)
4. Organic Synthesis, The Disconnection Approach, Stuart Warren, John Wiley & Sons (2004)
5. Organic Synthesis, C. Willis and M. Wills, Oxford Chemistry Primers (1996)
6. The Logic of Chemical Synthesis, E. J. Corey and Xue-Min Cheng, Wiley-Interscience (1995)
7. Advanced Organic Chemistry, Part B: Reactions and Synthesis, F. A. Carey and R. J. Sundberg, 3rd Edition, Plenum Press (1993)
8. Greene's Protective Groups in Organic Synthesis 4th ed., P. Wuts and T. Greene, John Wiley & Sons (2006)

Paper III CH(PO) 303T(ELECTIVE IIIA):
SPECTROSCOPY, CHEMICAL KINETICS AND PHOTOCHEMISTRY

PO-(CB1)07:X-RaySpectroscopy & Diffraction techniques
PO-(CB1)08: Chemical Kinetics– II
PO-(CB1)09: Photochemistry – II

PO(CB1)-07: 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.

X-ray diffraction: Bragg condition. Miller indices, d-spacing formula, Lattice planes and number of d-spacings, experimental methods of X-ray diffraction. Laue method and Debye-Scherrer method. Primitive and nonprimitive unit cells. Indexing the reflections. Identification of unit cells from systematic absences in diffraction pattern. Structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis. Typical examples.

Electron diffraction. Scattering intensity versus scattering angle. Wierl equation. Measurement technique. Elucidation of structure of simple gas phase molecules.

PO(CB1)-08: Chemical kinetics – II: **15Hrs**

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.

Enzyme kinetics: Michaelis - Menten mechanisms of enzyme catalyzed reactions involving one and two intermediates. Steady-state approximation. Derivation of kinetic equations. Evaluation of kinetic parameters. Enzyme- substrate complex: Fischer's lock and key and Koshland's induced fit hypotheses.

Specificity of enzyme-catalyzed reactions. pH dependence of enzyme-catalyzed reactions – the kinetics and the equations involved. Enzyme reversible and irreversible inhibition. Discussion of equations involved.

PO(CB1)-09: Photochemistry – II **15Hrs**

Formation of excimers and exciplexes – PE diagram and quantum yields. Energy transfer mechanism for bimolecular quenching. Long-range coulombic energy transfer – critical transfer distance. Short-range electron exchange energy transfer. Triplet-triplet energy transfer and sensitization.

E-type and P-type delayed fluorescence. Evaluation of triplet energy splitting ΔE_{ST}. 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 photo-redox reactions, examples. Photochemical cleavage of water.

BOOKS SUGGESTED:

1. X-ray diffraction procedures for polycrystalline and amorphous materials, H. P. Klug & L. E. Alexandar, John Wiley (1954).
2. Physical Chemistry, Ira N. Levine, Sixth Edition, McGraw-Hill (2009).
3. Chemical Kinetics, K. J. Laidler, Second Edition, McGraw-Hill (1973).
4. Kinetics and Mechanism, A. A. Frost & R. G. Pearson, John Wiley & Sons (1981).
5. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman & J. Kuriacose, McMillan (2000).
6. Chemical Kinetics and Reaction Mechanisms, J.H. Espenson, Second Edition, McGraw-Hill (1995).
7. Physical Organic Chemistry, N.S. Isaacs, Second Edition, Longman Scientific & Technical (1995).
8. The Physical basis of Organic Chemistry, Howard Maskill, Oxford University Press (1985).
9. Atkin's Physical Chemistry, P. Atkins & Juliode Paula, Oxford University Press (2010).
10. Essentials of Molecular Photochemistry, A. Gilbert & J. Baggott, Blackwell Scientific Publications (1991).

PAPER III CH(PO) 303T(ELECTIVE IIIB): CATALYSIS

PO(CB2) -07: Homogeneous catalysis

PO(CB2) -08: Micellar catalysis, Phase transfer & Photo catalysis

PO(CB2) -09: Heterogeneous catalysis

PO(CB2)-07: 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.

Acidity functions: Types of acidity functions. Hammett acidity function. Measurement of Hammett acidity function (*Ho*), usefulness of Hammett acidity function in understanding the mechanism of an acid catalyzed reactions. Zucker-Hammett hypothesis and its applications. Bunnett – Olson's criteria of acid-base catalyzed reactions with examples.

Catalysis by transition metal ions and their complexes. Use of Ziegler –Natta and metallocene catalysts as homogeneous catalysts for polymerization of olefins. Application of metal ion catalysis to the hydrogenation of alkenes, hydroformylation, oxidation and isomerization reactions. Asymmetric Catalysis–Introduction, Catalysts, Commercial Applications, Asymmetric Hydrogenation, Enantioselective Isomerization: L-Menthol, Asymmetric Epoxidation.

PO(CB2)-08: Micellar catalysis, Phase transfer and Photo catalysis — 15 Hrs

Micelles: Classification of surface-active agents. Micellization and micellar interactions. Structure of micelles – spherical and laminar. Critical micellar concentration (CMC). Factors affecting the CMC of surfactants.

Reverse micelles. Reactions assisted by micelle formation. Examples of micelle-catalyzed reactions and their mechanisms.

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.

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.

PO(CB2)-09: Heterogeneous catalysis — 15 Hrs

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

Steps in heterogeneous catalyzed reactions. Diffusion and adsorption. Mechanism of surface-catalyzed reactions. Adsorption isotherms - Langmiur Hinshelwood model, Rideal - Eley mechanism, Kinetics and thermodynamics of catalysed reactions. Catalytic activity – the determining factors. Structure sensitive and structure insensitive catalysts.

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalysts-Determination of surface acidity by indicator method, IR spectroscopic method and TPD methods. Surface characterization by XRD, LEED, TEM & AFM, XPS, AES, techniques.

Auto exhaust emissions- catalytic converters. Catalytic hydrogenation and oxidation reactions.

Cracking and reforming. Fischer-Tropsch synthesis of methanol.

BOOKS SUGGESTED:

1. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing
2. Heterogeneous Catalysis, C. Satterfield, McGraw Hill (1980).
3. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, Narosa Publishing House (2002).
4. Catalysis, J. C. Kuriacose, Macmillan (1980).
5. Colloidal and surface chemistry, M. Satake, Y. Hayashi, Y. Mido, S.A. Iqbal and M.S. Sethi, First Edition, Discovery Publishing Pvt. Ltd (2003)
6. Physical Organic Chemistry by L.P. Hammett, chapter 9, McGraw Hill (1940).
7. Chemical Review, M.A. Paul and F.A. Long "*Ho* and related indicator acidity functions" 57, 1-45, (1957).
8. Phase Transfer Catalysis, Fundamentals, Applications and Industrial perspective, C. M. Stark, C. Liotta & M. Halpern, Springer Science & Business Media (1994).
9. Phase Transfer Catalysis, E. V. Dehmlow & S. S. Dehmlow, Verlag Chemie, Weinheim (1980).
10. Phase Transfer Catalysis in Organic synthesis, W. P. Weber & G. W. Gokel, Springer (1997).
11. Hand book of phase transfer catalysis Edited by Y. Sasson and R. Neumann, Springer (1997).
12. Catalysis in Micellar and Macromolecular systems, J. H. Feudler & E. J. Feudler, Acad. Press (1975).
13. Reaction Kinetics in Micelles, E. H. Codes (ed), Plenum (1973).
14. Micelles – Theoretical and Applied aspects, V. Moroi, Springer New York, NY (1992).
15. Physical Chemistry of surfaces, A.W. Adamson and A.P. Gast, Wiley (1976).
16. Polymer supported Catalysts, C. U. Pittman Jr, vol 8, Comprehensive Organometallic Chemistry
17. Principles and Practice of Heterogeneous Catalysis, J. M. Thomas and W. J. Thomas, Second Edition, Wiley, VCH (2015).
18. Spectroscopy in catalysis – An introduction by J. W. Niemantsverdriet, 3rd Edition, Wiley (2007).
19. Modern methods of Organic Synthesis: Ahluwalia.

PAPER IV CH (PO) 304T(ELECTIVE IVA): NEW SYNTHETIC REACTIONS CONFORMATIONAL ANALYSIS AND ^{13}C NMR SPECTROSCOPY.

PO (CB2)-10: New Synthetic Reactions
PO (CB2)-11: Conformational Analysis – II (Cyclic systems)
PO (CB2)-12: ^{13}C NMR Spectroscopy

PO(CB3)-10: New Synthetic reactions **15 Hrs**

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.

2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey 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.

PO(CB2)-11: Conformational Analysis-II (Cyclic systems) **15 Hrs**

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*-Methyl piperidine, tropane, tropine, pseudotropine, decahydroquinoline and 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.

PO(CB2) - 12: ^{13}C 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.

Spectral editing techniques in ^{13}C-NMR: principle and applications of APT, INEPT and DEPT methods.

