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

Semester III
Paper I : CH (IC) 301T: Bonding, Group Theory and its applications

Prof. B. Sireesha

Lesson Plan: IC-09: Group Theory, Normal Mode Analysis and Spectral Activity	
Lecture No	**Topic**
1	Properties of a point group, closure rule-abelion and non-abelion groups, associative rule, inverse rule and identity rule
2	Group multiplication table, the rearrangement theorem, GMT of C_3, C_4
3	Group multiplication table for C_{2V}, C_{2h}, C_{3V} and C_5 point groups
4	Sub groups-Langrange's theorem, Classes, similarity transformation. Properties of conjugate elements
5	Definition, classes for C_{2V}, C_{3V} with examples
6	Matrices and vectors, types of matrices, multiplication and direct product, matrix representation of symmetry elements-E, σ, *i*, Cn
7	Matrix representation of symmetry element- Sn. Matrix representation of Points groups- C_2v, C_3v etc
8	Product and square rule, Matrices of C_{2h}, C_{2V}, C_{3V} and C_{4V}, block factorization
9	Transformation matrices, reducible and irreducible representations, character of a representation
10	Properties of irreducible representation, orthognality principle, construction of character table- C_{2V}
11	Character tables of C_{2h}, C_{3V} and C_{4V} groups
12	Mulliken symbolism, rules for IRs. Symmetry species for translations and rotations, standard reduction formula
13	The direct product, rules of direct products, normal mode analysis, Cartesian coordinate method, C_2v, alternate method
14	Internal coordinate method C_{2V}- H_2O, IR and Raman activity
15	Normal mode/Internal coordinate method for C_{2h} and C_{3V} with examples

Paper I **Prof. B. Sireesha**

Lesson Plan: IC-10: Molecular Orbital Theory of Metal Complexes	
Lecture No	**Topic**
1	Revision of CFT, Limitations of CFT, Adjustments of CFT to allow for covalence
2	Experimental evidences for metal-ligand orbital overlap – ESR and NMR studies of few metal complexes
3	Adjusted CFT, introduction to MOT, atomic and molecular wave functions
4	Symmetry classification of metal and ligand orbitals in cubic environment (tetrahedral and octahedral) geometries
5	Symmetry classification of metal and ligand orbitals in non-cubic environment -square pyramidal, trigonal bipyramidal and square planar geometries
6	Linear Combination of Atomic Orbitals (LCAO) concepts. Concept of Ligand Group Orbitals LGO's
7	Construction of LGO's for Octahedral, Tetrahedral and Square Planar geometries (sigma orbitals)
8	Construction of LGO's Pi-Orbitals for Octahedral geometry –Four steps
9	Construction of LGO's Pi-Orbitals for Tetrahedral and Square Planar geometries
10	Construction of MOED –Oh metal complexes with σ only orbitals and σ and π orbitals
11	Construction of MOED –Oh metal complexes with, σ, π and π* orbitals
12	Construction of MOED for Td metal complexes with σ only obitals, and σ and π orbitals
13	Construction of MOED for square planar metal complexes with σ only obitals, and σ and π orbitals
14	Construction of MOED –Oh metal complexes with σ, π and π* orbitals of Sqaure planar geometry
15	MO electronic configuration and calculation of magnetic moment

Paper I **Prof. B. Sireesha**

Lesson Plan: IC-11: Electronic Spectroscopy of Metal Complexes	
Lecture number	**Topic**
1	Classification of Electronic Spectra for Metal Complexes, Types of electronic transitions in metal complexes, Selection Rules
2	Details of Electric Dipole Transitions, Electric quadrupole transitions, Magnetic Dipole Transitions, their intensities
3	Orbital Selection Rules-With the ground and excited electronic energy levels with totally symmetric terms. Examples with allowed and forbidden transitions
4	Orbital Selection Rules- With the ground and excited electronic energy levels with non- symmetric terms. Examples with allowed and forbidden transitions
5	Spin Selection Rules, Working of all the point groups to find out the allowed and forbidden transitions
6	Relaxation in Selection Rules- d-p mixing, vibronic coupling, lifting the cubic symmetry, intensities of Laporte and spin allowed and forbidden transitions along with relaxed selection rule
7	Nature of Electronic Spectral Bands: Band Widths and Band Intensities, factors effecting band intensities with suitable examples for each
8	Factors Influencing Band Shapes: Jahn-Teller Effect, Spectrochemical Series-trends and reasons for the position of ligands in the series, Nephelauxetic Effect, nephelauxetic ratio calculation of Racah Parameter (B) and Nephelauxetic Ratio (β)
9	Orgel Diagrams for d^1-d^9 Configurations, energy level diagrams, expected transitions, combined diagrams, 10Dq values and Calculation of 10Dq Values
10	Crystal Field Spectra of O_h Metal Complexes of 3d Metals, electronic spectra of low spin and high spin complexes
11	Crystal Field Spectra of T_d Metal Complexes of 3d Metals with suitable examples
12	Charge Transfer Spectra. Types of CT transitions, representation with molecular orbitals, examples
13	Strong Field Configurations: working out by trial and error method, The Method of Descending Symmetry
14	Correlation Diagrams for d^2 and d^8 configurations in octahedral and tetrahedral geometries
15	Tanabe-Sugano Diagrams significance, advantage over Orgel diagrams, Tanabe-Sugano diagrams for d^2 and d^8 Configurations

Paper I **Prof. B. Sireesha**

Lesson Plan: IC-12: Infrared and Raman Spectroscopy	
Lecture No	**Topic**
1	Conditions for Infrared and Raman Spectroscopies, selection rules
2	Direct product: Rules, excercises
3	Symmetry requirements for overtones, binary and ternary combination bands with examples of SO_2, BCl_3
4	Partial Normal mode analysis-Structure Fitting (eg. ClF_3, PCl_3, BCl_3
5	Determination of Coordination Sites and Linkage Isomers (eg NO_2^- , SCN^-)
6	Assigning Denticity of Ligands (eg SO_4^{2-}, CO_3^{2-})
7	Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes. (eg. Cis and trans ML_4X_2)
8	Prediction of Diagnostic Fundamentals in Isomers of Metal Complexes and Distinguishing Isomers of Metal Complexes (eg. Cis and trans ML_2X_2, fac and mer-ML_3X_3)
9	Effect of Coordination on Ligand Vibrations – general discussion
10	Effect of Coordination on NH3, H2O vibrations
11	Effect of Coordination on Glycine, Carbonyl vibrations
12	Effect of Coordination on halides
13	Raman effect and molecular structure- CO, HCN, CO2, N2O, H2O
14	Principles and theory of Resonance Raman Spectroscopy,
15	Application of Resonance Raman Spectroscopy to Structural Elucidation of the active Sites of Heme and Non-Heme Oxygen Carriers

Paper: II- CH(IC) 302T: Organo Metallic Chemistry of Transition Metal Complexes

Paper: II **Dr.P. Muralidhar Reddy**

Lesson plan: IC-13: Mono, Di and Tri hapto Complexes	
Lecture No	**Topic**
1	Nomenclature and Classification based on the number of Coordinated Carbons (hapticity) and number of electrons donated by the Ligand.
2	16 and 18 electron rules. Electron counting covalent and ionic models.
3	η^1 – Complexes: Introduction, General methods of Preparation
4	Bonding of Ligand to Metal: αand βInteraction and agostic interaction
5	Stability and decomposition pathways –η^1 Complexes –Tertiary Phosphine – Transition Metal Alkyl and Aryl Complexes of Pt
6	Ortho-effect – Bonding in Metal – Carbene and Carbyne Complexes
7	η^2 –Complexes: Introduction, General methods of preparation of Metal – Alkene Complexes
8	η^2 –Complexes: Structure and Bonding in η^2 Complexes
9	η^2 –Complexes: Zeises salt – Trans Effect – Definition and significance, Examples and applications
10	Rotation of Olefin Around Metal-Olefin Bond- Factors affecting rotation, Experimental observations
11	η3 - Complexes: Introduction to Metal-Allyl Complexes
12	η3 - Complexes: General methods of preparation of Metal – Allyl Complexes
13	η3 - Complexes: Structure and Bonding in η3 Allyl Complexes
14	η3 - Complexes: Fluxionality-Definition and significance, Examples and applications
15	Problem-solving session, provide additional reading materials and resources for students to explore topics in more depth.

Paper: II **Dr.M.Kavitha**

Lesson Plan: IC-14: Tetra, Penta, Hexa, Hepta and Octahapto Complexes	
Lecture No	**Topics**
1	Overview of organometallic chemistry. Importance and applications of organometallic complexes. Brief introduction to bonding in organometallic compounds
2	Structure and bonding in η4 complexes
3	Detailed study of butadiene and cyclobutadiene complexes Stability and reactivity of η4 complexes
4	General methods of preparation of metallocenes
5	Focus on ferrocene: structure, bonding, and electronic configuration
6	Reactions of ferrocene including electrophilic substitution, Friedel-Crafts reactions
7	Introduction to η6 complexes
8	Dibenzenechromium: preparation, structure, and bonding
9	Reactions of bis(arene)-metal complexes
10	Introduction, Preparation methods of η7 complexes
11	Structural aspects and bonding in C_7H_7 complexes. Reactivity and applications
12	Preparation, structure, and bonding in cyclooctatetraene complexes
13	Detailed study of uranium complexes (e.g., Uranocene)
14	Properties, stability, and reactions of η8 complexes
15	Recent advancements in organometallic chemistry. Industrial applications and significance of various organometallic complexes

Paper-II **Prof. G. Vijaya Charan**

Lesson Plan: IC-15: Catalytic Role of OTMC-I	
Lecture No	**Topic**
1	Definition and explanation of Oxidative addition reactions with suitable examples, mechanism of Oxidative addition by concerted, non-concerted and free radical pathways.
2	Detailed study of Stereochemistry of oxidative addition reactions by physicochemical techniques such as NMR, IR Spectroscopy. Reductive Elimination: Definition, types-Intra molecular elimination and Inter molecular elimination by using specific examples with mechanism.
3	Definition and types of insertion reactions:1,1 insertion,1,2 insertion,1,3 insertion,1,4 insertion reactions.
4	Hydrogenation of Olefins by using Wilkinsons catalyst $[RhCl(PPh3)_3]$ with mechanism.
5	Definition and mechanism of the transfer hydrogenation with suitable examples.
6	Synthesis and mechanism of hydrosilation of olefins with suitable examples.
7	Isomerization of olefins-Alkene -1is isomerized to cis-trans alkene-2 catalytically using $[HCo(CO)_4]$, $[HRh(CO)(PPh_3)_3]$.
8	Ziegler –Natta catalyst- synthesis, polymerization of olefins, and applications
9	Oligomer formation and the reactions of Oligomerization of alkanes and conjugated dienes, oligomerization of butadiene in presence of catalyst Nickel phosphine, Zeigler Natta catalyst.
10	Alkene Metathesis undergoes bond reorganization and redistribution of alkylidene species with mechanism by using suitable examples.
11	Synthesis of Dupont-1,4-hexadiene with detailed mechanistic pathway.
12	Oxidation of Olefins to Carbonyl Compounds, ethylene oxidation to acetaldehyde using $Pdcl_2$, $Cucl_2$.
13	Oxidation of Hydrocarbons to Alcohols and Acids, Oxidation of Aldehydes by using catalysts.
14	oxidation of Cyclohexanol to adipic acid, oxidation of Cyclohexanone to adipic acid and glutamic acid.
15	oxidation of p-Xylene by using cobalt catalyst to terephthalic acid.

