

3 – Year Integrated Ph.D. Programme in Chemistry

Paper-I

Title: Research Methodology

Max Marks: 100

Duration: 6 months

Unit – I Spectroscopic Techniques

Molecular Fluorescence Spectroscopy:

Theory: Resonance Fluorescence, single/triplet excited states, Jablonoski diagrams, spectra.

Deactivation processes: Vibrational relaxation, intersystem crossing, internal conversion, fluorescence and phosphorescence, Quantum yield, effect of temperature, solvents and pH on fluorescence.

Instrumentation: Fluorometer and spectrofluorometer, phosphorimeter, light sources filters and monochrometers, detectors, cells and cell compartment.

Atomic absorption spectroscopy:

Theory: Atomic absorption, spectra, atomic line width, sample atomization, continuous atomizers, discrete atomizers, Flame atomization, types of flames, flame structure, common fuels and oxidants. Laminar flow burners, fuel and oxidant regulators, electro thermal atomizers (graphane furnace).

Instrumentation: Radiation sources, Hollow cathode lamp, electrodeless discharge lamps, single and double beam spectrophotometers, spectral interferences, Methods for correcting matrix interferences and chemical interferences.

Unit-II Separation and Electroanalytical Techniques

Separation Techniques :

Introduction to Separation Techniques Introduction to sample pre treatment.

Sample Preparation: Grinding, homogenization and drying of the sample. Dissolution and digestion of insoluble species. General theory of separation efficiency.

Classification of separation techniques: Separation based on size, mass or density, complexation, Change of state and partitioning between phases.

Chromatographic Techniques Gas Chromatography , Liquid Chromatography and High Performance liquid Chromatography. Ion Exchange Chromatography. Classical and High performance techniques. Size Exclusion Chromatography, Super Critical Fluid Chromatography. Affinity and Chiral Chromatographic Techniques.

Coupling of Chromatographic and Spectroscopic techniques: GC-MS, GCFTIR, LC-MS and LC-NMR. **Classical Electrophoresis, Gel and Capillary Electrophoresis:** Introduction classical electrophoresis : Factors affecting ion migration. Principle and application of gel and capillary electrophoresis. Introduction and application of high performance capillary electrophoresis and capillary electro chromatography.

Field Flow Fraction (FFF): Principles of separation, sub-techniques and application of FFF.

Electrochemical Techniques:

Potentiometry: Principles, Instrumentation . Indicator and reference electrodes, glass pH electrode and Ion-selective electrodes. Applications of Potentiometry.

Coulometric methods: Controlled potential coulometry and coulometric titrations, Principles, Instrumentation and applications.

Amperometric titrations: Basic and applications, Amperometric sensors

Voltammetry; Principles of Linear sweep voltammetry and cyclic voltammetry, stripping methods. Voltammetric instruments and Voltammetric electrodes. Applications.

Polarography: Basics: diffusion current, half-wave potential, Ilkovic equation, DME. (Applications in organic/inorganic analysis)

Unit – III Thermal Techniques and Rheology

Thermal Techniques

Thermogravimetry (TG/TGA), Differential Thermal analysis (DTA), Differential scanning calorimetry (DSC) and Thermometric titrations. Basic and instrumentation and applications.

Rheology:

Introduction to Rheology and rheometry. Definition of terms. Shear stress, shear rate, viscosity (shear viscosity and Kinematics viscosity), deformation and strain, shear modules.

Viscoelasticity: flow behavior and flow curves viz Newtonian, shear thinning and shear thickening. Model functions for flow curves. Effect of rheological additives in aqueous dispersions. Rheological behavior of surfactants and polymer systems

Unit – IV Literature survey, Data Analysis and Research Ethics:

Literature survey:

Use of Google, Scifinder, Scopus and Pubmed for searching the literature

Date Analysis and Data Analysis Software

Accuracy and precision. Significant figures. Rounding off. Determination of errors. Indeterminate errors. Mean, Median, range, variance and standard deviation. Propagation of errors. Reliability of results. Types of probability distribution: Normal distribution and Binomial distribution. The confidence limit. Tests of significances; the Q test, t- test, F- test. Correlation and regression. Least squares fitting: linear and nonlinear.