BOOKS SUGGESTED:

1. Advanced Organic Chemistry, Part B: Reactions and Synthesis, F. A. Carey and R. J. Sundberg, 3rd Edition, Plenum Press (1993)
2. Guidebook to Organic Synthesis, Mackie, Raymond K, New York: Wiley (1990)
3. Name Reactions, A Collection of Detailed Mechanisms and Synthetic Applications Fourth Ed., Springer (2009)
4. Stereochemistry of Organic Compounds: Principles and Applications by D. Nasipuri, New Age International (P) Limited Publishers (2005)
5. Stereochemistry of Organic Compounds by Ernest L. Eliel, Samuel H. Wilen and Lewis N. Mander, Wiley India Publishers (2008)
6. Stereochemistry: Conformation and Mechanism, by P. S. Kalsi, New Age International (P) Limited Publishers (2022)
7. Spectrometric Identification of Organic Compounds by R. M. Silverstein and F. X. Webster, 6th Ed., (1998)
8. Nuclear Magnetic Resonance in Chemistry: A Multinuclear Introduction by William Kemp, Springer Link Publishers (1986) and MacMillan Publishers (1988).
9. Nuclear Magnetic Resonance: Basic principles by Atta-ur-Rahman, Springer Publishers (2012)
10. Basic One- and Two-Dimensional NMR Spectroscopy 5th Ed. by Horst Friebolin, Wiley Publishers (2010)

PAPER IV CH(PO) 304T(ELECTIVE IVB: ADVANCED ORGANIC CHEMISTRY

PO(CB2)-10: Carbohydrates and Proteins
PO(CB2)-11: Principles of Green Chemistry and Synthesis
PO(CB2)-12: Organic Nanomaterials and Supramolecular Chemistry

PO(CB3)-10: Carbohydrates and Proteins — 15 Hrs

Carbohydrates

Introduction to the importance of Carbohydrates. Types of naturally occurring sugars. Deoxy sugars, amino sugars, branched chain sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. Synthesis of amino, halo and thio sugars. Conformational structures of sucrose. Structure and biological functions of starch, cellulose, glycogen and chitin.

Proteins

Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods.

PO(CB2)-11: Principles of Green Chemistry and Synthesis — 15 Hrs

Introduction of Green Chemistry: Principles of Green Chemistry. Introduction to alternative approaches.

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 diydroxylation reactions. b) Organic Synthesis using Ionic liquids: Introduction, applications- Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction.

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.

PO(CB2)-12: Organic Nanomaterials and Supramolecular Chemistry — 15 Hrs

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation. **Molecular Devices:** Photochemical devices, Liquid crystals.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Single walled CNTs (SWCNTs) and multi walled MWCNTs) and Graphene.

Supramolecular Chemistry:

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, Calixarenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcerands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catenanes, Molecular necklace, dendrimers, properties and applications.

BOOKS SUGGESTED:

1. P.T. Anastes & J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).
3. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M.A. Ryan & M. Tinnes and, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers (2004).
6. Enantioselective Organocatalysis, Peter I Dallco, Willey-VCH (2014).
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications (2007).
9. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications (2009).
10. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications (1995)
11. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999).
12. Nanochemistry by G.B. Sergeev; Elsevier (2006).
13. Nanochemistry: A chemical approach to nano materials, G.A. Ozin & A.C. Arsenault; RSC publishers (2005).
14. Carbohydrate Chemistry by Barton Volumes.
15. Carbohydrate chemistry by G.J. Boons, Blackie Academic and Professional (1998)
16. The chemistry of natural products: vol. V - carbohydrates by S.F. Dyke (1960).
17. Organic Chemistry by McMurry, 1st Edition (1984).
18. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon First Edition (2005).

LABORATORY COURSES

Paper-VCH (PO) 351 P: Chemical Kinetics **4Hrs/week**

- **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 acetone – iodine reaction by titrimetry
  1. Order w.r.t.[iodine]
  2. Order w.r.t. [acetone]
  3. Order w.r.t. [H^+]
- **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 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-butyl chloride by conductometry:**
  1. 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

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.

BOOKS SUGGESTED:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2 Fifth Edition, Longman (1989).
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati, Eighteenth Edition, S. Chand & Company (2018).
3. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age International (2007).
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books (2012).
5. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
6. Advanced Practical Physical chemistry: J.B. Yadav, Krishna Prakashan Media (P) Ltd (2015).

PAPER -VI CH(PO) 352P: Synthesis of Organic compounds **4Hrs/week**

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), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin ($NaBH_4$ reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Synthesis of BINOL.

BOOKS SUGGESTED:

1.A textbook of practical organic chemistry by A I Vogel, Vol 1&2.
2.Unitized experiments in organic chemistry by R Q Brewster and others.
3.Handbook of organic analysis by H T C Clarke.
4.Practical Organic Chemistry by Mann and Saunders.

Paper-VII CH (PO) 353P: (Potentiometry and Graphical Analysis of Data & Molecular Visualization using Software Tool) **2Hrs/ week**

- 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).
  5. Mixture of halides vs $AgNO_3$
  6. Mixture of KI and KSCN vs $AgNO_3$
- Graphical Analysis of Data

  The data obtained in all the experiments are to be analyzed by the students by usual graphical methods and with software tools like MS EXCEL and/or ORIGIN.
- Molecular visualisation and/or energy calculations using Chem draw software tool.

a) cyclohexane b) amino acids (acidic and basic) c) naphthalene and/or anthracene

BOOKS SUGGESTED:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2 Fifth Edition, Longman (1989).
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati, Eighteenth Edition, S. Chand & Company (2018).
3. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age International (2007).
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books (2012).
5. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
6. Advanced Practical Physical chemistry: J.B. Yadav, Krishna Prakashan Media (P) Ltd (2015).

PAPER VIII CH (PO) 354 P: Separation and Identification of Organic Compounds 2Hrs/week

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 (m. p/b. p), 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.

SEMINAR

M.Sc. SEMESTER - IV
PHYSICAL ORGANIC CHEMISTRY SPECIALIZATION
(for the batches admitted in academic year 2023& later under CBCS pattern)

PAPER I CH(PO) 401T(CORE): THERMODYNAMICS AND ELECTROCHEMISTRY

PO-13: Non-equilibrium Thermodynamics
PO-14: Statistical Thermodynamics
PO-15: Electrochemistry-II

PO-13: Non-equilibrium Thermodynamics — 15 Hrs

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.
Application of Onsager relations to electrokinetic phenomena – electroosmotic pressure and streaming current. The Onsager relations and the principle of detailed balance. Liquid junction potentials – derivation of equation for liquid junction potential in terms of transport numbers using Onsager relations. Steady states. Principle of minimum entropy production.
Irreversible thermodynamics as applied to biological systems - examples.
Application to thermoelectric circuits. Seebeck and Peltier effect.

PO-14: Statistical Thermodynamics — 15 Hrs

Concepts of distribution and probability. Estimation of probability and the most probable distribution. Systems composed of noninteracting particles. Derivation of Boltzmann distribution law. The molecular partition function. Systems composed of interacting particles.

The concept of ensemble and canonical ensemble. Canonical partition function and its relation to molecular partition function. The factorization of molecular partition function – translational, rotational, vibrational and electronic partition functions. Derivation of expressions for translational, rotational (diatomic) and vibrational partition functions. Relationship between partition functions and thermodynamic functions. The relationship between partition functions and thermodynamic functions. Law of equipartition energy.

Specific heats of solids – Einstein equation of heat capacity of solids – derivation. Explanation of heat capacity at very low and very high temperatures – Dulong and Petits Law. Debye theory.
The entropy of a monoatomic ideal gas. The Sackur-Tetrode equation- derivation. Mean translational and vibrational energies.

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.

PO-15: Electrochemistry – II — 15 Hrs

The electrode-electrolyte interface: The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Quantum aspects of charge transfer at the interfaces. Tunneling.

Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation. Tafel equation - low field - equilibrium, Nernst equation. The symmetry factor and its significance.

Corrosion: Electrochemical corrosion. Short-circuited energy producing cell. The definition and final expression of corrosion current and corrosion potential. Homogeneous theory of corrosion. Evans diagrams. Potential-pH (Pourbaix) diagrams of iron. Methods of corrosion rate measurement. Mechanism of anodic dissolution of iron. Protection against corrosion. Corrosion inhibition by organic molecules.

Electro-organic synthesis: Reduction of carboxylic acids, the polymerization of acrylonitrile to adiponitriles in the synthesis of nylon. Reduction of nitro compounds.

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 (1999).
3. Advanced physical chemistry by Gurtu and Gurtu, Pragati Prakashan (2021).
4. Physical chemistry by Puri and Sharma, 48th Edition, Vishal Publishing Company (2021).
5. Elements of Statistical Thermodynamics, L. K. Nash, Addison – Wesley Publication Company (1974).
6. Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wiley Publication Company (1962).
7. Statistical Thermodynamics, M. C. Gupta, Seond Edition, New Age International (2007).
8. Physical Chemistry, Ira N. Levine, Sixth Edition, McGraw Hill (2008).
9. Modern Electrochemistry, J. O. M. Bockris & A. K. N. Reddy, Plenum.
10. Modern Electrochemistry 2B, Bockris & Reddy, Second Edition, Springer New York, NY (2001).
11. Industrial Electrochemistry, D. Pletcher, Chapman & Hall (1984).
12. Introduction to Electrochemistry, S. Glasstone, EAST-WEST Press Pvt. Ltd, New Delhi (2006).
13. Electrochemistry – B K Sharma Goel, Meerut, India(1973)
14. Fundamental principles of Modern Electroplating, Lowenheim, Third Edition, John Wiley & Sons (1974).