Paper-II **Prof. G. Vijaya Charan**

Lesson Plan: IC-16: Catalytic Role of OTMC-II	
Lecture No	**Topic**
1	Reactions of Carbon monoxide and Hydrogen: Introduction, reactions with specific examples.
2	Hydroformylation –Addition of H_2 and CO to unsaturated systems to yield linear and branched aldehydes by using $[Co_2(CO)_8]$, $[Rh(H)(CO)(PPH_3)_2]$, $[Ru(CO)_3(PPH_3)_2]$ catalysts with mechanism.
3	Carbonylation-introduction of CO into organic and inorganic substrates by using catalysts to produce acetic acid.
4	Syngas and Reactions of Syngas. reactions involving CO and H_2 as building blocks for basic organic chemicals, based on catalytic hydrogenation of CO to produce methanol, ethanol, ethylene glycol etc.
5	Water gas shift reaction (WGS) using homogeneous catalysts and its applications.
6	Applications of Metal Clusters in Catalysis, Hydroformylation of Ethylene using $[HRu_3(CO)_{11}]$.
7	Hydrogenation of Olefins. Use of $[Fe_4C(CO)14]$ as a model for Fischer-Tropsch process.
8	Recent Developments in Homogeneous Catalysis
9	Phase Transfer Catalysis (PTC) – Homogeneous Transition Metal Catalyzed Reactions under Phase Transfer Conditions and applications.
10	Bio Catalysis, Enzyme Analogue Catalysis: Introduction, Examples of Enzymatic Conversions.
11	Reduction of >C=O and >C=C< bonds.
12	Templates: Introduction, Metal Cations as Templates, Covalent molecules as Templates.
13	External and Internal Templates -reactions with mechanism.
14	Homogeneous Catalysts and their Heterogenization.
15	Immobilization by Aqueous Catalysis.

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

Paper: IIIa **Dr.M. Kavitha**

Lesson Plan: IC-17: Data Handling	
Lecture No	**Topic**
1	Introduction and basic concepts
2	Concept of accuracy and precision, few examples to identify data accuracy and precision, accuracy measures and precision measures
3	Introduction about errors, identify and differentiate between determinate and indeterminate errors
4	Minimization of determinate errors
5	Statistical validation of data, Mean, Median, Average deviation and standard deviation, coefficient of variation and variance
6	Calculation of mean, median and standard deviation
7	Computation rules with examples
8	Concept of Significant figures, identifying the significance of zero Students F test, calculations
9	Students F test, calculations
10	Confidence limit, calculation of confidence limit
11	Q test for the rejection of result with few solved problems
12	Students t test, t test under different conditions, Calculations
13	Regression analysis, method of least squares
14	Calculation of correlation coefficient
15	Detection limit and calculations

Paper-IIIa **Dr. P Muralidhar Reddy**

Lesson Plan: IC-18: AAS, AES, ICP-AES

Lecture No	Topic
1	Atomic Absorption Spectroscopy (AAS): An Introduction to Optical Atomic Spectroscopy- atomization - Principles of AAS,
1	Instrumentation- Flame Atomization- Electro Thermal Atomization- Graphite Furnace Technique
3	Flame AAS and furnace AAS, resonance line sources, sensitivity and detection limits in AAS.
4	Interferences –chemical and spectral, evaluation methods in AAS
5	Applications of AAS in qualitative and quantitative analysis.
6	Atomic Emission Spectroscopy (AES): Principles of AES, Instrumentation
7	Evaluation methods, Application of AES in quantitative analysis - Raies Ultima or RU lines
8	Advantages & disadvantages of AES - Comparison Between Atomic Absorption and Emission Spectroscopy
9	Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES): Limitations of AES
10	Principles of plasma spectroscopy, plasma as an excitation source. Inductively coupled plasma source
11	ICP-AES – Instrumentation –sequential spectrometers- Simultaneous spectrometers
12	Qualitative information- Quantitative information- Application of ICP-AES, Comparison with AAS and AES
13	Flame Photometry: - Basic concept- structure of flame –Interferences - Principle, and Theory
14	Instrumentation and Applications of Flame Photometry
15	Comparison of AAS, AES, ICP-AES and Flame Photometry

Paper-IIIa **Prof. P. Saritha Reddy**

Lesson Plan: IC-19: Diffraction Methods	
Lesson No	**Topic**
1.	Introduction to Diffraction methods: X-ray diffraction, Electron and Neutron diffraction
2.	X-ray Diffraction: Generation of X-rays, X-ray tubes: Continuous andcharacteristic spectra, Choice of Radiation- Selection based on application, Filters and monochromators
3.	Crystal structure, Unit cells and types of unit cells(FCC, BCC, HCC) lattice points
4.	Identification of lattice planes, Weiss indices , Miller indices, Probles on identification of lattice planes.
5.	Constructive interference and destructive interference of waves, in phase and out of phase, diffraction by diffraction grating.
6.	Crystals and diffraction of X-rays, Bragg's law, Problems based on Bragg's law.
7.	X-Ray Diffraction techniques- Powder methods and Single crystal methods. Debye Scheerer method- Principle and apllications
8.	Guinier focussing method and Powder diffractometer methods-principle and interpretation of results
9,	Single crystal methods- Rotation method, Weissenberg method and Precession methods-methodology and applications
10.	Indexing the reflections and Systematic absences- The relation between intensities of diffracted X-rays and arrangement of atoms in a crystal
11.	Electron density studies by X-rays- Patterson maps and direct methods- study of Platinum Pthalocyanine Silyl thioacetate and Tetraalkylbiphosphate
12.	Advantages and limitations of X-ray diffraction studies
13.	Electron diffraction studies- Principles, Radial distribution curves-Interpretation of results for PBrF2S, PF3S, PF2HS
14.	Limitations of Electron diffraction -study of $HClO_4$, Silylmonothioacetate and Germylmonothioacetate and HgCl2molecules, Advantages.
15.	Neutron Diffraction: Principle, Application in Hydrogen bonding studies, combined use of X – ray and Neutron diffraction studies, Advantages and limitations.

Paper-IIIa **Dr. P Muralidhar Reddy**

Lesson Plan: IC-20: Advanced Mass spectrometry

Lecture No	Topic
1	Mass Spectrometry basic introduction- Block diagram of mass spectrometer- Types of ionization methods- Types of ions in mass spectrometer
2	Mass Analyzers: Quadruple Mass Analyzers-Principle of operation, Instrumentation and applications
3	Mass Analyzers: Ion traps, Time of flight (TOF) mass analyzers - Principle of operation, Instrumentation and applications
4	Mass Spectrometry / Mass Spectrometry: Tandem Mass Spectrometry, Instrumentation, Applications; LC-MS-MS and GC-MS-MS
5	Hyphenated Techniques: GC-MS: Basic principles of gas chromatography and mass spectrometry (GC-MS) -Integration of GC and MS
6	Instrumentation and Interfaces-Direct coupling interface, Open split interface
7	Application based on gas chromatography/mass spectrometry-Analysis of metabolite of drug Imipramine.
8	Principle of LC-MS- Basic principles of liquid chromatography and mass spectrometry, Integration of LC and MS
9	LC-MS- Instrumentation – Interfaces- Moving belt interface, particle beam interface, thermospray interface, Electrospray interface, atmospheric pressure chemical ionization interface.
10	ICP – MS - Principle of Inductively Coupled Plasma Mass Spectrometry Instrumentation, and Applications in environmental and biological analysis
11	Matrix-assisted laser desorption/ionization-Time of flight Mass spectrometry (MALDI-TOF-MS): Introduction
12	MALDI- TOF-MS - Principle, Matrix, Sample Preparation for MALDI-MS - Dried droplet Crystallization, Thin layer method, Sandwich Crystallization
13	MALDI- TOF-MS - Instrumentation
14	Applications of Matrix-assisted laser desorption/ionization-Time of flight Mass spectrometry in chemistry and biology
15	Provide additional reading materials and resources for students to explore topics in more depth. Online resources and videos for supplementary learning

PaperIVa:CH(IC)304T:AnalyticalTechniques-

II

Paper-IVa **Prof.P. Saritha Reddy**

Lesson Plan: IC-25 Thermal Methods

Lecture No.	Topic
1	Introduction to Thermal methods of Analysis: Overview of different thermal techniques - TGA, DTA, DSC, Combined thermal instruments and their importance in material science.
2.	Thermogravimetric Analysis (TGA): Principle of TGA, MethodologyThermogram with examples.
3.	Instrumentation –Thermobalance – Balance, sample holder, Furnace, Temperature control, Data acquisition system and Working function of eachcomponent.
4.	Applications of TGA - Analysis of polymers, pharmaceuticals, and inorganicmaterials, Thermal stability studies and Compositional analysis.
5.	Study of Oxalates, Nitrates, and Chromates by TGA - Thermal decomposition mechanisms. Determination of Carbon Black in Polythene
6.	Differential Thermal Analysis (DTA): Principle of DTA- Definition and working principle, Comparison with TGA , Instrumentation and Methodology
7.	Applications in the study of polymers, ceramics and metal industry, phasediagrams, determination of melting and boiling points. Differential thermogram of sulphur. TG and DTA of manganese phosphine monohydrate.
8.	Differential scanning calorimetry (DSC): Principle, instrumentation, power compensated DSC instruments and Heat flow DSC instruments
9.	Methodology, DSC experiment calibration and data analysis. Determinationof Glass transition temperature and heat capacities, crystallinity and its rate.
10.	Problems based on Thermal Techniques
11.	Thermometric titrations: Principle, apparatus, applications to acid base,precipitation, complexometric, redox and non-aqueous titrations.
12.	Combined thermal instruments: Introduction to TGA/MS Principle,instrumentation and applications
13.	TGA/FTIR: Principle, instrumentation and applications
14.	High resolution TGA: Instrumentation, applications and advantages
15.	Microthermal analysis: Principle, instrumentation and applications

Lesson Plan: IC-26: Surface Analysis Methods/ Microscopic analysis	
Lecture No	**Topic**
1	Introduction, types of surface measurements
2	Photon Probe Techniques: X-Ray Photoelectron spectroscopy, Principle
3	Instrumentation of XPS, applications.
4	Electron Probe Techniques: Scanning electron microscopy (SEM) – Principle, Instrumentation
5	Transmission Electron Microscopy (TEM) - Principle, Instrumentation, applications
6	Energy Dispersive X-ray Spectroscopy (EDX) - Principle, Instrumentation, applications
7	Electron Probe X-ray analysis (EPXMA) - Principle, Instrumentation, applications.
8	Auger electron spectroscopy (AES) - Principle, Instrumentation, applications
9	Introduction to ion probe techniques
10	Rutherford backscattering spectrometry (RBS) - Principle, Instrumentation, applications
11	Secondary ion mass spectrometry (SIMS) – Fundamental aspects of sputtering
12	Principle of SIMS, Instrumentation, applications
13	Introduction to Scanning probe microscopy Techniques: Scanning Tunneling Microscopy – Principle
14	STM Instrumentation and applications
15	Atomic Force Microscopy - Principle, Instrumentation, applications

Paper-IVa **Dr.P. Muralidhar Reddy**

Lesson Plan: IC-27: Advanced Separation Techniques	
Lecture No	**Topic**
1	Solid Phase Extraction (SPE)- Principle of SPE, Methodology, Applications
2	Solvent Extraction in Flow Injection Analysis- Principle and methodology- Applications in metal ion extraction using chelating agents (Dithizone, 8-hydroxyquinoline, cupferron)
3	Organic Reagents in Inorganic Analysis- Theoretical basis for the use of organic reagents, Extraction of metal ions using organic reagents (acetylacetone, thionyl trifluoroacetone, tri-n-octyl phosphine oxide)
4	Affinity Chromatography- Principle of affinity chromatography, Technique and instrumentation, Applications
5	Chiral Chromatography- Principle of chiral chromatography, Technique and instrumentation, Applications
6	Principles of Gel Filtration Chromatography-Basic principles, Instrumentation
7	Retention Behavior and Resolution-Factors affecting retention, Methods to improve resolution
8	Selection of Gel Type and Applications- Types of gels used, Applications in biological and polymer sciences
9	Ion Exclusion Chromatography- Principle and applications
10	Supercritical Fluid Chromatography (SFC)-Principles of SFC; Basic principles and theory
11	Instrumentation of SFC-Detailed analysis of instrumentation, Stationary and mobile phases used, Detectors used in SFC
12	Advantages and Applications of SFC-Benefits over other chromatographic techniques Applications in pharmaceuticals, environmental analysis, and food science
13	Principles of GC-FT-IR- Basic principles of Gas Chromatography coupled with Fourier Transform Infrared Spectroscopy
14	Instrumentation of GC-FT-IR- Detailed analysis of instrumentation, Integration of GC and FT-IR
15	Applications of GC-FT-IR- Applications in environmental analysis, forensic science, and material characterization