Introduction to origin and Microsoft excel: Graphing, statistics and fitting in origin & excel.

Research Ethics:

Scientific conduct: ethics with respect to science and research, intellectual honesty & research integrity: scientific misconducts and misrepresentation of research data.

Publication Ethics: Best Practices, conflict of interest; publication misconduct (Fabrication, Falsification and Plagiarism), authorship and contribution acknowledgement, Hybrid mode of publication. Conflict of interest, complaints and appeals.

Open access: Predatory publishers & journals, UGC Regulations-meaning & concept.

Recommended Books:

1. Principles of Instrumental Analysis, 4th Edition, D.A. Skoog, J.J. Leary, Saunders College Publishing
2. Modern Analytical Chemistry, 1st Edition, David Harvey, Mc Graw – Hill Education, 2000
3. Analytical chemistry, 5thEdn. G.D. Christian; John Wiley 2001
4. Fundamentals of Analytical Chemistry, 8thEdn. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Thomson Learning Inc.
5. Principles and practices of Analytical Chemistry, 5thEdn. F. W. Fifield, D. Kealey, Blackwell Sciences
6. Analytical Chemistry, 2ndedn., R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmur; Wiley, 2004.
7. Modern Chemical Techniques; C.B. Faust, RSC, 1998
8. Thomas G.Mezger. The Rheology Handbook, 3rd edition, Vincentz Networks 2011. Verlag GmbH & Co. Germany.
9. Rheology for Chemists: An introduction, J. Goodwin, R. Hughes, Ed-2, RSC Publishing, 2008.
10. Willard, Merit and Dean, “Instrumental methods of Analysis”, John Wiley and Sons, New York.
11. Skoog and West, “Fundamentals of Analytical Chemistry”, John Wiley and Sons, New York, 1994.
12. Jeffery, Basset, Mendham & Denny, “Vogels Text Book of Quantative Analysis”, ELBS, 1989.
13. Alexander Findley, “Practical Physical Chemistry”, revised by B.P. Levitt, Longman, London, 1973
14. Shoemaker, Garland & Niber, “Experiments in Physical Chemistry”, McGraw-Hill Book Company, 1998.
15. Automated Data Analysis Using Excel, Brain D. Bissett, Chapman and Hall/CRC, 2007.
16. Origin 2015: Graphing and Analysis from www.originlab.com, An interactive booklet.
17. Practical Skills in Chemistry, J. R. Fean, A.M. Jones, D. Holmes, R. Reed, J. Weyers and A Jones, Pearson Education Ltd., Prentice Hall, 2002.
18. Philosophy of Science by Alexander Bird (1998) Routledge, Taylor & Francis ISBN 9781857285048.
19. 2. Ethics in Competitive Research: Do not get Scooped; do not get plagiarized by Praveen Chaddah (2018) ISBN 9387480860
20. 3. National Academy of Sciences, National Academy of Engineering and Institute of Medicine (2009)., National On being a Scientist: A guide to responsible conduct in Research : third edition, National Academies Press.

3 – Year Integrated Ph.D. Programme in Chemistry

Paper-II

Title: Recent Trends in Chemistry

Max Marks: 100

Duration: 6 months

Unit – I Green & Sustainable Chemistry

Green Chemistry-

Introduction: Need for Green Chemistry and the role of chemists.

Principles of Green Chemistry. Tools of Green Chemistry: Selection of starting materials, Catalysts, Alternative Solvents, Appropriate reagents, Percentage atom utilization. Microwaves and Sonication.