PAPER II CH(PO) 402T(CORE): HETEROCYCLIC CHEMISTRY
NEW TECHNIQUES IN ORGANIC CHEMISTRY AND ASYMMETRIC SYNTHESIS

PO-16: Five and six membered heterocycles with two hetero atoms
PO-17: New techniques and concepts in organic synthesis
PO-18: Asymmetric Synthesis

PO – 16 : 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 – 17: New techniques and concepts in organic synthesis — 15 Hrs

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.

Solid phase oligodeoxynucleotide synthesis: Phospho-triester, phosphite-triester and phosphoramidite pathway

Oligosaccharide synthesis: Glycosidation: Cylicoxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.

Phase Transfer catalysis: Onium and crown ethers as PTC.

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

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

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.

Determination of absolute configuration: Mosher's method.

PO-18: Asymmetric synthesis — 15 Hrs

Introduction: Brief revision of classification of stereo selective reactions

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

Prochiral nomenclature: Pro-chirality and Pro-R, Pro-S, Re and Si. Conditions for stereoselectivity: 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; 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: 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 IPC_2BH and $IPCBH_2$.

Chiral catalyst controlled asymmetric synthesis: Sharpless Asymmetric epoxidation. Asymmetric hydrogenations using chiral Wilkinson catalyst (Using chiral phosphines ligand).

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

BOOKS SUGGESTED:

1. Heterocyclic Chemistry, T. Gilchrist, published by Pitman (1985).
2. An introduction to the Chemistry of heterocyclic compounds, R. M. Acheson, Wiley(1976).
3. Heterocyclic Chemistry, J. A. Joule & K. Mills, Wiley-Blackwell(2010).
4. Handbook of Heterocyclic Chemistry, A. R. Katritzky Pergamon Press (1985)
5. Organic Chemistry Vol. I and Vol. II by I. L. Finar Longmans Green and Co. Ltd. (1959).
6. Biotransformations in Organic Chemistry by K Faber Springer Berlin, Heidelberg (2011).
7. Organic Synthesis: Special techniques. V. K. Ahulwalia and Renu Aggarwal, Alpha Science(2001)
8. Asymmetric synthesis: The Essentials by Nogradi, Wiley.
9. Asymmetric organic reactions by J D Morrison and H S Moscher, ACS (1976).
10. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey aube, Elsevier Science(1996).
11. Stereo differentiating reactions by Izumi, Kodansha and Acdemic Press(1977) later was also published by Elsevier Science (2012).
12. Stereochemistry of Carbon Compounds by Ernest L. Eliel & Samuel H. Wilen, McGraw-Hill(1962).

PAPER III CH (PO) 403T(ELECTIVE IIIA): ADVANCED SPECTROSCOPY

PO(CB1) - 19: Photoelectron Spectroscopy (PES) and Electron spin Resonance Spectroscopy (ESR)
PO(CB1) - 20: NMR, NQR and Mössbauer Spectroscopy
PO(CB1) - 21: 2D NMR and ORD spectroscopy

PO(CB1) – 19: Photoelectron Spectroscopy (PES) and Electron Spin Resonance Spectroscopy (ESR)

15 Hrs

Photoelectron Spectroscopy

Principle and Instrumentation, Types of Photoelectron Spectroscopy – UPS & XPS. Binding Energies, Koopman's Theorem, Chemical Shifts.

Photoelectron Spectra of Simple Molecules: N_2, O_2, F_2, - Vibrational Structure of PES Bands, Potential energy curves, Interpretation of Vibrational spectral data for ionized (M+) species, Prediction of Nature of Molecular Orbitals.

ESCA in qualitative analysis, Principles of Auger electron spectroscopy.

Electron Spin Resonance

Introduction, principle, instrumentation, selection rules, interpretation of Lande's factor 'g'. Hyperfine and super hyperfine Coupling. Anisotropy in 'g' values and hyperfine coupling constants. Zero field splitting, Kramer's degeneracy and quadrupolar interactions.

Study of free radicals and transition metal complexes. Evidence for covalency in complexes, ex. Cu(II) Bis-salcylaldimine, Bis-acetylacetanatovanadyl(II) and hexachloroiridium(IV) complexes.

PO(CB1) –20: NMR, NQR and Mossbaur Spectroscopy 15 Hrs

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.

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.

PO-(CB1) –21: 2D-NMR Spectroscopy and ORD Spectroscopy 15 Hrs

2D-NMR spectroscopy:

Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMOCOSY (^{1}H-^{1}H COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY (^{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.

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.

BOOKS SUGGESTED:

1. Physical Chemistry, Ira N. Levine, McGraw Hill
2. Atkin's Physical Chemistry, P. Atkins & Julio de Paula, Oxford University Press
3. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press (1977).
4. Principles of Instrumental Analysis, Skoog and Leary, Saunders College Publishing (1992).
5. International series of Monographs, Vol. 53: Photoelectron Spectroscopy, Edited by D. Becker and D. Betteridge, (1972).
6. Structural methods in inorganic chemistry, E.A.V. Ebsworth, John Wiley & Sons (1987).
7. Solid state chemistry and its applications. A. R. West, John Wiley & Sons (1991).
8. Modern Spectroscopy, J. M. Hollas, Fourth Edition, John Wiley & Sons (2004).
9. Fundamentals of Molecular Spectroscopy, Banwell & McCash, Fourth Edition, McGraw Hill Education (2017).
10. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (1962).
11. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (1988).
12. Basic principles of Spectroscopy, R. Chang, McGraw Hill (1971).
13. Molecular Structure and Spectroscopy by G Aruldhas, Second Edition, PHI Learning Private Ltd. New Delhi (2008).
14. NMR Spectroscopy: Basic principles, concepts and applications in chemistry, H. Gunther, John Wiley-VCH publishers (2013).
15. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood (1990).
16. NMR Basic Principles, Atta-ur-Rahman, Springer Verlag (2012).
17. Two-dimensional NMR Spectroscopy-Applications for chemists and biochemists, edited by W. R. Croasmun & R. M. K. Carlson, Second Edition, Wiley-VCH (1994).
18. Organic Chemistry, John McMurry, Eighth Edition, Congage Learning (2011).
19. Spectroscopic Identification of Organic Compounds by RM Silverstein, G C Bassler and T B Morrill, Second Edition, John Wiley & Sons (1967).
20. NMR in chemistry - A multinuclear Introduction, William Kemp, Mc Millan (1988).
21. Introduction to Organic Spectroscopy by Pavia, Lampzman, Third Edition, Thomson Education (2001).
22. Basic one and two-dimensional NMR spectroscopy, Horst Friebolin, Third Edition, Wiley-VCH (1998).
23. Textbook of organic chemistry, Vol 2, I L Finar, Fifth Edition, Pearson (2011) First Edition by Longmans Green and Co. Ltd.(1959)
24. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman.
25. An introduction to the chemistry of terpenoids and steroids, William Templeton, Butterworths, London (1969).
26. One- and two-dimensional NMR spectroscopy, Atta-Ur-Rahman, Second Edition, Elsevier (1991).
27. Stereochemistry of Carbon Compounds, Ernest L. Eliel & Samuel H. Wilen, Mc Graw Hill (1962).

PAPER IV CH (PO) 403T(ELECTIVE IIIB): TOTAL STEREOSELECTIVE SYNTHESIS OF NATURAL PRODUCTS, BIOMOLECULES and PHYSICAL PRINCIPLES OF SPECTROSCOPY and VIBRATIONAL SPECTROSCOPY

PO(CB1) - 19: Total Stereoselective Synthesis of Natural Products
PO(CB1) - 20: Biomolecules
PO(CB1) – 21: Physical principles of spectroscopy & Vibrational spectroscopy

PO(CB1)-19: Total stereoselective synthesis of Natural products **15 Hrs**

Takasago synthesis of Menthol. Hoffmann-LaRoche synthesis of Biotin. Corey's synthesis of Prostaglandins (E2, F2α) and Paeoniflorin. Sharpless synthesis of L-Hexoses. Danishefsky synthesis of Indolizomycin. Nicolaou's synthesis of Taxol. Myer's synthesis of Dynemicin A.

PO(CB1) - 20: Biomolecules **15 Hrs**

Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis. Lock and Key model and Induced- Fit model. Enantiomer discrimination by Three-point Contact model. Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition. Enzymes in organic synthesis. Immobilised enzymes.

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 nucleosides and nucleotides.

Lipids: Lipid structure- acylglycerols, phosphoglycerides and sphingolipids. Biosynthesis and chemical Synthesis of lipids.

PO(CB1) - 21: 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 – Structure determination of XY_4 molecules, Phase transitions.

BOOKS SUGGESTED:

1. Steroids by L. F. Fieser and M. Fieser, Van Nostrand Reinhold Inc., U. S. (1959).
2. The Alkaloids: Chemistry and Physiology by R. H. F. Manske and H. L. Holmes, Academic Press (2016).