Paper-IVa **Dr.M. Kavitha**

Lesson Plan: IC-28: Optical Methods	
Lecture No	**Topic**
1	Introduction to Spectroscopy
2	Optical Rotatory dispersion principles, optical rotation, circular birefringence
3	Circular Dichroism Principle
4	CD, ORD Instrumentation
5	Cotton Effect
6	Octant Rule, Examples of substituted cyclohexanone
7	Experimental techniques CD
8	Use of CD in the conformational studies of metal complexes, DNA and DNA-metal complexes
9	Principles of fluorescence spectroscopy. Characteristic of fluorescence emission
10	Fluorescence life time, quantum yield
11	Fluorescence Quenching, Structures of various Fluorophores
12	Static and Dynamic Quenching, Comparison
13	Fluorescence polarization and polarization spectra of a fluorophore
14	Application of Fluorescence Quenching
15	ligand/drug/metal complex DNA binding studies by Fluorescence Quenching

Paper I **Prof. B. Sireesha**

Lesson Plan: IC-33: Multinuclear NMR	
Lecture No	**Topic**
1	Theory and principle of NMR, The magnetic properties of other nuclei, 13C-NMR-chemical shifts
2	^{13}C-NMR continuous wave NMR: NMR recorded in frequency domain, pulsed Fourier Transform NMR, Un-decoupled NMR, broad band coupled NMR. Ex: Ethyl Phenyl acetate etc
3	Broad band decoupled spectra, single frequency off resonance decoupled (SFORD) NMR, Selectively decoupled NMR spectrum: principles and applications
4	Factors effecting chemical shifts in ^{13}C-NMR spectroscopy-diamagnetic, paramagnetic and neighbour anisotropic terms
5	Factors-hybridization, electro-negativity of substituents, steric and vander-Waals effects electron deficiency – carbonium anions with suitable examples
6	Factors: mesomeric effect – Aniline, benzonitrile, intra-molecular anisotropic effects- cyclohexane and toluene, heavy atom effect, conjugation isotropic effect, hydrogen bonding, effect of pH, solvent shifts
7	Chemical and magnetic equivalence definitions, examples- $H_2P_2O_5$, ethane etc. virtual coupling in cis $[Pd(P(CH_3)_3)_3I_2]$, $[PdI_2(PMe_3)_2)]$
8	Spin dilute systems- satellites –Pt and Sn complexes low abundance active isotopes resulting in satellite peaks. NMR time scale and its uses
9	Stereochemical non-rigidity: application of NMR in identifying the fluxional behavior in molecules and complexes – with examples of PF_5, $[Rh(PR_3)_5]^{5+}$, $[Fe(Cp)_2(CO)_2]$, ΔR, the ring contribution to ^{31}P chemical shifts, taking examples of phosphorous chelates
10	Interpretation of ^{1}H-NMR spectral signals $[PtHCl(PEt_3)_2]$ and coupling constants, $[Pt(CH_3)_3(NH_3)_3]$ – facial and meridonial isomers, BH4− coupling with 10B and 11B, NH^{4+} coupling with ^{14}N and ^{15}N, CH_3CN
11	^{1}H-NMR –spectra of $[6h(C_7H_8Mo(CO)_3]$ and $[7h(C_7H_7Mo(CO)_3]$, B_2H_6 – coupling with ^{11}B and $^{29}SiH_3$-SiH_3 – satellite peaks
12	^{19}F-NMR spectrum of BF_4^-, (coupling with ^{11}B, ^{10}B. H_2PF_3, $J_{P-H} > J_{P-F}$ and $J_{P-F} > J_{P-H}$ spectra. ^{31}P-NMR spectrum of $Mo(CO)_3(PPh_3)_3$ – facial and meridonial isomers, $[Rh(PPh_3)_3Cl]$ Wilkinsons catalyst – J_{Pb-Rh}, J_{Pb-Pa} and J_{Pa-Rh}, J_{Pa-Pb} coupling
13	^{31}P-NMR spectra of trans $[PtCl_4(PEt_3)_3$-satellite Peak. $^{31}PF_2H(^{15}NH_2)_2$ when $J_{P-H} > J_{P-F}$ and $J_{P-F} > J_{P-H}$ cases-interpretation of 90 line spectrum
14	^{13}C-NMR spectrum of $[^4hC_8H_8Ru(CO)_3]$ delocalization of electron density due to 1,2 shift. ^{13}C-NMR spectrum of iron carbonyls –$Fe(CO)_5$, $Fe_2(CO)_4$ – bridging and terminal carbonyls, $Fe_3(CO)_{12}$
15	^{13}C-NMR spectrum of $FeICp(CO)_2$, $^{13}C^{15}NCo(DMG)_2$pyridine, ^{13}C and ^{1}H- NMR & ^{13}C-NMR spectrum of bonded phenyl ligand (C_6H_5)

Paper -I **Dr.M. Kavitha**

Lesson Plan: IC-34: Advanced NMR techniques	
Lecture No	**Topic**
1	Introduction to NMR Spectroscopy
2	Spin-Lattice (T1) and Spin-Spin Relaxation (T2)
3	Spin Echo Polarization Transfer
4	Spin Echo Measurements
5	Attached proton test (APT spectra) by Gated Spin Echo
6	Cross polarization
7	INEPT spectra, DEPT spectra
8	INADEQUATE spectra (Incredible Natural Abundance Double Quantum Transfer Experiment)
9	Two Dimensional NMR: Basic principles
10	Types of 2D NMR: J- resolved spectroscopy
11	a)homo and b) Heteronuclear J- resolved spectroscopy
12	Correlation spectroscopy ; Homo nuclear shift correlation spectroscopy (COSY)
13	Hetero nuclear shift correlation spectroscopy (HETCOR)
14	NOESY(Nuclear Overhauser Enhancement Spectroscopy), HOESY (two dimensional heteronuclear NOE)
15	Advantages of 2-D NMR

Lesson Plan: IC-35: Applications of ESR to Metal Complexes	
Lecture No.	**Topic**
1.	Introduction to Electron spin resonance spectroscopy, ESR active species, Principle of ESR
2.	Instrumentation- Source – Klystron, Isolator, Wave meter ,Attenuator Circulator or Magic T, Sample cavity, Magnet system, Crystal detectors.Auto amplifier or phase sensitive detectors and Oscilloscope and Pen recorder
3.	Preparation of sample, Types of instrument, Presentation of the spectrum
4.	Hyperfine interaction, Nuclear spin quantum number, Hyperfine splting, Selection rules
5.	Application of ESR to the study of simple free radicals – Methyl, hydroxy methyl, cyclopentadienyl, diphenylpicrylhydrazyl free radicals
6.	Super hyperfine splitting, Zero field spliiting and Kramer's degeneracy with examples
7.	Importance of g value, Factors affecting g values, Interpretation of g in cubic, axial and rhombohedral geometries.
8	Calculation of g values with simple examples. Intensities of '$g_{\parallel}$ and $g_{\perp}$peaks.
9.	Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis –Salicylaldimine, Cu(II)- diethyldithiophosphinate, Vanadyldithiophsphinate,
10.	Evidence for Metal-Ligand Bond Covalency- Copper(II) tetraphenylporphyrin , Co(II)- phthalocyanine and $K_2[IrCl_6]$.
11.	ESR spectra of $[(NH_3)_5 Co O_2 Co (NH_3)_5]^{5+}$ in determination of itsstructure.
12.	Effective Spin - Orbitally Non-degenerate and Degenerate States.ESR Spectra of d^1-d^9 Transition Metal Complexes with examples.
13.	ESR Spectra of d^1-d^9 Transition Metal Complexes with examples.
14.	Interpretation of 'g' and 'A' values from ESR spectral data in- i) MnF_6^{4-}, ii)CoF_6^{4-}, and CrF_6^{3-}.
15.	ESR spectra of dinuclear Cu(II) complexes.

Paper I **Prof. B. Sireesha**

Lesson Plan: IC-36 Mossbauer and Nuclear Quadrupole Resonance Spectroscopy	
Lecture No	**Topic**
1	Mossbauer Spectroscopy**:** Principle, theory, Mossbauer effect, recoil energy, Doppler effect, Sources
2	Instrumentation, working of the components, experimental considerations and presentation of the spectrum, Isomer Shifts –factors effecting isomer shift
3	Quadrupole splitting- number of quadrupole states, electric field gradient, reason for quadrupole splitting, Selection Rules, examples
4	Magnetic hyperfine splitting – paramagnetic, ferro and antiferromagnetic compounds, Selection Rules, iron six line spectra
5	Applications: Iron Compounds**:** Low-spin and High-spin Fe(II) and Fe(III) Complexes – $FeCl_3.6H_2O$, $FeSO_4.7H_2O$. FeF_2
6	Iron Compounds: interpretation of Mossbauer spectra of $FeCO_3$, FeF_3, $[Fe(CN)_6]^{3-}$, $[Fe(CN)_6]^{4-}$, $[Fe(CN)_5NO]^{2-}$
7	π-bonding Effects in Iron complexes - Study of High-spin Low-spin Cross-over with and example of $[Fe(o\text{-}phen)_2(SCN)_2]$ diamagnetic and covalent Compounds
8	Structural aspects of Iron Carbonyls $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$; Iron-Sulfur Proteins- Ferridoxin and Rubredoxin using Mossbauer spectra
9	Tin Compounds**:** Sn isotopes, Energy of γ radiations, Sn(II) and Sn(IV) compounds, isomer shift values of Tin halides and organo-tin compounds symmetric and asymetrically substituted Sn com
10	Iodine Compounds**:** Isomer Shifts of ^{127}I and ^{129}I – graphical representation, applications to alkali metal iodides, Mb spectrum of molecular Iodine, Mossbauer spectra of IF_6^- and IF_6^+
11	Nuclear Quadrupole Resonance Spectroscopy**:** Principle, nuclear quadrupole resonance, electric field gradient, quadrupole splitting, number of quadrupole energy levels
12	Energy of quadrupole levels, calculation of energies of quadrupole level and energies of transitions with I=1/2, 1, 3/2 and 5/2
13	Nuclear quadrupole resonance experiment, Instrumentation, Structural information from NQR spectra
14	Interpretation of NQR spectra of $PFCl_4$, PCl_4Ph, Ga_2Cl_7
15	Interpretation of NQR spectra $TeCl_4$ and interpretation of nuclear quadrupole coupling constants, Revision