Green Chemistry-Practice: Green Solvents and Reaction conditions: Supercritical fluids, Aqueous reaction conditions, Immobilized Solvents and irradiative reaction conditions. Examples of Green materials, reagents and some specific reactions

Unit – II Homo & Heterogeneous Catalysis using Organometallics

Introduction, History and Importance of Organometallic Compounds as reagents, additives and Catalysis

Mechanism of Catalysis using Organometallics:- Oxidative addition, insertion reactions, Reductive elimination and Water gas Shift reaction (WGSR)

Catalytic Mechanism of Hydrogenation, Hydroformulation, oxidative and isomerization of alkenes, Olefin metathesis

Fischer-Tropsch Synthesis and Zeigler Natta Polymerization of alkenes

Unit – III Chemistry of Materials

Liquid Crystals: Mesomorphism, types of liquid crystals, properties of liquid crystals, Characterization by optical polarization microscopy, Applications – Liquid crystal displays, thermography, optical imaging and ferroelectric liquid crystals

Langmuir – Blodgett Films: Introduction and general preparative techniques. LB Films of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications – nonlinear optical effects, conduction, photoconductivity and sensors.

Block Copolymers: Introduction: Classification, micellization of diblock and triblock copolymers. Introduction to PH-, thermo- and Photo-responsive block copolymers. Linear-dendrimer block copolymers: introduction, structural peculiarities of their aggregates, potential applications

Unit – IV Novel Materials

Bio-inspired smart materials: Introduction to bio-inspired materials. Examples and applications of following bio-inspired materials: bioceramics, bioglasses, self-healing, PH-responsive, photo-responsive, stress-responsive and electric-responsive materials.

Nanomaterials: Introduction with examples and applications of nanoparticles, nanofibers (nanowires, nanotubes and nanorods) and nanoplates.

Graphene: Introduction. Overview of electrochemistry of graphene. Graphene based electrochemical sensors for enzymes, DNA and heavy metals

Recommended Books:

1. Green Chemistry – An introduction Text; IIndEdn. ; Mike Lancaster; RSC; 2010.
2. Green Chemistry- Theory and Practice; P. T. Anastas and J.C. Warner; Oxford ; 2000.
3. Inorganic Chemistry; 4thedn.; Huheey; E. Keiter; Addison- Wesley; 1983
4. Metallo-Organic Chemistry; A.J. Pearson; Wiley.
5. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Books / Cole; 1985
6. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and Sons, Inc. 2001.
7. Smart Materials. M. Schwartz, CRC Press, 2008.
8. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley
9. Bloc Copolymers, N. Hadjichristidis, S. Pispas and G.A. Floudas , Wiley, New York, 2003.
10. The Physics of Block Copolymers, I. W. Hamley,. Oxford University Press, Oxford, 1998
11. P. Alexandridis and J.F. Holzwarth, Curr. Opin Colloid Interface Sci. 5, 312, 2000.
12. Green Chemistry – Environment Friendly Alternatives; Rashmi Sangh & M.M. Srivastava; Narosa ; 2007.
13. Nanotechnology, An introduction, J.J. Ramsden, Elsevier, 1st Edition, 2011.
14. Essentials of Nanotechnology, J.J. Ramsden, Jeremy Ramsden and Ventus Publishing Aps, 2009

3 – Year Integrated Ph.D. Programme in Chemistry

(Supervisor Specific Specialized Papers)

Course No. : 03

Max Marks: 100

Title: Specialized Paper

Duration :6 months

Unit I: Oscillatory Chemical reactions

Introduction: History; Fundamentals; Apparatus: Analytical techniques- Spectroscopic methods; Potentiometric methods. Batch reactors, Semi batch reactors; Flow reactors; Pumps; Reactor for Chemical waves.

Types of Oscillatory Chemical reactions- Belousov-Zhabotinsky reaction; FKN mechanism; Effect of Substrate; metal ion; acid; additives (alcohol, Surfactants, ketones, etc). Briggs-Rauscher reaction; Bray-Liebhafsky reaction; Chlorite-Iodate oscillator; pH Oscillators.