3. The Chemistry of the Terpenes by A. R. Pinder, Wiley Publishers (1990).
4. Total synthesis of Natural Products by J. Apsimon Vol 1-5, John Wiley & Sons.
5. Principles of Organic Synthesis by R. O. C. Norman and J. M. Coxon, Routledge Taylor & Francis Group (1993)
6. Classics in Total Synthesis: Targets, Strategies, Methods by K. C. Nicolaou and E. J. Sorensen, 6th Ed. VCH Publishers (2014)
7. Classics in Total Synthesis: Targets, Strategies, Methods by K. C. Nicolaou and S. A. Snyder, VCH Publishers (2003)
8. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
9. NMR in Chemistry: A Multinuclear Introduction by William Kemp, MacMillan Publishers (1988)
10. Nuclear Magnetic Resonance: Basic principles by Atta-ur-Rahman, Springer Publishers (2012)
11. Basic One- and Two-Dimensional NMR Spectroscopy 5th Ed. by Horst Friebolin, Wiley Publishers (2010).
12. Textbook of organic chemistry, Vol II by I L Finar, Longmans Green and Co. Ltd.(1959).
13. Enzyme structure and mechanism by Fersht and Freeman, published by W H Freeman (1977).
14. Bio-Organic chemistry by Hermann Dugas, Springer (1981)
15. Nucleic acids in Chemistry and Biology, G M Blackbum MI Gait, IRL Press Oxford Univ.(1990)
16. Lehninger Principles of Biochemistry by D L Nelson and M M Cox, Macmillan(2005)
17. Biotransformations in Organic Chemistry by K Faber Spreinger Berlin, Heidelberg(2011).
18. Modern Spectroscopy, J. M. Hollas, John Wiley & Sons(1987)
19. Fundamentals of Molecular Spectroscopy, Banwell & McCash, Fourth Edition, McGraw Hill Education (2017).
20. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (1962).
21. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (1988).
22. Basic principles of Spectroscopy, R. Chang, McGraw Hill (1971).
23. Physical Methods for Chemistry, R. S. Drago, Affiliated East West Press **(1977).**
24. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age International (2015).
25. Introduction to Raman Spectroscopy, J. R. Ferraro & K. Nakamoto, Academic Press (2012).
26. Molecular structure and Spectroscopy, G. Aruldhas, Second Edition, PHI Learning Pvt. Ltd (2008).

LABORATORY COURSES

Paper-IV CH (PO) 451P: Instrumentation — 4 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 $CuSO_4$ vs strong base.
  4. Mixture of halides (chloride + iodide) vs $AgNO_3$.
  5. Formic acid, acetic acid, chloroacetic acid, dichloroacetic acid and Trichloroacetic acid
  6. and their mixtures vs strong base.
  7. Precipitation titration: K_2SO_4 vs $BaCl_2$.
- 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.

Colorimetry/Spectrophotometry

- Estimation of Cu(II) using EDTA.
- Estimation of Fe(III) using thiocyanate.
- Estimation of Fe(II) using 1,10-phenanthrolin.
- 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.
- Estimation of Mn(II) by spectrophotometry using periodate.
- Determination of *pKa* of methyl red indicator.
- Simultaneous determination of dichromate and permanganate in a mixture.

Paper-V CH (PO) 452P: Spectroscopic Identification of Organic Compounds — 4 Hrs / week

Identification of unknown organic compounds by interpretation of IR, UV, ^1H - NMR, ^{13}C NMR, and mass spectral data. A minimum of 15 representative examples should be studied

Paper-VI CH (PO) 453P: *pH* metry, Separation of mixtures and chromatography — 2 Hrs/ week

- 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
- **Separation of ternary mixtures and column chromatography**

Separation of any two ternary mixtures by qualitative analysis (by chemical methods) and column chromatography

BOOKS SUGGESTED:

1. A textbook of practical organic chemistry by A I Vogel, Vol 1&2 Fifth Edition, Longman (1989).
2. Senior practical physical chemistry. B. D. Khosla, V.C. Garg, Adarsh Gulati, Eighteenth Edition, S. Chand & Company (2018).
3. Experimental Physical Chemistry: V. Athawale and P. Mathur, New Age International (2007).
4. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan, Viva Books (2012).
5. Practical in Physical Chemistry: P.S. Sindhu, Laxmi Publications.
6. Advanced Practical Physical chemistry: J.B. Yadav, Krishna Prakashan Media (P) Ltd (2015).
7. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster, 8th Edition Wiley (2014).
8. The systematic identification of organic compounds by Shriner et.al. 6th Edition Wiley (1980).

PROJECT CH (PO) 454P **12 hrs/ week**

IV Semester Project Assessment for 175 Marks

Marks Distribution for Project Assessment

INTERNAL ASSESSMENT

Research Design Seminar	1 credit	25 marks
Progress Seminar	1 credit	25 marks

SEMESTER END ASSESSMENT

Dissertation	1 credit	50 marks
Final presentation	2 credits	50 marks
Viva Voce during final presentation	1 credit	25 marks

M.Sc. CHEMISTRY

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

FOR STUDENTS ADMITTED FROM THE YEAR 2023-24 ONWARDS

M.Sc. CHEMISTRY (PHARMACOINFORMATICS SPECIALISATION)

Syllabus for III and IV Semesters

[Under Restructured CBCS Scheme]

(for the batches admitted in academic year 2023-24 onwards under CBCS pattern)

Grand total marks and credits (all 4 semesters) 2400 marks – 80 credits

(Approved in the P.G. BOS meeting held on 27-01-24)

Semester - III					
	Instruction Hrs/week	Internal assessment marks	Semester marks*	Total	Total Credits
CH(CPI) 301T (Core)	3	50	50	100	3
CH(CPI) 302T (Core)	3	50	50	100	3
CH(CPI) 303T (Elective)	3	50	50	100	3
CH(CPI) 304T (Elective)	3	50	50	100	3
CH 351P (PI LAB)	4		50	50	2
CH 352P (PI LAB)	4		50	50	2
CH 353P (PI LAB)	2		25	25	1
CH 354P (PI LAB)	2		25	25	1
Seminar	2	---	---	50	2
Total	26			600	20

Semester – IV					
	Instruction Hrs/week	Internal assessment marks	Semester marks*	Total	Total Credits
CH(CPI) 401T (Core)	3	50	50	100	3
CH(CPI) 402T (Core)	3	50	50	100	3
CH(CPI) 403T (Elective)	3	50	50	100	3
CH 451P (PI LAB)	4		50	50	2
CH 452P (PI LAB)	4		50	50	2
CH 453P (PI LAB)	2		25	25	1
CH 454P (Project)	12	50	125	175	6
Total	31			600	20

Grand total marks and credits (all 4 semesters) 2400 marks - 80 credits

M.Sc. SEMESTER III
PHARMACO INFORMATICS SPECIALISATION
(for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH(CPI)301T (CORE): DATA MINING AND SCRIPTING
CPI - 01: Data Mining & Python Scripting
CPI - 02: Chemical Information Sources and Searches
CPI - 03: Structure based drug design

PAPER II CH(CPI)302 T (CORE): CHEMICAL INFORMATION & COMPUTATIONAL CHEMISTRY.
CPI – 04 : Computational Chemistry – I
CPI – 05 : Computational Chemistry – II
CPI – 06 : Ligand based drug design

PAPER III CH(CPI) 303T (ELECTIVE IIIA) : PHARMACEUTICAL ANALYSIS –I
CPI(CB1) - 07: Spectral Methods in Pharmaceutical Analysis
CPI(CB1) - 08: Chromatography in Pharmaceutical Analysis - I
CPI(CB1) - 09: Chromatography in Pharmaceutical Analysis - II

PAPER III CH(CPI) 303T (ELECTIVE IIIB) : GREEN CHEMISTRY AND NEW TECHNIQUES
CPI(CB1) - 07: Principles of Green chemistry and Green Synthesis
CPI (CB1) -08: Organic nanomaterials and Supramolecular chemistry
CPI (CB1) -09: New techniques and concepts in organic synthesis

PAPER IV CH (CPI) 304T (ELECTIVE IVA) : SYNTHETIC REAGENTS, ^{13}C AND 2D NMR
CPI(CB2) -10: Synthetic Reagents-I
CPI(CB2) -11: Synthetic Reagents-II
CPI(CB2) -12: ^{13}C NMR and 2D NMR spectroscopy

PAPER IV CH (CPI) 304T (ELECTIVE IVB): MODERN ORGANIC SYNTHESIS
CPI(CB2) -10: Asymmetric synthesis
CPI(CB2) -11: Synthetic strategies
CPI(CB3) -12: New Synthetic reactions

LABORATORY COURSES

PAPER V CH(CPI) 351P: Molecular Modeling Lab
PAPER VI CH(CPI) 352P: Synthesis of Organic Compounds
PAPER VII CH(CPI) 353P: Mixture separation
PAPER VIII CH(CPI) 354P: Spectral Problem solving

SEMINAR

M.Sc. SEMESTER - IV
PHARMACO INFORMATICS CHEMISTRY SPECIALIZATION
(for the batches admitted in the academic year 2023 -24 and later under CBCS pattern)