Paper-II: CH(IC) 402T: Bioinorganic Chemistry

Paper II **Prof. B. Sireesha**

Lesson Plan: IC-37: Metal ions Interactions with Nucleic acids and their constituents	
Lecture No	**Topic**
1	Introduction, nucleic bases- purines and pyrimidines, ribose and deoxyribose sugars
2	Nucleosides, nucleotides, structure and bonding, nomenclature, structures, bonding-glycosidic bond and phosphor-ester bonds
3	Proton binding sites of nucleic acids and constituents in solution
4	Covalent structure of polynucleotides, secondary structure of DNA, hydrogen-bonding between A-T and G-C
5	Syn and anti-conformations of nucleotides, available binding sites in each of the confirmation in purines and pyramidines
6	Structural features of B, A and Z forms of DNA, helical structures, right and left handed nature, number of base pairs
7	Comparison of B, A and Z forms of DNA in structure and other features
8	Major grooves and minor grooves, Information from grooves, hydrogen bonding and base pairing
9	General factors influencing metal ion binding in solution-basicity of bases, nature of donor atoms and metal ions, stacking of bases
10	Factors: indirect Chelation, kinetic factors, pH, N(7) Vs N(1) of purines, hydrogen bonding
11	Stability of phosphate metal ion complexes in solution, metal ion binding in nucleotides, AMP, BMP, CMP, UMP and TMP, diphosphates and triphosphates
12	Nucleotide metal ion interactions-binding sites, structures
13	Intra-molecular equilibrium constant, K_I, equations, structures of macro-chelated form, concept of open and closed systems, calculation of percentage of closed isomers
14	Outer sphere and inner sphere isomers of M-ATP complexes, structure and linkages
15	Metal ion interactions with DNA and RNA, stability of nucleotide chain. Concept of T_M

Lesson Plan IC-38: Transport of Electrons and Metal ions	
Lecture No.	Topic
1.	Introduction to Bioinorganic chemistry: Importance of metal ions in biology. Significance and types of electron transferases.
2.	Iron-sulphur proteins. Introduction, [1Fe-0S]-rubridoxins - Structural and spectral aspects.
3.	[2Fe-2S] and [3Fe-4S] Iron sulphur proteins – Structural and spectral aspects.
4.	Structural and spectral aspects of [4Fe-4S] and High potential iron proteins
5.	[8Fe -8S] proteins - Structural and spectral aspects.
6.	Electron transport by Cytochromes – Types of cytochromes and study of their structural aspects.
7.	Study of mechanism of electron transport by cytochromes.
8.	Blue copper proteins- Structural aspects of Azurin and Plastocyanin and their role in electron transport.
9.	Structure and activity of Fe-S enzyme Acotinase
10.	Introduction to transport and storage of metal ions.
11	Iron transport by Transferrin –Study of structure and function of Transferrin.
12.	Iron storage by Ferritin- Structure and mechanism of action of Ferritin.
13.	Iron transport by Siderophores in Bacteria- structure and mechanism of action.
14.	Transport of Na^+ and K^+ across the cell membrane by Na^+-K^+-ATPase, Mechanism
15.	Transport of calcium across the sarcoplasmic reticulum by Ca^{2+}-ATPase.

Paper:II

Dr.M. Kavitha

Lesson Plan: IC-39: Metallo Enzymes of Iron, Zinc and Nickel	
Lecture No	**Topic**
1	Introduction to Protein Structure
2	Structural and Mechanistic Aspects of Cytochrome P450
3	Cytochrome oxidase, Reactions and catalytic cycle
4	Structural and mechanistic aspects of Catalases and Peroxidases
5	Role of Iron in metalloenzymes
6	Structural and Mechanistic Aspects of Carbonic Anhydrase
7	Structure of Carboxy peptidase and catalytic cycle
8	Structural and Mechanistic Aspects of Leucin – aminopeptidase
9	Structural and Mechanistic Aspects of Thermolysin
10	Structural and Mechanistic Aspects of Alcohol Dehydrogenase
11	Role of Zinc
12	Introduction of Nickel enzymes, Role of Nickel
13	Urease Structure and catalytic cycle
14	Structural and Mechanistic Aspects of Hydrogenase
15	Structural and Mechanistic Aspects of Factor F 430

Dr.P. Muralidhar Reddy

Paper: II

Lesson Plan: IC-40: Metallo-Enzymes of Cobalt, Copper, Molybdenum and Manganese	
Lecture No	**Topic**
1	Cobalt Enzymes - Cobalt in Vitamin B12 – Definitions of some terms- Anaemia- Megaloblastic Anaemia- Pernicious Anaemia- Gastric Atrophy- Causes of Vit-B12 deficiency- Dietary sources of Vit –B12
2	Recommended dietary allowances (RDA)- Absorption- Storage of Vit-B12- Industrial production of Vit – B12- Excess intake of Vit-B12-Symptoms of Vit-B12 deficiency- Function of Vit-B12.
3	Discovery of Vit-B12- Natural synthesis of Vit-B12- Research- Phase-I- Phase-II and Phase - III
4	Structural Features of Vitamin B12 with reference to coordination of Cobalt - Different Oxidation States of Cobalt-Different forms of Vit-B12
5	Various forms of Vitamin B12 and Active Enzyme forms – Isomers of Vit-B12- Properties of Vit – B12r and Vit-B12s
6	Types of Reactions Catalysed by i) Methyl Cobalamin ii) Deoxyadenosyl Cobalamin
7	Mechanism of the Methyl Malonyl CoA conversion to Succinyl CoA by Deoxyadenosyl Cobalamin
8	Methyl Cobalamin catalyzed reactions – Homocystine to Methionine- Acetate synthetase- Methane synthetase
9	Role of the Apoenzyme - Unique features of Cobalt to suit Vitamin B12.
10	Copper Enzymes-Types of Copper in Biological Systems. Structural and Mechanistic Aspects of Superoxide Dismutase
11	Structural and Mechanistic Aspects of Laccase and Galactose oxidase
12	Molybdenum Enzymes: Biological Roles and Mechanistic Aspects of Nitrogenase – Nitrogen cycle
13	Structural and Mechanistic Aspects of Xanthineoxidase and Sulfite oxidase.
14	Manganese Enzymes: Arginase- Structure and function
15	Manganese Enzymes: Water – oxidase - Structure and function

CH(IC)403T(ElectiveIIIa):Medicinal InorganicChemistry,Spectroscopic Analysis of Drug/Metal Complexes and Applications of Nanomaterials

Paper-IIIa **Prof G. Vijaya Charan**

Lesson Plan: IC-41: Metal complexes in Clinical Chemistry	
Lecture No	**Topic**
1	Theory and mode of action of therapeutic chelating agents with examples.
2	Single ligand Chelation Therapy introduction and examples.
3	Aminopolycarboxylic acids structure and bonding of APC, examples glycine, imino diacetic acid, EDTA, DTPA and TRIEN.
4	Desferrioxamine-structure and bonding and advantages.
5	Penicillamine-structure and bonding advantages and side effects.
6	Triethylenetetramine structure and bonding, advantages.
7	Mixed ligand chelation therapy -Combination therapy with 2 chelating agents' examples and advantages.
8	Metallothionines in detoxification-cysteine residues binding to metal ions through thiol groups and types of MTs, Structure and functions.
9	Importance of Role of metal ions in the action of antibiotics.
10	Bleomycin: structure, bonding and activity of BLM.
11	Adriamycin-Structure, bonding- binding to DNA and inhibiting replication and transcription.
12	Tetracyclines structure, bonding, mode of action and side effects.
13	Gold-Containing drugs used in therapy, mechanism of action, examples of gold compounds to treat Rheumatoid arthritis.
14	Copper-histidine - A therapeutic agent for Menkes disease -structure of 5 & 6 coordinated cu-histidine complex and mechanism of action.
15	Anti-viral chemotherapy-viral cycle, steps in viral cycle, chelating agents with antiviral activity, Importance of metal peptide interaction with DNA and cleavage examples of metal peptide complexes.

Paper-IIIa **Dr. P. Muralidhar Reddy**

Lesson Plan: IC-42: Metal complexes as Drugs and Anticancer agents	
Lecture No	**Topic**

1	Thermodynamic and Kinetic Principles- Basic concepts of thermodynamics and kinetics in Pt(II) chemistry, Cis and trans influences
2	Steric and Electronic Tuning of Reactivity- Factors affecting steric and electronic properties Examples of steric and electronic tuning in Pt(II) complexes
3	Thermodynamic and Kinetic Aspects- Stability and reactivity of Pt(II) complexes, Influence of ligands on thermodynamic and kinetic behavior
4	Discovery and Applications- Historical perspective on the discovery of platinum-based drugs, Clinical applications of platinum complexes
5	Structure-Effect Relationships- Correlation between structure and anticancer activity, Examples of structure-activity relationships in platinum drugs
6	Cisplatin (cis-Pt(NH3)2Cl2) Mode of Action- Mechanism of action of cisplatin, Interaction with nucleic acids and proteins
7	Potential Binding Sites- Binding sites on nucleic acids, bases, and proteins, Role of binding in drug activity
8	Drug Resistance Mechanisms- Mechanisms of resistance to platinum-based drugs, Strategies to overcome drug resistance
9	DNA Repair Mechanisms- Role of DNA repair in drug resistance, Mechanisms of DNA repair in the presence of platinum complexes
10	DNA Binding-Mechanism of DNA binding by metal complexes, Factors influencing binding affinity
11	DNA Structural Changes-Unwinding, shortening, and bending of the double helix, biological consequences of these changes
12	Organic Intercalators and Transition Metal Complexes as Donor-Acceptor Pairs-Mechanism of action, Examples and applications
13	Introduction to Non-Classical Platinum Agents, Definition and examples of non-classical platinum agents
14	Mechanisms of Action-Comparison with classical platinum agents, Unique mechanisms of non-classical agents
15	Clinical Applications and Future Directions- Current clinical applications, Research trends and future prospects

Paper: IIIa

Dr.M. Kavitha

Lesson Plan: IC-43: Spectroscopic analysis of drug/metal complexes binding to DNA

Lecture No	Topic
1	Introduction to DNA binding sites
2	Cooperativity and Anti-cooperativity in DNA- ligand binding
3	Excluded Site Model
4	UV-Vis Absorption Spectroscopy to study DNA-ligand interactions
5	Application of Fluorescence quenching in general and ligand/drug/metal complex DNA binding studies, Fluorescence titrations and binding constants
6	Salt back titrations interpretation of the data
7	Binding Analysis, Binding isotherms, Calculation of binding constant
8	Dependence of Kobs on salt concentration, cation effects on ligand nucleic acid equilibria, Competitive effects of monovalent and divalent cations for binding
9	Record's polyelectrolyte theory and its importance
10	Equilibrium dialysis. Partition analysis
11	competitive equilibrium dialysis to assess B & Z DNA binding. Competition dialysis to assess base and sequence specificity
12	viscosity studies
13	Tertiary structure of DNA
14	Various forms of DNA, Supercoiled DNA(Form-I), Nicked DNA (Form-II), and Linear DNA(Form-III)
15	DNA cleavage activity with ligand/metal complexes-Analysis by Gel electrophoresis

Paper: IIIa **Dr.M. Kavitha**

Lesson Plan: IC-44: Applications of Nanomaterials

Lecture No	Topic
1	Introduction to Nanotechnology
2	Applications of Nanotechnology in Electronics
3	Biological Applications
4	Consumer and domestic applications with examples
5	Energy related application: photo-volatile cells
6	Energy storage nanomaterials
7	Nano Sensors in Agriculture
8	Nano Sensors in food industry
9	Nano Sensors in health and medical field
10	Nano Sensors in military
11	Introduction to Applied Nanobiotechnology
12	nano biomedical science drug delivery
13	Nano materials in drug targeting
14	Nano materials in biosensors, bioimaging
15	neutron capture therapy

Paper-IV: CH(ID) 404T: Interdisciplinary Course (Environmental and Applied Analysis)

Lesson Plan: IC-49: Clinical and Pharmaceutical Analysis	
Lecture No	**Topic**
1	Analysis of Carbohydrates and their significances -Folin-Wu method -principle, procedure calculation and clinical significance.
2	Estimation of Glucose by O-Toluidine Method-Principle, procedure, calculation and clinical significance. Estimation of Glucose by Oxidase method Principle, procedure, calculation and clinical significance.
3	Analysis of lipids and their significances –Test for cholesterol-ZAK' S method - Principle, procedure, calculation and clinical significance. Test for cholesterol by Enzymatic method - Principle, procedure, calculation and clinical significance.
4	Analysis of proteins and their significance – Estimation of total protein in serum. Principle, procedure, calculation and clinical significance.
5	Analysis of Major metabolites and their significance – Determination of Blood urea and Creatinine in urine- Principle, procedure, calculation and clinical significance.
6	Analysis of ions and their significance: Estimation of Na, K, Ca, bicarbonates and phosphate in serum.
7	Analysis of Hormones and their significance-ELISA and RIA.
8	Determination of Diclofenac by non-aqueous titration Calcium in Vitamin D and Calcium formulations by Complexometric titrations.
9	Sulphanilamide by potentiometry.
10	Pethidine hydrochloride and Frusemide by UV-Vis spectroscopy.
11	Aspirin, paracetamol and codein in APC tablets by NMR.
12	Phenobarbitone in tablets by IR spectroscopy.
13	pivalic acid in dipivefrin eye drops by GC.
14	Assay of hydrocortisone cream. by HPLC method
15	Impurity profiling of Propranolol by GC-MS and famotidine by LC-MS.