Unit II: Patterns, Waves and Chaos

Stability analysis; Arsenous acid-Iodate reaction; Propagator-Controller systems; Wave initiation; Waves in two dimensions- Target patterns and Spirals; Three dimensional waves; Chemical waves and patterns in open systems; Chemical waves in Non-uniform media;

Complex oscillations; Mixed mode oscillations; chemical chaos; One dimensional maps; characterising chaos; controlling chaos. Stirring and Mixing Effects.

Unit III: Polymer Systems

Introduction: Sources of feedback; Thermal Oscillations; Emulsion polymerisation; Radical polymerisation; Biopolymers; Synthetic polymers; Frontal polymerization-Mechanism.

Polymerization coupled to Oscillatory reactions; Ordering phenomena in Phase separation of Polymer mixture; Photo-Crosslinking of Polymer blends; Coupled Oscillators; Oscillator death; Biorhythmicity; Compound Oscillation.

Unit IV: Applications of Nonlinear Chemical Dynamics

Biological Oscillators: Neural Oscillators-Bursting; Microtubule polymerization; Synthesis of polymers using oscillatory reactions; Analytical monitoring of various chemical entities viz. antioxidants, metals, drugs, etc. Ion exchangers : Role of Ion exchangers in changing oscillatory parameters; Pattern formation using ion exchangers; Corrosion chemistry: Synthesis of corrosion inhibition polymers using oscillatory reactions; Turing patterns; Future directions.

BooksRecommended:

1. An Introduction to Nonlinear Chemical Dynamics- Oscillations, waves, patterns and chaos; J. A. Pojman and M. Burger, 1998
2. Chemical Waves and Patterns, Raymond Kapral and Kenneth Showalter, Springer, 2012.
3. Oscillations and Travelling waves in Chemical Systems, M. Burger and R. J. Field, Wiley Interscience, 1985.
4. Nonlinear Dynamics with Polymers, Fundamentals, Methods and Applications, edited by John A. Pojman and Qui Tran-Cong-Miyata, Wiley-VCH, 2010

3 – Year Integrated Ph.D. Programme in Chemistry

Course No. : 03

Max Marks: 100

Title: Specialized Paper

Duration :6 months

Unit 1. Liquids and Solutions

Viscosity, Newtonian and non-Newtonian behavior, Stokes–Navier equation, Einstein’s law of viscosity, intrinsic viscosity and particle size, viscometers. Light scattering by colloidal solutions, aggregation number by light scattering and fluorescence spectral methods. Isothermal and adiabatic compressibility of liquids and solutions.

Non-ideal solutions: Virial equation of state, second virial coefficient as a measure of non-ideality, excluded volume. Regular solution and Flory- Huggins statistical theory with their application to binary liquid mixtures. DLVO- theory for stability of colloids.

Unit 2. Micelles and Microemulsions

Micellization of surfactants, critical micelle concentration (cmc), structure and shape of micelles, aggregation number. Factors affecting cmc in aqueous media and their role in micellization. Equations for cmc based on theoretical grounds. Thermodynamics of micellization, pseudophase model and mass action model, self-assembly.

Macroemulsions, Microemulsions and Nanoemulsions: formation and stability. Structure-dynamics and transport properties of microemulsions. Applications of microemulsions in food, textile, agro-chemical, pharmaceutical and petroleum industries with focus on their role in environmental remediation, biotechnology and chemical reactions.

Unit3. Importance of Micelles and microemulsions in growing Technological Advancements.

Micellar Solubilization: Experimental methods of studying solubilization and factors affecting it. Solubilization of drugs into micelles and its importance. Effect of surfactants on membrane permeability with respect to drugs. Drug delivery systems and controlled release.

Reactivity in surfactant systems: Micellar reactions; hydrolysis, oxidation, reduction, luminescence and fluorescence, reactions involving metal ions, enzyme catalyzed reactions and oscillatory reactions.