PAPER I CH(CPI) 401T (CORE): PHARMACOKINETICS & PHARMACODYNAMICS
CPI - 13 : Biopharmaceutics
CPI - 14 : Pharmacokinetics
CPI - 15 : Pharmacodynamics

PAPER II CH(CPI) 402T (CORE): PHARMACEUTICAL ANALYSIS –II
CPI-16: Clinical and Pharmaceutical Analysis
CPI-17: Spectral and Electroanalytical Techniques in Pharmaceutical Analysis
CPI-18: Titrimetry, Chemical & Extraction methods in Pharmaceutical Analysis

PAPER III CH(CPI) 403T (ELECTIVE III A): INTELLECTUAL PROPERTY RIGHTS & RESEARCH METHODOLOGY
CPI(CB1) - 19: Introduction to IPR
CPI(CB1) - 20: Patent Search and IP Reports Generation
CPI(CB1) - 21: Research Methodology

PAPER III CH(CPI) 403T (ELECTIVE III B): PRINCIPLES OF DRUG DISCOVERY, DRUG TARGETS AND CHEMISTRY OF PHARMACOLOGY
CPI(CB1) - 19: General Principles of Pharmacology and drug Targets, drugs acting on ANS and CNS
CPI(CB1) - 20: Drugs Acting on Cardio Vascular and Respiratory System
CPI(CB1) - 21: Drugs acting on metabolic process, cell wall, genetic material and immune system

LABORATORY COURSES

PAPER IV CH(CPI) 451P : Quantitative Analysis of Pharmaceuticals
PAPER V CH(CPI) 452P : Computational and Python Scripting
PAPER VI CH(CPI) 453P: TLC and column chromatography

CH(CPI) 454P: PROJECT WORK

M.Sc. SEMESTER - III
PHARMACOINFORMATICS Specialization
(for the batches admitted in academic year 2023 and later under CBCS pattern)

PAPER I CH(CPI)301T(CORE):DATA MINING AND SCRIPTING

CPI - 01: Data Mining and Python Scripting
CPI - 02: Chemical Information Sources and Searches
CPI - 03: Structure Based Drug Design

CPI – 01: Data Mining and Python Scripting — 15hrs

Introduction to Data Mining, working principles of Data Mining, Architecture form of data Mining, Difference between Data Mining and Machine learning techniques, Supervised and unsupervised learning methods and its application to QSAR. Data Visualization: Visualizing Data mining models, Decision Tree. Data warehousing: Data mining and analytic technology, comparing different Models using visualization.

Introduction to Computers and it's components, Operating System (Windows & Linux). Introduction to Python & Bio-Python, Data-types, Variables – Declaration and Use, Operators – Assignment, Logical, Arithmetic etc., Conditional Statements – If else and Nested If else and elif, Python Collections (Arrays) – List, Tuple, Sets and Dictionary, Loops – For Loop, While Loop & Nested Loops, Accessing MySQL database - getting id, Sequence from a Database Object, matching a sequence in a Database Object.

CPI – 02: Chemical Information Sources and Searches — 15hrs

Introduction to information sources and searching strategies, tactics for searches, Advantages and Limitations of computer searching, Keyword based general bibliographic searches, Chemical connectivity and structure searches (2D), Chemical structure, property and shape based searches (3D), Searching for the synthesis (or) reactions of specific compounds or classes of compounds, Searching of chemical abstracts.

Types of Publications: Journals, Technical reports, Patents, Conference Papers, Dissertations, Electronic Publications.

Types of databases: Public databases - NCBI, RCSB, CSD, Expasy, Swiss-Prot and Paid databases - CAT'STN and SciFinder.

Web-based cross platform solutions for Cheminformatics: BLAST, ClustalW, SAVES, ProSA.

CPI – 03: Structure Based Drug Design — 15hrs

Database similarity searches - Pair-wise alignment: Global sequence analysis (Needleman-Wunsch), Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment - Homology Modeling: Query sequence, Template selection, Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling, Model optimization, Energy minimization - Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA - Active site Identification - Docking, Docking Algorithms: Genetic Algorithm - Molecular Interactions, Scoring functions - Virtual Screening: Ligand Based and Structure Based. De novo ligand design and its limitations.

SUGGESTED BOOKS

1. MySQL (TM): The Complete Reference by Jeremy D. Zawodny and Derek J. Balling. O'Reilly & Associates, April 2004.
2. Data Mining: Concepts and Techniques by Jiawei Han and Micheline Kamber, Third Edition, 2012, Elsevier Inc.
3. Data Mining Techniques by Arun K. Pujari. 2001
4. Python All-in-One For Dummies, John C. Shovic, Alan Simpson, Wiley, 2021
5. Advanced Guide to Python 3 Programming, John Hunt, Springer International Publishing, 2023

PAPER II CH(CPI)302 T (CORE): Chemical Information & Computational Chemistry.

CPI – 04 : Computational Chemistry – I
CPI – 05 : Computational Chemistry – II
CPI – 06 : Ligand Based Drug Design

CPI – 04 : Computational Chemistry – 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.

CPI – 05: Computational Chemistry – 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.

CPI – 06: Ligand Based Drug Design **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) - 3D QSAR: CoMFA and CoMSIA - Differences between 2D and 3D QSAR. Chemical connectivity and structure searches (2D), Chemical structure, property and shape based searches (3D)

SUGGESTED BOOKS:

1. Molecular Modelling: Principles and Applications, by Andrew Leach, Longman Publications.
2. Computational Chemistry, Guy H. Grant & W. Graham Richards, Oxford University Press.
3. Computational Chemistry: Introduction to the theory and Applications of Molecular and Quantum Mechanics, Errol Lewars, Springer Publications.
4. Molecular modelling – Basic Principles and Applications by Hans Dieter Holtje and Gerd Folkers, Wiley-VCH, 1996
5. Introduction to Computational Chemistry by Jensen, Wiley Publishers, second edition
6. Introduction to Bioinformatics by Arthur M. Lesk, Oxford University Press (Indian. Edition), 2002
7. Principles of Medicinal Chemistry Vol. II by Dr. SS Kadam Pragati books Pvt. Ltd; 2007
8. Principles of Medicinal Chemistry, by Patrick.
9. Burger's Medicinal Chemistry and Drug Discovery, 5th Edition.
10. Text book of Drug design and Vol.1 discovery 3rd Edition by POVL krogsgaard- larsen tommy liljefors and ULF madsen.

PAPER III CH(CPI) 303T (ELECTIVE IIIA) : PHARMACEUTICAL ANALYSIS –I

CPI(CB1) - 07: Spectral Methods in Pharmaceutical Analysis
CPI(CB1) - 08: Chromatography in Pharmaceutical Analysis - I
CPI(CB1) - 09: Chromatography in Pharmaceutical Analysis - II

CPI(CB1) - 07: Spectral Methods in Pharmaceutical Analysis **15hrs**

(A) Ultraviolet and Visible Spectroscopy: Introduction, UV spectra of some representative drug molecules: Steroid enones, Ephedrine [the benzoid chromophore], ketoprofen [extended benzene chromophore], Procaine [amino group auxochrome], Phenyleprine [hydroxylgroup auxochrome]. Applicationof UV-Vis Spectrophotometry to Pharmaceutical quantitative Analysis: Assay of Penicillin by derivatization.

(B) Infrared Spectroscopy- Introduction, Sample preparation, Application of IR Spectrophotomety in Structure Elucidation, interpretation of IR spectra of Paracetamol, aspirin, dexamethasone and phenoxymethylpencillin potassium. Near IR analysis (NIRA): Introduction, Examples of NIRA application–determination of active ingredients in multi-component dosage forms, moisture determination.

(C)Nuclear Magnetic Resonance Spectroscopy - Introduction, ^{1}H NMR:,^{1}H-NMR spectral analysis of Benzocaine, Phenacetin, Clofibrate and phenylephrine.^{13}C-NMR: ^{13}C-NMR spectrum of Salbutamol sulphate,

CPI(CB1) - 08: Chromatography in Pharmaceutical Analysis - I **15hrs**

Thin Layer Chromatography– Introduction, Instrumentation, TLC Chromatogram, Stationary Phases, Eluotropic series and Mobile phases, Modification of TLC, Adsorbents, detection of compounds on TLC plate following development, Applications of TLC analysis – qualitative identity tests, limit tests. High performance TLC (HPTLC), Applications of HPTLC– Assay for rifampicin (R), isoniazid (I) and pyrazinamide(P).

High performance Capillary Electrophoresis – Introduction, Instrumentation, control of separation. Application of capillary electrophoresis in pharmaceutical analysis - Separation of Atenolol and related impurities - Analysis of Non-steroidal anti-inflammatory drugs - Micellar Electrokinetic Chromatography, Analysis of flavonoids by MECC.

CPI(CB1) - 09: Chromatography in Pharmaceutical Analysis - II **15hrs**

Gas Chromatography – Introduction, Instrumentation, Selectivity of Liquid Stationary Phases, Use of Derivatization in GC, Application of GC in quantitative analysis, Determination of manufacturing and degradation residues by GC, Determination of pivolic acid in dipivefrin eye drops, Determination of residual solvents, Application of GC in Bioanalysis.