Lecture No.	Topic
Lesson Plan: IC 50: Food and Agricultural Analysis	
1	Chemical additives, Division of color additives (Coal-tar dyes, vegetable colours and mineral colours).
2	Chemical preservatives and synthetic sweetening agents (organic-ether extractable and non-ether extractable) SO2, Sodium Benzoate,
3	Analysis of Sorbic acid and Benozoic acid.
4	Antioxidants: Types of Antioxidants used in foods, Analysis of Butylated hydroxy toluene (BHT), propyl – gallates (PG) TLC & GC.
5	Analysis of Octyl gallates (GO) and dodecyl gallates (DG) by TLC & GC.
6	Food adulteration: Common adulterants in food, contamination of food stuffs.
7	Microscopic examinations for food adulterants.
8	Importance of soil analysis in agriculture and environmental science. Overview of soil properties: pH, conductivity, cation exchange capacity (CEC) and total organic matter. Techniques and instruments used in soil analysis.
9	Principles of pH measurement of soil and its significance. Conductivity and its correlation with soil salinity.
10	Understanding Cation Exchange Capacity and its role in soil fertility. Methods for determining total organic matter.
11	Importance of nitrogen, phosphorous, potassium, sulfur, calcium, magnesium, and trace elements in soil. Analytical methods for these nutrients - Kjeldahl method for nitrogen, colorimetry for phosphorous.
12	Fertilizer Analysis :Moisture determination using Karl Fischer titration. Determination of ammonical nitrogen and ammoniacal nitrate nitrogen in fertilizers.
13	Fertilizer Analysis : Methods for determining total phosphates (P2O5) and potassium in fertilizers. Estimation of micronutrients (e.g., Zn, Cu, Fe, Mn) using Atomic Absorption Spectroscopy (AAS).
14	Pesticide Analysis : Overview of pesticide residues and their impact on food safety. Analysis of organo-chlorine pesticides, Cypermethrin) using Gas Chromatography (GC).
15	Pesticide Residue Analysis in Vegetables and Food Grains : Determination of Malathion, Methyl parathion, and DDT residues.Techniques for extracting and analyzing pesticide residues in food samples.

Lesson Plan: IC-51: Analysis of Air and Water Pollutants	
Lecture No	**Topic**
1	Introduction to Air Quality Standards- Overview of air quality standards (WHO, EPA, local standards), Importance and objectives of air quality analysis
2	Sampling and Analysis Techniques for Air Pollutants- Sampling methods for air pollutants Analysis techniques for SO2: UV-Vis, IR spectroscopy, Analysis techniques for H2S: Spectrophotometry, Non-dispersive IR spectrophotometry
3	Analysis Techniques for Other Pollutants- NO-NOx: Chemiluminescence technique, Colorimetric technique (Saltzman method), CO & CO2: IR spectroscopy, Atomic Absorption Spectroscopy (AAS), Gas Chromatography (GC)
4	Hydrocarbons Analysis-Analysis of hydrocarbons using GC and GC-MS, Aromatic hydrocarbons in automobile exhaust, petrol, and air
5	Analysis Techniques for Other Pollutants- O3: Chemiluminescence, Spectrophotometry, Particulate matter analysis: Sampling and measurement techniques
6	Objectives and Methods of Sampling and Preservation- Objectives of air pollutant analysis Sampling, preservation, and pre-concentration methods
7	Physical Analysis of Water Pollutants- Colour, odour, temperature, pH, Electrical Conductivity (EC), redox potential, Total Dissolved Solids (TDS): Turbidimetry
8	Chemical Analysis of Anions in Water- Analysis of CN-, Cl-, F-, NO2-, NO3-: Spectrophotometry, Analysis of SO4, PO4: Spectrophotometry
9	Objectives of Water Pollutant Analysis- Importance of water quality analysis, Objectives and significance
10	Biochemical Oxygen Demand (BOD)- Definition and significance, Methods of determination
11	Chemical Oxygen Demand (COD)-Definition and significance, Methods of determination
12	Total Organic Carbon (TOC) and Dissolved Oxygen (DO)- Definition and significance, Methods of determination
13	Introduction to Toxic Metals- Importance and impact on health and environment, Sources of toxic metals in water
14	Analysis Techniques for Toxic Metals- Atomic Absorption Spectroscopy (AAS), Spectrophotometry
15	Analysis of Specific Toxic Metals- Techniques for analyzing Hg, As, Pb, Cd, Be, Al, Cr Case studies and real-world applications

Paper-IVa **Dr. P. Muralidhar Reddy**

Lesson Plan: IC-52: Drinking Water and Sewage Water Treatment	
Lecture No	**Topic**
1	Hardness: causes, measurement of hardness, Degree of hardness, units- types of hardness – parts per million, milligrams per litre, Degree clark, Degree French-conversion of hardness
2	Estimation of temporary and permanent hardness, Alkalinity of water and its estimation.
3	Treatment of Water for Municipal Supply: Characteristics of potable water/Domestic water,
4	WHO standards and Indian Standards.
5	Water for Domestic use and Treatment of Water for Municipal Supply - Aeration, Sedimentation with coagulation, Filtration, Sterilization and Disinfection:
6	Physical Methods-Boiling, Exposure to Sunlight, Disinfection with UV light, Chemical Methods – Ozonization, Chlorination, Breakpoint chlorination and Dechlorination.
7	Desalination of Brackish Water: Treating saline water: distillation, electrodialysis, reverse osmosis (RO).
8	Mineral Water and Purified Water - Typical Manufacturing Process, Flow Sheet Diagram of Mineral Water Manufacturing Process,
9	Purified Water-Purification methods-Distillation, Double distillation, Deionization - Co-current deionization, Counter-current deionization, Mixed bed deionization
10	Demineralization, Uses of purified water- Laboratory use, Industrial uses and other uses; Health effects of drinking purified water
11	Sewage Water Treatment: Domestic sewage - Physical, Chemical, and Biological Characteristics of Domestic Sewage, Municipal sewage
12	Sewage Composition and Contaminants and Sewage Treatment -Types of contaminants in sewage-Impact on environment and healt
13	Sewage Treatment - On-Site Sewage Treatment Systems - Types of on-site systems Design and operation- Advantages and limitations
14	Off-Site Sewage Treatment Systems-Types of off-site systems, Design and operation, Advantages and limitations
15	Sewage Treatment Processes- Preliminary treatment, Primary treatment, Secondary treatment, Tertiary treatment, Case Studies and Real-World Applications- Examples of successful sewage treatment plants

M.Sc (ORGANIC CHEMISTRY)- FINAL YEAR

SEMESTER -III

PAPER-I : SYNTHETIC REAGENTS, ADVANCED NMR, CONFORMATIONAL ANALYSIS AND ORD

UNIT-I : SYNTHETIC REAGENTS-I

Lecture 1: Importance of protections, deprotections in synthesis and various types of deprotections.

Lecture 2: Protection of 1,2-diols by acetal, ketal and carbonate formation

Lecture 3: Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl,fmoc and triphenyl methyl groups

Lecture 4: Protection of carbonyls by acetal, ketal and thiol acetal (Umpolung)groups.

Lecture 5: Protection of carboxylic acids by ester and ortho ester (OBO) formation.

Lecture 6: Preparation and application of Organolithium and Organo copper reagents.

Lecture 7: Application of organoboranes in C-C bond formations

Lecture 8: Organosilicon reagents, Peterson's olefination and stabilization of α-carbanions and β-carbocations

Lecture 9: Utility of trimethyl silyl halides, cyanides and triflates

Lecture10:Organophosphorous reagents and wittig synthesis with stabilized, non-stabilised and semistabilised ylides

Lecture11: E-Stereoselectivity with Horner-Wordsworth-Emmons reaction and synthesis, application of Nysted reagent.

Lecture12:Application of Tebbe reagent and Petasis reagent

Lecture13: Importance of Rh based carbene complexes and the different stereochemical models.

Lecture14: Rh catalyzed cyclopropanations and its applications

Lecture15: Introduction to Rh catalysed C-H activation andits synthetic utility.

UNIT-II : SYNTHETIC REAGENTS-II

Lecture 1: Introduction to Cr(vi) oxidations and applications of Jones reagent, PCC, PDC.

Lecture 2: Hypervalent iodine based oxidations using IBX.

Lecture 3 :Hypervalent iodine based oxidations using DMP

Lecture 4: Oxidations with TEMPO, TPAP and the selectivities.

Lecture 5: DMSO based oxidations (Swern oxidation) and application of CAN.

Lecture 6: Oxidative cleavage of 1,2-diols with HIO_4 and $Pb(OAc)_4$.

Lecture 7: Oxidations with DDQ and SeO2

Lecture 8: Heterogenous catalytic hydrogenation and functional group selectivities.

Lecture 9: Homogenous catalytic hydrogenation, its functional group selectivities and decarbonylations.

Lecture10: Applications of diimide reductions

Lecture11: Development and applications of Birch reductions

Lecture12: Reductions with LiAlH4 and its modified versions.

Lecture13: Reductions with NaBH4 and its modified versions.

Lecture14: Reductions with electrophilic metal hydridesBH3, AlH3, DIBAL

Lecture15: Reductive cleavages with Tri ^{n} butyul tin hydride.

UNIT-III : ^{13}CNMR AND 2D-NMR SPECTROSCOPY

Lecture-1	**^{13}CNMRspectroscopy** Introduction.
Lecture-2	Types of ^{13}C nmr spectra:undecoupled,proton-decoupled and off-resonance decoupled (ORD) spectra.
Lecture-3	^{13}C chemical shifts, factors affecting the chemical shifts.
Lecture-4	chemical shifts of organic compounds. Calculation of chemical shifts of alkanes,
Lecture-5	Calculation of chemical shifts of alkenes and alkynes.
Lecture-6	Homonuclear (^{13}C,^{13}CJ)andheteronuclear(^{13}C,^{1}HJand ^{13}C, ^{2}H J) coupling.
Lecture-7	Applications of ^{13}C-NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules.
Lecture-8	^{13}C- NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.
Lecture-9	Introduction of **2D-NMR spectroscopy**.
Lecture-10	Principles of 2D NMR, Classification of 2D-experiments.
Lecture-11	Correlation spectroscopy (COSY) HOMOCOSY (^{1}H-^{1}H COSY)
Lecture-12	TOCSY (Total Correlation Spectroscopy), HeteroCOSY (^{1}H,^{13}C COSY,HMQC)
Lecture-13	long range ^{1}H,^{13}C COSY (HMBC)
Lecture-14	Homonuclear and Heteronuclear 2D-J-resolved spectroscopy.
Lecture-15	NOESY and 2D- INADEQUATE experiments and their applications.