Unit 4. Surfactant-Surfactant and surfactant-polymer interactions

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, various models of mixed micelle formation (Clint, Rubingh, Motamurra, Blankschtein, and Rubing-Holland models) and mixed monolayer formation (Rosen’s model). Importance and practical applications of mixed surfactant systems.

Surfactant-Polymer Interactions: Effect of polymers on aggregation behavior of surfactants and the factors governing their interaction. Phase behavior of polymer-surfactant mixtures. Characterization of polymer-surfactant systems by various techniques like viscosity, light scattering, spectroscopic and conductance measurements.

Books recommended

1. J.N. Murell and E. H. Boucher, "Properties of Liquids and Solutions," John Wiley & Sons Ltd., 1982
2. P.W. Atkins. "Physical Chemistry", ELBS, Oxford, 1994.
3. P.C. Heimenz, "Principles of Colloid and Surface Chemistry", Marcel Dekker Inc. New York, 1986.
4. M. J. Rosen, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 1989.
5. R. D. Vold and M. J. Vold, "Colloid and Interface Chemistry", Addison-wesley, 1982.
6. .D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
7. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998
8. B.K.Paul&S.P.Moulik,*Current Science*,Vol.80,p 990-,2001;*Advances in Colloid and Polymer Science*,Vol.78,p 99,1998
9. John Flanagan & Harjinder Singh, *Critical Reviews in Food Science and Nutrition*,Vol.46,pp221-237,2006.
10. M.J.Lawrence&G.D.Rees,*Advanced Drug Delivery Reviews*,Vol,45,p 898,2000.
11. T.N.Dantas,A.A.D,Netoetal.,*Energy Fuels*,DOI:10.1021/ef900952y,2010.

3 – Year Integrated Ph.D. Programme in Chemistry

Course No. : 03

Max Marks: 100

Title: Specialization Paper

Duration :3 hours

Unit-I: Foundations of Molecular Orbital Theory:

Quantum mechanics and the wave function. The Hamiltonian Operator; General features, the Variational Principle, the Born-Oppenheimer Approximation. Construction of trial wave functions; the LCAO basis set approach, the secular equation. Huckel theory; fundamental principles, application to the Allyl systems. Many –electron wave functions; Hartree-product wave functions, the Hartree Hamiltonian, electron spin and antisymmetry, Slater determinants, the Hartree-Fock Self-consistent Field Method.

Unit-II: *Ab Initio* Implementation of Hartree-Fock Molecular Orbital Theory:

Basis sets; Functional forms, contracted Gaussian functions, Single- ζ , Multiple- ζ , and Split- Valence, polarization functions, diffuse functions, the HF limit, effective core potentials, Technical aspects; SCF convergence, symmetry, open shell systems, efficiency of implementation and Use.

Unit-III: Writing in LaTeX

LaTeX: Basics, LaTeX input files, Document classes, Page styles, Packages, Commonly used LaTeX commands, Typesetting text and mathematical formulae, Constructing tables, Producing mathematical graphics using the picture environment, Using graphics in LaTeX, The Figure environment, Creating presentations with LaTeX classes.

UNIT – IV: Working with Gaussian

Resource management; % mem, %rwf, %chk, % nproc. Number of processors for different methods. Route card description syntax. Creation of input files; single point energy and properties, geometry optimization, frequency, reaction path following /searching. Levels of theory; Molecular Mechanics, Semi-empirical, Density Functional theory, Ab-initio, Hybrid etc. Basis set. Basis set types- all electron: Pople, Dunning,Huzinaga etc.; effective core potential. Molecular coordinates; Cartesian coordinates; Z-matrix. Building with Gauss View; remote login, loading of proper module, launching of GaussView. Syntax for submitting calculations; Interactive, Batch and Queue commands. Common errors; memory errors, disc errors, SCF failure, Coupled cluster iteration failure, optimization failure. Output visualization and interpretation of output files.