High Performance Liquid Chromatography– Introduction, Instrumentation, Structural factors which govern rate of elution of drugs from HPLC columns, Application of HPLC to the quantitative analysis of drugs in formulations, Assay of hydrocortisone cream with one point calibration against an internal standard, Assays involved in more specialized HPLC techniques, Assay of adrenaline injection by chromatography with an anionic ion-pairing agent.

SUGGESTED BOOKS:

1. Pharmaceutical Analysis by David G. Watson
2. Practical pharmaceutical chemistry Part I by Beckett &Stenlake
3. Pharmaceutical analysis by Ashtoshkar
4. Physical pharmacy by AN.Martin,J, Swarlbicketal

5. Biopharmaceutics and pharmacokinetics by Brahmanikar
6. Text book of physical pharmaceuticals by Subramaniyan
7. Inorganic pharmaceutical chemistry By Black
8. British Pharmacopoeia Vol I,II
9. Indian Pharmacopoeia Vol I,II
10. Bently's Text book of pharmaceutics by Rowlins
11. The science and practice of pharmacy by Remington
12. Thermal methods of Analysis-D.G Watson

PAPER III CH(CPI) 303T (ELECTIVE IIIB) : GREEN CHEMISTRY AND NEW TECHNIQUES

CPI (CB1) - 07: Principles of Green chemistry and Green Synthesis
CPI (CB1) - 08: Organic nanomaterials and Supramolecular chemistry
CPI (CB1) - 09: New techniques and concepts in organic synthesis

CPI (CB1) - 07: Principles of Green chemistry and Green Synthesis **15Hrs**

Introduction of Green Chemistry - Principles of Green Chemistry - Introduction to alternative approaches – **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 diydroxylation reactions. **b)** Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction. **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.

CPI (CB1) - 08: Organic nanomaterials and Supramolecular chemistry **15Hrs**

Organic Nanomaterials:

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nano-manipulation.

Molecular Devices: Photochemical devices, Liquid crystals.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Types of Fullerenes, CNTs (Zig-Zag, Armchair and Chiral), single walled CNTs (SWCNTs) and multi walled MWCNTs) and Graphenes.

Supramolecular Chemistry:

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 anology, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcirands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, properties and applications.

CPI (CB1) - 09: 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: cylicoxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahneglycosidation, convergent and linear oligosaccharide synthesis.

4. Phase Transfer catalysis: Onium and crwon ethers as PTC.

5. Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, elctrocylic-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.

SUGGESTED BOOKS:

1. P.T. Anastes& J.K. Warmer: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).
3. M.C. Cann& M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers
6. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
9. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
10. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications
11. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
12. Stereochemistry of organic compounds - Principles & Applications by D Nasipuri
13. Nanochemistry by G.B. Sergeev; Elsevier
14. Nanochemistry: A chemical approach to nano materials , G.A. Ozin& A.C. Arsenault; RSC publishers.

PAPER IV CH (CPI) 304T (ELECTIVE IVA) : SYNTHETIC REAGENTS ^{13}C AND 2D NMR

CPI(CB2) -10: Synthetic Reagents-I
CPI(CB2) -11: Synthetic Reagents-II
CPI(CB2) -12: ^{13}C NMR and 2D NMR spectroscopy

CPI(CB2) - 10: Synthetic Reagents I **15 Hrs**

i) Protecting groups:
a) Protection of alcohols by silyl ether(TBDMS,TBPS) and ester formation
b) Protection of 1,2-diols by acetal, ketal and carbonate formation
c) Protection of amines by t-butyloxycarbonyl, fmoc groups.
d) Protection of carbonyls by thiol acetal (Umpolung) groups.
e) Protection of carboxylic acids 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, 2) Horner-Wordsworth-Emmons reaction.
iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.
v) C-H Activation: Introduction, Rh catalysed C-H activation.

CPI(CB2) - 11: 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: Crv oxidants Jones reagent, PCC, PDC, IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation.
ii) Reductions:
a) Catalytic hydrogenation: Homogenous (Wilkinsons 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.

CPI(CB2) - 12: ^{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),

Hetero COSY ($^{1}H,^{13}C$ 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.

SUGGESTED BOOKS:

1. Some modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R AAtken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser&Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
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
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
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
26. Stereo selectivity in organic synthesis by R S Ward.
27. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
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 IV CH (CPI) 304T (ELECTIVE IVB): MODERN ORGANIC SYNTHESIS

CH CPI(CB2) -10: Asymmetric synthesis
CH CPI(CB2) -11: Synthetic strategies
CH CPI(CB2) -12: New Synthetic reactions

CPI(CB2) - 10: Asymmetric synthesis — 15 Hrs

Introduction: Brief revision of classification of stereo selective reactions
Prostereo isomerism: Topicity in molecules Homotopic, stereo heterotopic (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 enantio selectivityy.
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. Asymmetric Diels-Alder reaction.
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.

CPI(CB2) - 11: Synthetic Strategies — 15 Hrs

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target.Linear and convergent synthesis.Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. .
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.

CPI(CB2) - 12: New Synthetic reactions **15 Hrs**

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia- Lythgoe olefination and Petersons stereoselective olefination.
3. Multi-component Reactions: Ugi, Passerini, Biginelli and Bergman reactions.
4. Ring Formation Reactions: Pausan-Khand reaction, Nazerov cyclisation.
5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.
6. Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis(ROM), applications.

SUGGESTED BOOKS:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moschcr
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 AAtken
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 Jacj Li

LABORATORY COURSES

PAPER V CH(CPI) – 351P: Molecular Modeling Lab **4 Hrs/Week**

1. Drawing molecules, converting them to SMILES format and minimizing molecules in modeling software.
2. Calculating ADMET parameters of small molecules using different software and online tools.
3. 2D QSAR Studies (COX 1 and 2, DHFR inhibitors).
    a. Generating the molecule using relevant modeling software and minimizing the energy
    b. Obtaining the physicochemical parameters like QlogP, MR using the software
    c. Fitting the data to regression software (BuildQSAR) and generating a models in which correlate activity to its structure
    d. Projection of the best pharmacophore
4. Homology Modeling:
    a. Retrieving Query Sequence,
    b. Finding Template,
    c. Pair-wise alignment,
    d. 3D model generation,
    e. Energy minimization (Steepest Decent and Conjugant Gradient methods)
    f. Structure validation (Ramchandran plot, verify 3d, ProSA)
5. Molecular Docking of COX 1 and 2, DHFR inhibitors into respective receptors.
6. Virtual Screening of Asinex Ligand library for identification of new chemical entity.
7. Protein minimization and dynamics using NAMD/GROMACS
8. Multiple sequence analysis using ClustalX (cladogram, dendrogram, phylogram)
9. Active site Centroid (x,y,z coordinates) calculation by using Mercury software
10. XRD Protein Analysis using PDBSum server

PAPER VI CH(CPI) – 352P: Synthesis of Organic Compounds **4 Hrs/Week**

1. Synthesis of Drugs

Benzocaine (Anaesthetic), Antipyrine (Antipyretic), Sulphonamide (antibacterial), Clofibrate (Anti-lipidemic), 2-phenyl-Indole, Benzil-Benzillic acid rearrangement, Beckmann rearrangement 2,5-Dihydroxy acetophenone (Fries reaction), 7-hydroxy coumarin (Pechman synthesis), Vanillyl alcohol from vanillin ($NaBH_4$ reduction)

PAPER VII CH(CPI) – 353P: Mixture separation **2 Hrs/Week**

Mixture Separation – At least 06 mixtures

Separation of 02 component mixtures by chemical methods and their identification by chemical reactions

Separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% NaOH and *dil.* HCl, 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) Solid - Solid - 2 mixtures
b) Liquid - Liquid – 1 mixtures
c) Solid - Liquid - 1 mixtures

PAPER VIIII CH(CPI) – 354P: Spectral Problem solving **2 Hrs/Week**

Identification of unknown organic compounds by interpretation of IR, UV, ^{1}H-NMR, ^{13}C- NMR and mass spectral data. A minimum of 5 simple organic molecules should be studied initially as examples along with the spectral elucidation of the drugs as mentioned below to be studied. (Asprin, p-Chloroacetophenone, clofibrate, Ibuprofen, Phenylacetic acid, p-Methyl Benzoylchloride, L-Dopa, Benzocaine)

M.Sc. SEMESTER - IV
PHARMACOINFORMATICS SPECIALIZATION
(For the batches admitted in academic year 2023-24 onwards under CBCS pattern)

PAPER I CH(CPI) 401T (CORE): PHARMACOKINETICS & PHARMACODYNAMICS

CPI - 13 : Biopharmaceutics
CPI - 14 : Pharmacokinetics
CPI - 15 : Pharmacodynamics

CPI-13: Biopharmaceutics — 15hrs

Introduction - definition of pharmacokinetics, pharmacodynamics, ADME processes. Rate, Rate Constants and order of reactions - zero order kinetics, first order kinetics, mixed order kinetics. Routes of administration: Enteral (oral, sublingual, buccal, rectal) perenteral (intravenous, intramuscular and subcutaneous), topical (dermal, transdermal, ophthalmic, intranasal), advantages and disadvantages.