UNIT-IV: CONFORMATIONAL ANALYSIS

Lecture 1: Introduction to Conformational Analysis Cyclic Systems:
Lecture 2: Conformations of Cyclohexane Chair Boat and Twist-BoatEnergy Diagram:
Lecture 3: Mono-substituted Cyclohexanes Substitution Effects: Axial vs. Equatorial: Steric Strain:.
Lecture 4: Di-substituted Cyclohexanes Isomerism: Steric Effects Electronic Effects:
Lecture 5: Tri-substituted Cyclohexanes 1,3,5-Trimethyl CyclohexaneMenthols
Lecture 6: Conformations of Cyclohexanone Alkyl Ketone Effects Halocyclohexanones:
Lecture 7: Conformations of Cycloheptane Conformational Analysis Comparison:
Lecture 8: Stereochemistry of Bicyclo[3.3.0]octanes, Hydrindanes, and Decalins
Lecture 9: Conformational Structures of Perhydroanthracenes
Lecture 10: Conformational Structures of Piperidine and N-Methylpiperidine
Lecture 11: Conformational Structures of Tropane, Tropine, and Pseudotropine
Lecture 12: Conformational Structures of Decahydroquinoline and Quinolizidine
Lecture 13: Factors Governing Reactivity of Axial and Equatorial Substituents in Cyclohexanes
Lecture 14: Stereochemistry of Addition to the Carbonyl Group of a Rigid Cyclohexan one Ring
Lecture 15: Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) Spectroscopy

PAPER-II : MODERN ORGANIC SYNTHESIS

UNIT-I: ASYMMETRIC SYNTHESIS

Lecture 1: Introduction to Asymmetric Synthesis
Lecture 2: Prostereoisomerism - Topicity in Molecules
Lecture 3: Prochiral Nomenclature.
Lecture 4: Conditions for Stereoselectivity Symmetry Criteria: Transition State Theory:..
Lecture 5: Analytical Methods -Enantiomeric Excess:
Lecture 6: Analytical Methods - Chiral NMR: Derivatizing Agents: Solvents and Reagents:
Lecture 7: Analytical Methods -Chiral HPLC, Diastereomeric Ratio
Lecture 8: Chiral Substrate Controlled Asymmetric Synthesis Cram's Rule and Felkin- Anh Model:
Lecture 9: Chiral Auxiliary Controlled Asymmetric Synthesis ,Chiral Enolates: Evan's Oxazolidinone:.
Lecture 10: Chiral Auxiliary Controlled Asymmetric Synthesis Prelog's Rule
Lecture 11: Chiral Reagent Controlled Asymmetric Synthesis BINAL-HReduction Mechanisms
Lecture 12: Chiral Reagent Controlled Asymmetric Synthesis - IPC2 BH and IPCBH2:
Lecture 13: Chiral Catalyst Controlled Asymmetric Synthesis - Sharpless Epoxidation:
Lecture 14: Chiral Catalyst Controlled Asymmetric Synthesis Wilkinson Catalyst Hydrogenation Mechanisms:
Lecture 15: Asymmetric Aldol Reaction Aldol Reaction Zimmerman-Traxler Model

UNIT-II : SYNTHETIC STRATEGIES.

Lecture-1: Introduction: Terminology, Target, synthon, synthetic equivalent, functional group inter conversion, (FGI), functional group addition.
Lecture-2: Criteria for selection of target. Linear and convergent synthesis.
Lecture-3: Retrosynthetic analysis and synthesis involving chemo selectivity, region selectivity, reversal of polarity and cyclizations.
Lecture-4: Order of events: S-Salbutamol, Propoxycaine.
Lecture-5: One group C-C and C-X disconnections: Introduction .One group C-C disconnections inalcohols and carbonyl compounds.
Lecture-6: One group C-X disconnections in Carbonyl compounds,alcohols, ethers and Sulphides.
Lecture-7: One group C-X disconnections in Carbonyl compounds,alcohols, ethers and sulphides.
Lecture-8: Two group C-C and C-X disconnections: Introduction
Lecture-9: Introduction .Two group C-X disconnections in 1, 1-difunctionalised.
Lecture-10: 1,2-difunctionalised and 1,3-difunctionalised compounds.
Lecture-11: Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5- difunctionalised compounds.
Lecture-12: Michael addition and Robinson annulation. Control in carbonyl condensations: oxanamide and mevalonic acid.
Lecture-13: Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection.

Lecture-14: disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials.
Lecture-15: Retrosynthesis of Retronecene, longifoline.

UNIT-III : NEW SYNTHETIC REACTIONS.

Lecture 1: Pd catalyzed C-C couplings using Suzuki, Heck reaction and its applications
Lecture 2: Pd catalyzed C-C couplings using Sonogashira reaction and its applications
Lecture 3: Stille and Buchwald-Hartwig cross coupling reactions
Lecture 4: Ni and Pd catalysed Negishi-kumada cross couplings.
Lecture 5: C=C bond Formation with Shapiro and Bamford-Stevens reactions.
Lecture 6: C=C bond Formation with McMurray and Julia Lythgoe olefination reactions
Lecture 7: Peterson's olefination with stereoselectivities.
Lecture 8: Three and four component reactions such as Biginelli, Ugi, Passerini, Bergamann and Mannich reactions.
Lecture 9: Ring formation reactions with Pauson-Khand and Nazerov cyclisation.
Lecture10: 1,3-Dipolar additions and synthetic advantages of Click reaction.
Lecture11: Concept of Metathesis and olefin cross metathesis.
Lecture12:.Development of 1^{st}, 2^{nd}, 3^{rd} gen Grubbs catalysts and synthetic applications
Lecture13: Development of Hoveyda-Grubbs catalysts and synthetic applications
Lecture14: Synthetic applications of Baylis-Hilman reactionand Mitsunobu reactions.
Lecture15: Synthetic applications of Eschenmoser-Tanabe fragmentation, Stork-enamine reaction and Michael reactions.

UNIT IV: NEW TECHNIQUES AND CONCEPTS IN ORGANIC SYNTHESIS

Lecture 1.	Brief review of concept of organic synthesis and new techniques
Lecture 2.	Techniques in peptide synthesis: Solid phase peptide synthesis
Lecture 3.	Techniques in peptide synthesis: Commonly used resins and structures of Rink resin, Wang resin and Ellman resin
Lecture 4.	Synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis
Lecture 5.	Solid phase oligodeoxynucleotide synthesis: Phospho triester and phosphite triester
Lecture 6.	Solid phase oligodeoxynucleotide synthesis: phosphoramidite pathway
Lecture 7.	Oligosaccharide synthesis: Glycosidation: Cylicoxocarbeniumion, glycosyl donors and glycosyl acceptors, Kahneglycosidation
Lecture 8.	Oligosaccharide synthesis: Convergent and linear oligosaccharide synthesis
Lecture 9.	Phase Transfer catalysis: Onium and crwon ethers as PTC
Lecture 10.	Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction.
Lecture 11.	Polymerization cyclisation and Elctrocylic-Diels Alder reaction
Lecture 12.	Baldwin Rules:Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavouredcyclisations

Lecture 13.	Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors
Lecture 14.	Baldwin Rules:Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavouredcyclisations
Lecture 15.	Determination of absolute configuration: Mosher's method

PAPER-III A :BIOORGANIC CHEMISTRY

UNIT – I : CARBOHYDRATES

Lecture-1. Introduction to the importance of Carbohydrates.
Lecture-2. Types of naturally occuring sugars, Deoxy sugars, aminosugars,
Lecture-3. Branched chain sugars mrthyl ethers and acid derivatives of sugars.
Lecture-4. Determination of configuration and determination of ring size of D-glucose
Lecture-5. Determination of configuration and determination of ring size of D-Fructose.
Lecture-6. Conformational analysis of monosaccharides. 4C1 and 1C4 conformations of D-glucose.
Lecture-7. Reactions of six carbon sugars: Ferrier, Hanesian reaction and Ferrier rearrangement.
Lecture-8. Synthesis of amino, halo and thio sugars.
Lecture-9. Structure, ring size determination of sucrose and Maltose
Lecture-10. Conformational structures of sucrose, lactose, maltose.
Lecture-11. Conformational structures of cellobiose and gentobiose.
Lecture-12. Structure and biological functions of starch. cellulose,
Lecture-13. Structure and biological functions of glycogen and chitin.
Lecture-14. Role of sugars in cell to cell recognition
Lecture-15. Determination of blood groups.

UNIT II : NUCLEIC ACIDS AND LIPIDS

Lecture 1.	Brief explanation of Nucleic acids
Lecture 2.	Explained structures of Nucleotides, Nucleosides, Nucleotide bases and Sugars
Lecture 3.	Synthesis of nucleosides
Lecture 4.	Synthesis of nucleotides
Lecture 5.	Explanation Primary and Secondary structure of DNA
Lecture 6.	Explanation of Tertiary structure of DNA
Lecture 7.	Briefly explanation Types of mRNA, tRNA and rRNA
Lecture 8.	Briefly explained of Replication, transcription and translation.synthesis.
Lecture 9.	Discuss about the Genetic code and DNA finger printing
Lecture 10.	Explanation of Introduction and classification of lipids
Lecture 11.	Stereochemical notation in lipids.
Lecture 12.	Chemical synthesis and biosynthesis of phospholipids
Lecture 13.	Chemical synthesis and biosynthesis of glycolipids
Lecture 14.	Properties of lipid aggregates, micelles and bilayers
Lecture 15.	Properties of liposomes and biological membranes

UNIT-III : PROTEINS AND ENZYMES

Lecture-1: Introduction. Peptide bond,
Lecture-2: Classification and nomenclatue of peptides.
Lecture-3: Amino acid sequence of polypeptides and proteins
Lecture-4: Terminal residue analysis and partial hydrolysis
Lecture-5: Peptide synthesis by solution phase
Lecture-6: Solid phase synthesis methods.
Lecture-7: Proteins - Biologicalimportance
Lecture-8: Classification - Primary, secondary and tertiary structure of proteins.
Lecture-9: Enzymes: Definition. Classification based on mode of action.
Lecture-10: Mechanism of enzyme catalysis
Lecture-11: Lock and Key, Induced- Fit Three point contact models.
Lecture-12: Enzyme selectivity –chemo, regio, diastereo and enantio selectivity – illustration with suitable examples.
Lecture-13: Factors affecting enzyme catalysis. Enzyme inhibition- reversible and irreversible inhibition.
Lecture-14: Enzymes inorganic synthesis.
Lecture-15:Immobilised enzymes.

UNIT-IV: COENZYMES AND VITAMINS

Lecture-1. Introduction. Co-factors -cosubstrates -prosthetic groups.
Lecture-2. Classification — Vitamin derived coenzymes and metabolite coenzymes
Lecture-3. Structure and biological functionsof coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP)
Lecture-4. oxidized and reduced forms of I) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH)
Lecture-5.Ooxidized and reduced forms of Flavin adenine nucleotide FAD, FADH2
Lecture-6. Ooxidized and reduced forms Flavin mononucleotide (FMN, FMNH2)
Lecture-7. Ooxidized and reduced forms lipoic acid, biotin, tetrahydrofolate and ubiquinone.
Lecture-8. Adenosine triphosphate (ATP)and adenosine diphosphate (ADP),
Lecture-9. S-adenosyl methionine (SAM) and uridine diphosphosugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes.
Lecture-10. Vitamins: Introduction, classification and biological importance of vitamins.
Lecture-11. Structure determination and synthesis of vitamins A,
Lecture-12. Structure determination and synthesis of vitamins A, B1, and B2.
Lecture-13. Synthesis of vitamins - B6, C,
Lecture-14. Synthesis of vitamins - E .
Lecture-15. Synthesis of vitamins - K.Structure of vitamin B12.