Books recommended:

1. Computational Chemistry, A Practical Guide For Applying Techniques to Real World Problems: David Young: Wiley-Interscience:2001
2. Electronic Structure; Basic theory and practical methods: Richard M. Martin: Cambridge University Press:2004
3. Exploring Chemistry with Electronic Structure Methods: 2nd ed. James B. Foresman and Aeleen Frisch: Gaussian, Inc. 1996.
4. LaTeX by Leslie Lamport published by PEARSON Education (2004).

3 – Year Integrated Ph.D. Programme in Chemistry

Course No. : 03

Max Marks: 100

Title: Specialized Paper

Duration: 3 hours

Unit I: Ion – Exchange Materials:

Introduction: Historical development of ion –exchange materials. Basic types of ion-exchangers, miscellaneous exchangers. The Zeolites : Molecular sieve properties of the zeolites. Zeolites as ionic sieves. Selectivity in zeolite series. The Lindar molecular sieves – double sieve action. Exchange isotherms in the zeolites. Hydrous oxides and Salts of Polybasic Metals: The hydrous oxides. Quadrivalent metal oxides. Insoluble salts of polybasic metals; Zirconium phosphate. Preparation of zirconium phosphate. Physical and chemical properties of zirconium phosphate. The structure of zirconium phosphate. Intercalation and pillaring in zirconium phosphate. Ion exchange in Zirconium phosphate. Selectivity in Zirconium phosphate. Ion-sieve properties of zirconium phosphate.

Unit II:

(A) Ion-Exchange Kinetics:

Ion-Exchange Kinetics: Systems, Mechanism, and the Rate Controlling Step. Diffusion in Ion-Exchangers. Rate of Ion Exchange: Partial-diffusion control; Film diffusion control; Intermediate cases. Ion exchange accompanied by neutralization, complex formation, or other reactions. Multicomponent systems. Simplified rate equations.

(B) Ion – Exchange Selectively:

Introduction: General qualitative description of the selectively phenomenon. Quantitative definition of selectively; exchange; exchange involving monovalent ions only; Exchange involving multivalent ions. Experimentally observed features in Uni-Univalent Exchange. Approaches to the understanding of Ion –exchange Selectively. Factors underlying ion-exchange selectively; Non uniformity of exchange sites; Ion-water interactions; Ion – ion interactions. The effect of swelling.

UNIT-III:Low Temperature Synthetic Routes:

Co-precipitation, Sonochemical , Microemulsion; Solution combustion, Sol-gel.

Sol-gel: hydrolytic sol-gel, non-hydrolytic sol-gel, acid reflux, acid digestion, and mild hydrothermal or autoclave methods. Detailed mechanism of synthesis, Comparison. Advantages and disadvantages of different synthetic methods

Unit IV: Characterization techniques:

UV-Vis spectra: Beer's law. Limitation to Beer's law, Quantitative analysis: Calibration curve method, standard addition method, Quantitative analysis of mixtures. **Instrumentation:** Light sources, wavelength selectors (dispersion devices), sample containers, Detectors, Signal processor and read-out. Filter photometers, construction and working of Single beam, double beam and split beam spectrophotometers.

X-Ray Diffraction (XRD), Powder X-Ray Diffraction, Scanning Electron microscopy (SEM) and Transmission Electron Microscopy (TEM) : Principles and applications

Thermal Analysis: Differential Scanning Calorimetry (DSC), Calorimetry, Thermal Gravimetric Analysis (TGA), and Differential Thermal Analysis (DTA): Principle and applications