Plasma drug concentration *vs* time profile: pharmacokinetic parameters (Peak plasma concentration, time of peak concentration, AUC), pharmacodynamic parameters (MEC, MSC, Therapeutic range, onset of action, onset of time, duration of action, intensity of action). Dissolution: Definition and theories of drug dissolution, Diffusion layer model, Danckwert's model & interfacial barrier model. Factors influencing dissolution, dissolution tests for tablets and capsules (basket apparatus, paddle apparatus, flow through cell apparatus). *In vitro - In vivo* correlation of dissolution.

CPI -14: Pharmacokinetics — 15hrs

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). Methods of determination of drug absorption. Bioavailability.

ii) Distribution: Apparent volume of drug distribution. Factors affecting distribution, plasma protein binding.

iii) Metabolism: Sites of drug metabolism, metabolic rate constant, bioactivation and biotransformation of drugs (phase-I and phase-II reactions)

iv) Elimination: Types of elimination and overall apparent elimination rate constant and half-life, concept of clearance.

CPI 15: Pharmacodynamics — 15hrs

Introduction, targets for drug action, receptor concept. Pharmacological binding terms. Two state receptor model, receptor families - structure and signal transduction mechanisms- channel linked proteins, gating mechanism, G-protein coupled receptors, G-protein and their role, Targets for G-proteins, Kinase linked receptors, receptors that regulate gene transcription. Theories of concentration -response relationship, dose-response curves.

References:

1. Biopharmaceutics and Pharmacokinetics – An Introduction by Robert E. Notary, 2nd edition 1975, Marcel Dekkar Inc., New York
2. Applied BioPharmaceutics and Pharmaco Kinetics 5th Edition, Mc Grawhill Medical Publishing 2005 by Shargel, Wupong, Yu Andrew.
3. Pharacokinetics By Shobha Rani
4. Elements of Pharmacology. By Gandhi, Desani & Goyal.
5. The pharmacòlogical basis of therapeutics By Goodmann & Gilmann's
6. Pharmacology By Rang.
7. Physical Pharmacy By Martin
8. Biopharmaceutics and pharmacokinetics By Brahmanikar
9. Pharmacology By Lippincot
10. Modern Pharmacology with Clinical Applications. By R.Craig.
11. Compehensive pharmacy review by Leon Shargel
12. Advanced Pharmaco Kinetics – Venkateswarlu
13. Essentials of Pharmacokinetics and Pharmacodynamics, Thomas N. Tozer, Malcolm Rowland, Wolters Kluwer, 2016
14. Basic Pharmacokinetics and Pharmacodynamics An Integrated Textbook and Computer Simulations, Sara E. Rosenbaum, Wiley, 2016
15. Introduction to Medicinal chemistry. By Graham Patrick

PAPER II CH(CPI) 402T (CORE): PHARMACEUTICAL ANALYSIS –II

CPI - 16: Clinical and Pharmaceutical Analysis
CPI - 17: Spectral and Electroanalytical Techniques in Pharmaceutical Analysis
CPI - 18: Titrimetry, Chemical & Extraction methods in Pharmaceutical Analysis

CPI - 16: Clinical and Pharmaceutical Analysis 15hrs

Clinical analysis: Analysis of Carbohydrates and their significances – Fasting, random and post pandrial glucose tests, Estimation of Glucose in serum. Analysis of lipids and their significances – Test for cholesterol. Analysis of proteins and their significance – Estimation of total protein in serum. Analysis of Major metabolites and their significance – Determination of Blood urea and Creatinine in urine. Analysis of ions and their significance: Estimation of Na, K, Ca, bicarbonates and phosphate in serum. Analysis of Hormones and their significance-ELISA and RIA.

Pharmaceutical analysis: Determination of Diclofenac (non-aqueous titration), Calcium inVitamin 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).

CPI - 17: Spectral And Electroanalytical Techniques in Pharmaceutical Analysis 15hrs

Potentiometric Titrations: assay of Aspirin, assay of Iron (II) succinate in ferromyn tablets, Determination of fluoride in tablets and solutions by Flouride Ion Selective Electrode, Assay of Nitrazepam

Conductometric Titrations: Assay of antihistamine – Diphenylhydramine Hydrochloride using Silver Nitrate as titrant.

Thermal Method of Analysis: Classification of thermo-analytical techniques, Applications of DSC/DTA/TGA in pharmaceutical analysis- Detection of polymorphisim and pseudopolymorphisim in pharmaceutical by DSC/DTA. Analysis of Drug Phenacetin by DSC.

Spectrofluorimetry: Theory, Instrumantation, Appications – Determination of Hemisulphate in Proflavin cream

Atomic Absorption Spectroscopy: Prinicple, Instrumentation,Applications – assay of total Zinc in insulin Zinc suspension

CPI - 18: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis 15hrs

(A) Titrimetry and Chemical Methods - Introduction, Direct Acid/Base titrations in the aqueous phase, Indirect Titrations in aqueous phase – estimation of alcohols and hydroxyl values by reaction with acetic anhydride. Non-aqueous titrations – analysis of phenylephrine, Argentimetric Titrations – assays of Sodium chloride, potassium chloride, thiamine hydrochloride, Complexometric Titrations – metal salts estimations, Redox Titrations - assays of ferrous salts, hydrogen peroxide, sodium perborate and benzoyl peroxide by titration with $KMnO_4$, Iodometric Titrations – Asasy of phenolglycerol injection, Ion-pair Titrations, Diazotization Titrations – assay of sulphanilamide, Karl-Fischer Titrations. Potentiometric Titrations – assay of Aspirin, assay of Iron (II) succinate in ferromynS tablets, Determination of fluoride in tablets and solutions by Flouride Ion Selective Electrode.

(B) Extraction Methods - Introduction, Commonly used excipients in formulations - (i) tablets and capsules (ii) suspensions and solutions (iii) creams and ointments. Solvent Extraction methods, (i) extraction of organic bases and acids utilizing their ionized and un-ionized forms. Partition between organic solvents, ion-pair extraction. Solid phase Extraction – Introduction, Methodology,

types of adsorbents used in Solid phase Extraction – (i) Lipohilic silicagels. (ii) Polar surfaced modified silica gels.

References:

1. Pharmaceutical Analysis by David G. Watson
2. Practical pharmaceutical chemistry Part I by Beckett & Stenlake
3. Pharmaceutical analysis by Ashtoshkar
4. Physical pharmacy by AN.Martin,J, Swarlbick etal
5. Biopharmaceutics and pharmacokinetics by Brahmanikar
6. Text book of physical pharmaceuticals by Subramaniyan
7. Inorganic pharmaceutical chemistry By Black
8. British Pharmacopoeia Vol I,II
9. Indian Pharmacopoeia Vol I,II
10. Bently's Text book of pharmaceutics by Rowlins
11. The science and practice of pharmacy by Remington
12. Thermal methods of Analysis-D.G Watson

PAPER III CH(CPI) 403T (ELECTIVE III A): INTELLECTUAL PROPERTY RIGHTS & RESEARCH METHODOLOGY

CPI(CB1)-19: Introduction to IPR
CPI(CB1)-20: Patent Search and IP Reports Generation
CPI(CB1)-21: Research Methodology

CPI(CB1)-19 : Introduction to IPR **15 Hrs**

Introduction : Legal Rights and obligations, Concept of Property, Kinds of Property, General concept and Significance of Intellectual Property (IP), Intellectual Property Rights (IPR), Intellectual property, Introduction to IPR, contents of IPR and their protection, Recent Developments, IP Organizations.
Introduction to Patents, Trademarks, Copyrights, Trade secrets, Industrial designs and Geographical indications.
International organizations & treaties: introduction to various conventions and organizations, Paris Convention, World Trade organization (WTO)

CPI(CB1)-20: Patent Search and IP Reports Generation **15Hrs**

What is a patent search? Who needs a patent search? Patent Search Types and Methodologies, Novelty Searches, Validity Searches, Infringement Searches, State-of-the-art searches.
Searching in Patent Databases:
Free search databases: USPTO, EPSPACE, WIPO, Free Patents Online, Fresh Patents and JSPTO, Paid search databases: Micropat, Delphion, DialogPro, Patent Optimiser, Aureka and Patent Cafe, Patent Filing and Drafting, Patent filing procedures, Indian patent act, patent drafting, PCT applications, provisional and complete specifications.

CPI(CB1)-21: Research Methodology: **15Hrs**

Definition, objectives of research, types of research- significance of research, research and scientific method, importance of knowing how research is done.
Research process - formulating the research problem, extensive literature survey, development of working hypotheses, preparing the research design, determining sample design, collecting the data, execution of the project, analysis of data, hypothesis-testing, generalizations and interpretation, preparation of the report or the thesis.
Criteria of good research, problems encountered by researchers in India.
Defining the research problem, selecting the problem, necessity of defining the problem.
Research design, need for research design, features of a good design, Basic principles of experimental designs

References:

1. Fundamentals of Jurisprudence by Dhyani, Allahabad Publication, Central Law.
2. Jurisprudence of Legal Theory by Dwivedi S.P. Allahabad Central Law Agency.
3. Text Book on Jurisprudence by Hilari WC Cobrey, Oxford Publications.
4. Treaties on Intellectual Property Rights by Blackstone
5. W.T.O. by Myneni, Asia Law House.
6. W.T.O. by Vasudeva, Minerva Publications, Delhi.
7. Law of Practice of Intellectual Property in India by VikasVashistha, Bharat Law Publications, Delhi.
8. Intellectual property rights by B L Wadhera, Universal Law Publications.