PAPER-III B: FORENSIC CHEMISTRY&TOXICOLOGY

UNIT-I : FORENSIC CHEMISTRY-I

Lecture-1	Introduction - Types of cases / exhibits
Lecture-2	Forensic Chemistry - - Preliminary screening -
Lecture-3	presumptivetests(colourandspottests)-
Lecture-4	Examinationsproceduresinvolvingstandard methodsand instrumental techniques.
Lecture-5	Qualitative and quantitative forensic analysis of inorganic
Lecture-6	and organic material
Lecture-7	Chemical fertilizers (N,P,K)
Lecture-8	Insecticides (Endosulfan, Malathion, Carbaryl)
Lecture-9	Metallurgical analysis(Fe, Cu, Zn, Au, Ag)
Lecture-10	Natural products (tobacco, tea, sugars, rubber)
Lecture-11	Industrial chemicals - Sulphuric, Nitric and Hydrochloric acids,
Lecture-12	Sodium, Potassium hydroxide, Ammonium nitrate, Potassium chlorate.
Lecture-13	Organic solvents like Methanol, Ethanol, Acetone, Chloroform and Ether
Lecture-14	Organic chemicals like Acetanilide, P- Aminophenol,
Lecture-15	and Nitrobenzene etc. with reference to forensic work.

UNIT-II : :FORENSICCHEMISTRY-II

Lecture-1	Introduction
Lecture-2	Examination of petroleum products
Lecture-3	Distillation and fractionation
Lecture-4	various fractions and theircommercial uses
Lecture-5	Standard method of analysis of petroleum products
Lecture-6	Analysis of petroleumproducts for adulteration
Lecture-7	and arson residues. Chemistry of fire
Lecture-8	Investigation and evaluation of fires
Lecture-9	Causes of fire
Lecture-10	Analysis of arsonresidues by conventional andinstrumental methods
Lecture-11	Analysis of trace evidence
Lecture-12	Cosmetics, Dyes, Trap related evidence materials
Lecture-13	Paints, Pigments,Fibres
Lecture-14	Oils fats, Greases, Industrial dusts
Lecture-15	Chemicals and Plant materials.

UNIT -III :FORENSICTOXICOLOGY-I

Lecture-1	Toxicology- Introduction
Lecture-2	History- Scope
Lecture-3	Areas of Toxicology
Lecture-4	Role of forensic toxicologist
Lecture-5	Poisons- Classification of poisons
Lecture-6	Types of poisoning
Lecture-7	Sample collection and preservation oftoxicological
Lecture-8	exhibits in fatal and survival cases
Lecture-9	Storage of samples
Lecture-10	Signs and symptoms ofpoisoning
Lecture-11	Toxicological investigation
Lecture-12	examination of poisoneddeath
Lecture-13	Interpretationoftoxicologicaldata
Lecture-14	Courtroom testimonyin toxicological cases
Lecture-15	Case Histories.

UNIT -IV :FORENSICTOXICOLOGY-II

Lecture-1	PrinciplesofToxicology-Introduction
Lecture-2	Pharmacokinetics
Lecture-3	Methodsoftransportation oftoxicant
Lecture-4	Absorption- Distribution-Storageoftoxicants
Lecture-5	Redistribution-Metabolism
Lecture-6	Oxidation–Reduction
Lecture-7	Hydrolysis–Conjugation
Lecture-8	Excretion-Otherroutesofelimination
Lecture-9	Toxicokinetics
Lecture-10	one and two compartmental model
Lecture-11	Toxicodynamics- Spectrum of undesired(toxic) effects
Lecture-12	Interaction of chemicals- Tolerance
Lecture-13	Dose response relationship
Lecture-14	Developmentaland reproductivetoxicity
Lecture-15	Mutagenicity- Toxicity testing.

PAPER-IV A : GREEN CHEMISTRY AND ORGANIC MATERIALS

UNIT-I : PRINCIPLES OF GREEN CHEMISTRY

Lecture-1: Green chemistry: Introduction.
Lecture-2: Principles of Green Chemistry:.
Lecture-3: Designing a Green Synthesis using these principles.
Lecture-4: Prevention of Waste/by-products
Lecture-5 : Maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy)
Lecture-6: Maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy)
Lecture-7: Prevention/minimization of hazardous/toxic products.
Lecture-8: Designing safer chemicals.
Lecture-9: Selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis.
Lecture-10: Energy requirements forreactions - use of microwaves, ultrasonic energy in organic synthesis;
Lecture-11: Prevention of unnecessary derivatization – careful use of protecting groups
Lecture-12: Use of catalytic reagents in preference to stoichiometric reagents;
Lecture-13: Designing of biodegradable products
Lecture-14: Prevention of chemical accidents.
Lecture-15: Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

UNIT II: GREEN SYNTHESIS

Lecture 1.	Brief explanation of Green chemistry
Lecture 2.	Microwave Assisted Organic Synthesis: introduction, benefits and limitations
Lecture 3.	Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction.
Lecture 4.	Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters
Lecture 5.	Microwave assisted Solvent-free reactions: Alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes
Lecture 6.	Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound
Lecture 7.	Ultrasound Assisted Organic Synthesis: Cannizaro reaction, Reformatsky reaction and Strecker synthesis
Lecture 8.	Organic Synthesis in Green Solvents: introduction and applications

Lecture 9.	Organic Synthesis in Green Solvents: Aqueous Phase Reactions: Diels-Alder Reaction and Heck reaction
Lecture 10.	Organic Synthesis in Green Solvents: Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and diydroxylationreactions.
Lecture 11.	Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement
Lecture 12.	Organic Synthesis using Ionic liquids: Suzuki Cross-Coupling Reaction and Diels- Alder reaction
Lecture 13.	Green Catalysts in organic synthesis: introduction and applications
Lecture 14.	Phase Transfer Catalysts in Organic Synthesis: Williamson ether synthesis and Wittig reaction
Lecture 15.	Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions

UNIT III : ORGANIC NANOMATERIALS

Lecture-1	Introduction of Organic Nanaomaterials
Lecture-2	The‘top-down’approach, the ‘bottom- up’approach and Nanomanipulation.
Lecture-3	Molecular Devices: Photochemical devices, Liquid crystals.
Lecture-4	Molecular wires, Rectifiers.
Lecture-5	Molecular switches and Molecular Muscles.
Lecture-6	NewCarbon family:TypesofFullerenes.
Lecture-7	TypesofCarbonnanotubes(Zig-Zag, Armchair and Chiral), Graphenes.
Lecture-8	Growth, Chemical Synthesis and optoelectronic properties of Fullerenes.
Lecture-9	CNTs (Zig Zag, Armchair and Chiral)
Lecture-10	singlewalled CNTs (SWCNTs) and multi walled (MWCNTs)and Graphenes.
Lecture-11	Structures of aromatics belts, nano car and molecularmachines.
Lecture-12	Optoelectronicmolecules:OLEDs.
Lecture-13	OrganicSolarCells(BasicOLEDmechanismand structures)
Lecture-14	NaturalBenzheterazoles
Lecture-15	syntheticmodificationsasoptoelectronicmolecules.

UNIT IV : SUPRAMOLECULAR CHEMISTRY

Lecture-1: Introduction: supramolecular chemistry.
Lecture-2: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions),Ionophore and molecular receptors.
Lecture-3: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation-π, anion-π, π-π and Van der Walls interactions),Ionophore and molecular receptors.
Lecture-4: Host-Guest Chemistry.
Lecture-5 Lock and key anology
Lecture-6: Structures and applications of Cryptands,Spherands,
Lecture-7: Structures and applications of Cryptands,Spherands,.
Lecture-8: Self-assembly: Ladder
Lecture-9: Cyclophanes, Carcerands and hemicarcirands.
Lecture-10: Polygons, helices, rotaxanes
Lecture-11: Catanenes, Molecular necklace, dendrimers
Lecture-12: Self-assembly capsules their synthesis, properties and applications.
Lecture-13; Enantioselective molecular recognition.
Lecture-14: Cyclodextrins, Crown ethers with chiral frame work, Chiral receptor from Kemp's triacid.
Lecture-15: Chiral receptors for tartaric acid.

PAPER-IVB : PESTICIDES

UNIT I: INTRODUCTION TO PESTICIDES

Lecture 1.	Brief review of Definition ,Classification and importance of pesticides
Lecture 2.	Pest control: Different methods –chemical – insecticides, fungicides,
Lecture 3.	Pest control: Different methods –chemical – herbicides, rodenticides, fumigants
Lecture 4.	chitin synthesis inhibitors and insect repellents
Lecture 5.	Biological–pheremones: Definition and classification
Lecture 6.	Synthesis of Disparlure, Exobrevicomin
Lecture 7.	Synthesis of Endobrevicomin, frontalin and grandiso pheromones, synthetic sex attractants
Lecture 8.	Insect juvenile hormones: JH-A, JH-B,Synthesis of juvabione
Lecture 9.	Structural formula and importance of methopren
Lecture 10.	Moultingharmones-structural formulae and mode of action of ecdysones
Lecture 11.	Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agricultiure
Lecture 12.	Structural formula and importance of Blasticidin-S, Kasugamycin
Lecture 13.	Avermectin-B, Invermectin, piercidins and phytoalexins
Lecture 14.	Environmental pollution from pesticides.iv) Integrated pest management.

Lecture 15.	Pesticide formulations: Dusts, Granules, Wettable powders, Emmulsions and Aerosols.

UNIT II: SYNTHETIC INSECTICIDES .

Lecture 1.	Organochlorine insecticides-synthesis and mode of action of methoxychlor
Lecture 2.	Synthesis and mode of action of perthan
Lecture 3.	Synthesis and mode of action of Dicofol and Heptachlor
Lecture 4.	Synthesis and mode of action of Dieldrin and Endosulfan
Lecture 5.	Organophosphorous insecticides–synthesis and mode action of Phosphoric acid derivatives
Lecture 6.	Synthesis and mode action of phosdrin and Dichlorophos,
Lecture 7.	Synthesis and mode action of parathion
Lecture 8.	Synthesis and mode action of Zolone, Aninphomethyl,
Lecture 9.	Synthesis and mode action of TEPP and Sachradan.
Lecture 10.	Carbamate insecticides- synthesis and mode of action of carbamyl
Lecture 11.	Synthesis and mode action of Furadan and Baygon
Lecture 12.	Synthesis and mode action of Aldicarb and Zectron
Lecture 13.	Formulation and residue analysis of organochlorine
Lecture 14.	Formulation and residue analysis of organophophorous
Lecture 15.	Formulation and residue analysis of carbamate insecticides

UNIT III : NATURAL INSECTICIDES AND HERBICIDES

Lecture 1.	Insecticides of palnt origin–synthesis and importance of pyrethrins (I and II), Rotenone and Nicotine
Lecture 2.	Main constituents Neem-structural formula of Azadirachtin
Lecture 3.	Synthesis of polygodial and warbunganol(Antifeedants)
Lecture 4.	Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin, Cypermethrin,
Lecture 5.	Synthesis of Fenvalerate, Decemethrin and pyrithrelone
Lecture 6.	Concept of Bioinsecticides– Bacillus thiuringiensis.
Lecture 7.	Concept of pro-insecticides-structure and mode of action of pro-pheremones and pre-pro-insecticides
Lecture 8.	Herbicides– synthesis,applications and mode of action of Aryloxyalkyl carboxylic acid derivative:2,4-D, MCPA,
Lecture 9.	synthesis,applications and mode of action of 2,4,5-T and 2,4,5-TP
Lecture 10.	Synthesis and mode action of Carbamates propham and chloropham
Lecture 11.	Synthesis and mode action of Urea derivatives –Monouron and diuron
Lecture 12.	Synthesis and mode action of Aliphatic acids Dalapon,TCA
Lecture 13.	Synthesis and mode action of Aromatic acids -2,3,6-TBA,Dicomba and Amiben
Lecture 14.	Nitrogen heterocyclic dericvatives –Simazine,Atrazine, Amitrole,Maleic hydrazide Diquat and paraquat,
Lecture 15.	Nitrogen heterocyclic dericvatives Phenols PCP and Dinoseb and Benzonitrile compounds

UNIT IV: FUNGICIDES AND RODENTICIDES

Lecture 1.	Fungicides–classification
Lecture 2.	Synthesis application and mode of action of Carbamates
Lecture 3.	Synthesis application and mode of action of Quinones-chloranil,
Lecture 4.	Synthesis application and mode of action of Dichlone and Benquinox
Lecture 5.	Synthesis application and mode of action of perchloromethylmercaptan derivative –captan and folpet
Lecture 6.	Synthesis application and mode of action of perchloromethylmercaptan derivative – Difolatan and Mesulfan
Lecture 7.	Synthesis application and mode of action of Benzimidazoles-carbendazim, Benomyl and Thiabandazole
Lecture 8.	Rodenticides, Anticoagulents-synthesis and application of warfarin, Coumachlor
Lecture 9.	synthesis and application of Vacor and Coumatetrallyl,
Lecture 10.	Synthesis and application of Dicoumarol and Bromodiolen
Lecture 11.	Acute poisons application of pindone and Ratindan
Lecture 12.	Acute poisons application of Sodium Fluoroacetate
Lecture 13.	Acute poisons application of Barium fluoroacetate
Lecture 14.	Acute poisons application of Antu and Tetramine
Lecture 15.	Acute poisons application of pindone and castrix

(LABORATORY) PAPER V : SYNTHESIS OF ORGANIC MOLECULES,

ISOLATION OF NATURAL PRODUCTS & TLC.