Books Recommended:-

1. Ion Exchange-A series of Advances: Vol. 1. Jacob A. Marinsky: Marcel Dekker: 1969
2. Ion Exchange-A series of Advances: Vol. 2. Jacob A. Marinsky: Marcel Dekker: 1969
3. Inorganic Ion Exchangers: C. B. Amphlett: Elsevier: 1969
4. Ion Exchange: Dmitri Muraviev, Vladimir Gorshkov and Abraham Warshawsky: Marcel Dekker: 2000
5. Introductory Raman Spectroscopy: 2nd ed. John R. Ferraro, Kazuo Nakamoto and Chris W. Brown: Academic Press: 2005
6. Modern Analytical Chemistry: David Harvey: Mc Graw Hill: 2000).
7. Infrared and Raman Spectra of Inorganic and Co-ordination Compounds: 5th ed. Kazuo Nakamoto: John Wiley: 1997
8. Principles of Instrumental Analysis: 4th ed. Douglas A. Skoog and James J. Leary: Saunders: 1992

3 – Year Integrated Ph.D. Programme in Chemistry

Course No. : 03

Max Marks: 100

Title: Specialized Paper

Duration :3 hours

UNIT 1: Organic Solvents and Reagents:

Purification, drying and handling of the following common organic solvents and reagents:

DMSO, DMF, Pyridine, Ethyl Alcohol, Petroleum ether, Methanol, Ethyl acetate, Chloroform, Benzene and Methylene chloride.

Preparation and uses of following reagents:

Alkyl and Aryl lithium compounds, Aluminiumisopropoxide, Diazomethane, Raney nickel, Libberman-Burchard reagent, Tortelli reagent, Fieser reagent, Salkowski reagent, Dragendroff's reagent, Ceric ammonium sulphate.

UNIT II: Spectroscopy

- Problem based exercises on interpretation of spectral data using UV-IR**
H¹NMR, C¹³NMR and Mass
- Applications of advanced NMR techniques:** DEPT, COSY, 2DNMR
- ORD/CD:** Circular birefringence, ORD and CD Curves, relationship between ORD and CD and their applications. Distant rule. Displacement rule, rule of super position. Axial haloketone rule, Octant rule and its applications to ketos steroids.

UNIT III :Designing organic synthesis / Named reactions

Designing synthesis of following compounds using retrosynthetic approach.

ICI-DD7114, Ofornine, Phenylramidol, propanolol, Pre-moth-pheromone, Arildone, Cinflumide, Venlafaxine, Clobutinol, Thyroxine and salbutamol.

Named reaction

Arndt-Eisterthomologation, Bartoli Indole synthesis, Beckmann Rearrangement, Cope elimination, Barton- Zard reaction for the synthesis of pyrroles, Corey Chaykovsky reaction,

Corey Kim Oxidation, De-Mayo reaction, Dienone-Phenol rearrangement, Henery Notro aldol reaction, Jones Oxidation, Wittig rearrangement, Pechmann coumarin synthesis, Nef reaction.

UNIT IV : ALKALOIDS

Naming of Alkaloids, Classification, Properties, Distribution in nature. Biosynthesis of alkaloids, Qualitative tests, Chemical and Spectral methods of Structural elucidation.

β-carboline Alkaloids: Structure, Examples, Occurrence in nature, Pharmacology, Synthesis.

Applications:

Alkaloids in modern medicine, Alkaloids as drug leads.

Recommended Books:

- 1) Organic Chemistry- Finar Vol:II, ELBS-Longman 1975.
- 2) Organic Chemistry- Clayden, Greeves and Warren, Oxford University Press, 2001.
- 3) Organic Spectroscopy- Kemp, Macmillan and ETBC, 1995.
- 4) Mass Spectroscopy- Davis and Freavson, Jhon Wiley.
- 5) Spectroscopic Identification of organic compounds, 5th edition; Silverstein, Bassler, John Wiley, 1991.
- 6) Reagents for Organic Synthesis, M.Fieser and L.F. Fieser 1974.
- 7) Spectroscopic Methods in Organic Chemistry, 4th Edition D.H. Williams and Ian Fleming, Jhon Wiley, 1998.