9. Trade Marks Act by Mittal, Eastern Book Company.
10. Patent Law by Narayana P, Eastern Book Company.
11. Intellectual Property Rights by Cornish, Universal Publications.
12. Research Methodology- Methods and techniques, C. R. Kothari, New Age International (P) Ltd., Publishers

PAPER III CH(CPI) 403T (ELECTIVE III B): PRINCIPLES OF DRUG DISCOVERY DRUG TARGETS AND CHEMISTRY OF PHARMACOLOGY

CPI(CB1)-19: General Principles of Pharmacology and drug Targets, drugs acting on ANS and CNS
CPI(CB1)-20: Drugs Acting on Cardio Vascular and Respiratory System
CPI(CB1)-21: Drugs acting on metabolic process, cell wall, genetic material and immune system

CPI(CB1)-19: General Principles of Pharmacology and drug Targets, drugs acting on ANS and CNS **15hrs**

Introduction to molecular targets - lipids, carbohydrates, proteins (catalytic and non-catalytic) and nucleic acids. A brief introduction to the architecture of the Cells - Human Cell structure, Bacterial Cell wall, Cell membrane-membrane lipids, membrane proteins, membrane carbohydrates.

Pharmacology of Drugs Acting on ANS and CNS

Introduction - Transmission - Distribution and Functions of drugs acting on Autonomic Nervous System; Cholinergic agonists (Acetylcholine), Anti-cholinergic agents (Atropine), Anti Cholinesterase (Physostigmine), Local Anaesthetics (Procaine), Adrenergic stimulants (Dopamine), Adreno receptor antagonist (Doxazosin). Anti-Histamine agents (Cimetidine). Distribution and Functions of Drugs acting on Central Nervous System: CNS Neuro- transmitters; CNS Stimulants - Analeptics (Nikethamide), Psychomotor stimulants (Amphetamine), Anti-depressants (Imipramine), Hypnotics and Anxiolytics: Anti-psychotic Agents (Chlorpromazine), Anti-epileptic Agents (Phenytoin), General Anesthetics (Haloethanes (inhalation anasthetic)), Thiopentone (I.V. anasthetic). Neuro-degenerative disorders: Alzheimers disease (Donepezil), Parkinson disease (Levodopa).

CPI(CB1)-20 : Drugs Acting on Cardio Vascular and Respiratory System **15hrs**

General considerations - Pharmacology of drugs used in the treatment of congestive heart failure - Anti-arrythmics - Classification with examples, Anti-hypertensives, ACE inhibitors (captopril), beta1-blockers (Propranolol), Drugs acting on Ion channels - Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Amlodipine, Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine. α-Adreno receptor stimulant (Clonidine), α- Adreno receptor blocking agent (Prazocin), Anti-hyperlipedemic
(Clofibrate).

Pharmacology of Drugs affecting Respiratory System: Drugs used in the treatment of disorders of Respiratory Function and Bronchial Asthma - Broncho dilators - i) β–adrenergic agents (Albuterol) ii) Phosphodiestarase inhibitors (Aminophylline), Anticholinergic agents (Atropine), Corticosteroids (Beclomethasone), Inhibitors of mediator release (Cromolyn Sodium), Anti-tussives (Codeine) and Expectorants (Guaifenesin).

Pharmacology of Drugs affecting Gastro intestinal System - H^{+}/K^{+} - ATPase inhibitors (omeprazole) Pharmacology of purgatives/laxatives (Dulcolax), Anti-diarrhoeals (Lopramide).

CPI(CB1)-21 : Drugs acting on metabolic process, cell wall, genetic material and immune system **15hrs**

a) Drugs acting on metabolic process: Antifolates - Discovery and mechanism of action of sulphonamides, Structure of sulfomethoxazole, and dapsone. Diaminopyrimidines - trimethoprim, and drug synergism.

b) Drugs acting on cell wall: β-Lactam antibiotics - mechanism of action of penicillins and cephalosporins. Resistance to pencillins, broad spectrum penicillins - ampicillin and amoxicillin. β-Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactum.
Drugs acting on genetic material: Introduction, classification and mechanism of action.
a) DNA-intercalating agents - Anticancer and Antimalarial agents. Structural formulae of Daunomycin, Amsacrine and Chloroquine.
b) DNA-Binding and nicking agents: Antiprotozoal drugs, Metronidazole, and Tinidazole. **c) DNA-Polymerase inhibitors:** Antiviral agents - AZT.
d) DNA-Topoisomerase inhibitors: Anti-bacterial agents. Structural formulae of Ciprofloxacin and Norfloxacin
e) Inhibitors of transcribing enzymes: Anti-TB and anti-leprosy agents - structural formulae of Rifamycins.
f) Drugs interfering with translation process: Antibacterial drugs - Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin.
g) Drugs acting on immune system: Introduction to immune system. Immunosupressing agent-structural formula of Cyclosporin. Immunoenhancers - use of vaccines and strucrural formula of levamisol.

References:

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 Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 By Hanzsch.
5. Principles of medicinal chemistry. By William Foye
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Pharmacology and Pharmacotherapeutics, R.S. Satoskar and S.D. Bhandarker, Popular Prakashan, Mumbai.
9. Pharmacology, H.P. Rang, M.M. Dale & J. M. Ritter: Churchill Livingstone, 4th edition.
10. Basic and Clinical Pharmacology, 9th edition – Bertram. G. Katzung.
11. Pharmacology and Pharmacotherapeutics, R.S. Satoskar and S.D. Bhandarker, Popular Prakashan, Mumbai.
12. Pharmacology, H.P. Rang, M.M. Dale & J. M. Ritter : Churchill Livingstone, 4th edition.
13. Basic and Clinical Pharmacology, 9th edition – Bertram. G. Katzung. Reference Books
14. Essentials of Medical Pharmacology, K.D. Tripati, J. P. Brothers Medical Publishers.
15. Lewis's Pharmacology, by J. Crossl and, Churchill Livingstone.
16. Pharmacological Principles of Medical Practice, by Krantz and Care, Williams and Wilkins co.
17. Goodman and Gilman's, The Pharmacological Basis of Therapeutics. J. G. Hardman and Lee E. Limbard, Mc. Graw Hill, Health professions Division.
18. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
19. Introduction to Medicinal chemistry. By Graham Patrick.
20. Introduction to drug design. By R.B.Silverman
21. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.

Laboratory courses

PAPER IV CH(CPI) 451P : Quantitative Analysis of Pharmaceuticals **4 Hrs/Week**

Assay of pharmaceuticals - Redox titrations

Assay of ascorbic acid in raw material by iodometry
Assay of ascorbic acid in tablets by cerimetry
Determination of hydrogen peroxide in medicament by Permanganometry

Assay of pharmaceuticals - Non-aqueous titrations:

Assay of Ibuprofen in tablets

Potentiometric estimation of Sulphanilamide
Conductomeric estimation of Asprin

Colorimetric Estimations

Determination of Cholesterol
Determination of Glucose
Determination of Paracetamol
Determination of Creatinine

Determination of Sodium and potassium ions in pharmaceuticals by flamephotometry
Determination of Quinine sulphate & Riboflavin by florimetry.

PAPER V CH(CPI) 452P : Computational and Python Scripting **4 Hrs/Week**

1. Protein minimization and dynamics using NAMD/GROMACS
2. Multiple sequence analysis using ClustalX (cladogram, dendrogram, phylogram)
3. Active site Centroid (x,y,z coordinates) calculation by using Mercury software
4. XRD Protein Analysis using PDBSum server
5. Calculations: HOMO-LUMO calculations, DFT calculations, computational spectral data like IR, NMR, UV (Hyperchem), single point energy.
6. Dos and Linux commands
7. Python Scripting : if, if else, for, while
8. Python scripting for Translate DNA sequence into RNA sequence
9. Python scripting for Pairwise and Multiple sequence alignment
10. Python scripting for extracting FASTA sequence and Starting and ending AA number from PDB
11. Python scripting for centroid coordinate calculating in PDB
12. Python Scripting for linear regression of molecular data

PAPER VI CH(CPI) 453P: TLC and column chromatography **2 Hrs/Week**

Thin layer chromatography:

Determination of purity of a given sample, monitoring the progress of chemical reaction by comparing the Rf values with known standards.

Separation 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.

CH(CPI) 454P: PROJECT **12 Hrs/Week**

Marks Distribution for Project Assessment

INTERNAL ASSESSMENT

Research Design Seminar	1 credit	25 marks
Progress Seminar	1 credit	25 marks

SEMESTER END ASSESSMENT

Dissertation	1 credit	50 marks
Final presentation	2 credits	50 marks
Viva Voce during final presentation	1 credit	25 marks