Lecture 1: Synthesis of 2-Phenyl indole (Fischer indole synthesis).
Lecture 2: Synthesis of 7-hydroxy-3-methyl flavone (Baker- Venkatraman reaction).
Lecture 3: Synthesis of 2,5-Dihydroxy acetophenone (Fries reaction).
Lecture 4: Synthesis of 4- Chlorotoluene from p-toluidine (Sandmeyer reaction).
Lecture 5: Synthesis of Benzilic acid from benzoin (Benzillic acid rearrangement).
Lecture 6: Synthesis of Benzpinacol (photochemical reaction) and Photo-dimerization of maleic anhydride
Lecture 7: Synthesis of 7-hydroxy coumarin (Pechman synthesis).
Lecture 8: Synthesis of Benzanilide (Beckmann rearrangement).
Lecture 9: Synthesis of Vanillyl alcohol from vanillin ($NaBH_4$ reduction).
Lecture10: Nitration of Phenol and separation of 2- and 4-nitrophenols by steam distillation.
Lecture11: Isolation of Caffeine from tea leaves (solvent extraction).
Lecture12: Isolation of Piperine from pepper (Soxhlet extraction).
Lecture13: Extraction of Eucalyptus oil from leaves (steam distillation).
Lecture14: Extraction of Lycopene from tomatoes.
Lecture15:TLC theoretical aspects and monitoring the progress, identification of number of comounds in a mixture.

(LABORATORY) PAPER VI: SEPARATION AND IDENTIFICATION OF ORGANIC COMPOUNDS & COLUMN CHROMATOGRAPHY

Lecture-1. Introduction of Separation of two component mixtures by chemical methods and their identification by chemical reactions
Lecture-2. Separation by using solvent ether, 5 % aq. $NaHCO_3$, 5%aq. NaOH, dil. HCl and checking the purity of the two components by TLC,
Lecture-3. Identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur).
Lecture-4. Separation and Identification of Benzoic acid and Benzaldehyde .
Lecture-5. Separation and Identification of Phenol and Acetophenone
Lecture-6. Separation and Identification of Aniline and Naphthalene
Lecture-7. Separation and Identification of N-Methyl Aniline and Bromobenzine
Lecture-8. Separation and Identification of N,N-diMethyl Aniline and Ethyl benzoate
Lecture-9. Separation and Identification of beta-Naphthol and Nitrobenzine
Lecture-10.Separation and Identification of Chlorobenzoic acid and Naphthalene
Lecture-11. Separation and Identification of Chlorobenzoic acid and Benzaldehyde
Lecture-12 Separation and Identification of Cresol and Benzamide .
Lecture-13. Separation and Identification of ortho- Benzoic acid and Nitrobenzene
Lecture-14. Separation of three component mixtures by chemical methods. A minimum of two mixtures should be separated and analyzed.
Lecture-15. Column chromatography: Separation of a mixture of *ortho* and *para*-nitroanilinesand any one of the two component mixture using silica gel as adsorbent and chloroform as the eluent. It is monitored by TLC.

M.Sc ORGANIC CHEMISTRY-FINAL YEAR

SEMESTER-IV
PAPER-I: DRUG DESIGN AND DRUG DISCOVERY

UNIT-I : PRINCIPLES OF DRUG DESIGN AND DRUG DISCOVERY.

Lecture-1: Introduction to drug discovery
Lecture-2: Folklore drugs, stages involved in drug discovery- disease, drug targets, bio assay.
Lecture-3: Discovery of a lead- screening of natural products and synthetic compound libraries.
Lecture-4: Existing drugs as leads (me too drugs).
Lecture-5: Pharmacokinetics (ADME), pharmacodynamics.
Lecture-6: Nature of drug – receptor interactions and their theories – Occupancy theory.
Lecture-7: Induced – fit theory, Macromolecular purturbation theory and Two-state model of receptor activation.
Lecture-8: Natural products as lead structures in drug discovery – Pharmacophore -structure.
Lecture-9: pruning technique e.g. morphine.Discovery of lead structure from natural hormones

and neurotransmitters.

Lecture-10: Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril).

Lecture-11: Principles of design of agonists (e.g.Salbutamol), antagonists e.g. cimitidine) and enzyme inhibitors (e.g. captopril).

Lecture-12: Drug discovery without lead – serendipity- Penicillin and Librium as examples.

Lecture-13: Principles of prodrug design.

Lecture-14: Introduction to drug patents and Clinical trials.

Lecture-15: Introduction to drug patents and Clinical trials.

UNIT-II : LEAD MODIFICATION AND SAR STUDIES

Lecture 1: Lead identification and modification strategies.

Lecture 2: Definition and discussion on bioisoserism and its advantages.

Lecture 3: Discussion on variation of alkyl substituents, chain homologation and branching

Lecture 4: Discussion on variation of aromatic substituents and extension of structure.

Lecture 5: Discussion on ring expansion and ring contraction, ring variation,

Lecture 6: Discussion on variation and position of hetero atoms, ring fusion

Lecture 7: Discussion on simplification of the lead, rigidification of lead

Lecture 8: Discussion on Discovery of oxaminquine

Lecture 9: Development of salbutamol

Lecture10: Discovery of cimitidine

Lecture11: Development of captopril

Lecture12: Structure-Activity Relationship studies in sulfa drugs.

Lecture13: Structure-Activity Relationship studies in benzodiazepines.

Lecture14: Structure-Activity Relationship studies in taxol analogs.

Lecture15: SAR studies with XRD and computational studies.

UNIT-III : QSAR STUDIES and COMPUTER AIDED DRUG DESIGN

Lecture 1: Introduction to QSAR Studies

Lecture 2: Physicochemical Properties – pKa, Physicochemical Properties: pKa

Lecture 3: Electronic Effects and Hammett Constants (σ)

Lecture 4: Lipophilicity Constant (π)

Lecture 5: Steric Effects and Taft's Constant

Lecture 6: Linear and Nonlinear Relationships Between Biological Activity

Lecture 7: Hansch Analysis

Lecture 8: Craig's Plot

Lecture 9: Topliss Scheme

Lecture 10: Free-Wilson Approach

Lecture 11: Cluster Significance Analysis

Lecture 12: Case Study on QSAR Study of Pyranenamine

Lecture 13: Design of Crizotinib

Lecture 14: Introduction to Computer-Aided Drug Design (CADD)& Rigid Docking & Flexible

Lecture 15: Induced Fit Docking of Ligands' Definition Overview

UNIT-IV: COMBINATORIAL SYNTHESIS

Lecture 1: Introduction to Combinatorial Chemistry.
Lecture 2: Combinatorial Approach
Lecture 3: Combinatorial Libraries
Lecture 4: Combinatorial Technologies
Lecture 5: Solid Phase Synthesis.
Lecture 6: Types of Resins.
Lecture 7: Linkers.
Lecture 8: Reactants for Solid Phase Synthesis.
Lecture 9: Methods of Parallel Synthesis: Houghton's Tea Bag Procedure.
Lecture 10: Automated Parallel Synthesis.
Lecture 11: Mixed Combinatorial Synthesis: General Principles.
Lecture 12: Furkas Mix and Split Combinatorial Synthesis.
Lecture 13: Structure Determination of Active Compounds: Deconvolution.
Lecture 14: Examples of Combinatorial Chemistry.
Lecture 15: Planning and Designing of Combinatorial Synthesis.

PAPER-II : DRUG SYNTHESIS AND MECHANISM OF ACTION

UNIT I: DRUGS ACTING ON METABOLIC PROCESS, CELL WALL AND SPECIFIC ENZYMES.

Lecture 1: Basic concepts of mechanism of drug action.
Lecture 2: Different types of proteins as the macromolecular targets.
Lecture 3: Other macromolecular targets such as carbohydrates, lipids and nulceic acids.
Lecture 4: Classification of drugs. Enzyme inhibition and its types.
Lecture 5: Importance of Antifolates, Discovery and mechanism of action of sulphonamides.
Lecture 6: Synthesis of sulfomethoxazole, sulfodoxine, sulfaguanidine and dapsone.
Lecture 7: Bacterial resistance to sulfonamides and drug synergism and synthesis of Diaminopyrimidines -trimethoprim.
Lecture 8: Structure of bacterial cell wall and brief introduction to β-Lactam antibiotics.
Lecture 9: Mechanism of action of penicillins and cephalosporins.
Lecture10: Synthesis of pencillin-G and cephalosporin-C, cefalexin and cycloserine.
Lecture11: Resistance to pencillins and broad spectrum penicillins.
Lecture12: Synthesis and mode of action of cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin.
Lecture13: β-Lactamase inhibitors- Structural formulae and mode of action of clavulanic acid and sulbactum.
Lecture14: Discussion on H^+/K^+ -ATPase inhibitors- synthesis of Omeprazole.
Lecture15: Discussion on Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

UNIT II: DRUGS ACTING ON GENETIC MATERIAL AND IMMUNE SYSTEM

Lecture 1.	Brief review of Drugs acting on genetic material
Lecture 2.	Drugs acting on genetic material: Introduction, classification and mechanism of action.
Lecture 3.	DNA-intercalating agents-Anticancer and antimalarial agents
Lecture 4.	Structural formulae of Daunomycin, Adriamycin and Amsacrine
Lecture 5.	Synthesis of Amscarine, Nitracrine
Lecture 6.	Synthesis of Quinacrine and Chloroquine
Lecture 7.	DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole
Lecture 8.	Synthesis of Dimetridazole and Tinidazole.
Lecture 9.	DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.
Lecture 10.	DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.
Lecture 11.	DNA-Topoisomerase inhibitors: Anti bacterial agents.Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.
Lecture 12.	Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.
Lecture 13.	Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin
Lecture 14.	Drugs acting on immune system: Introduction to immune system. Immunosupressing agent structural formula of Cyclosporin.
Lecture 15.	Immunoenhancers-use of vaccines and strucrural formula of levamisol.

UNIT III : DRUGS ACTING ON RECEPTORS AND ION-CHANNELS

Lecture-1	Introduction to nervous system: structure of neuron, Nerve transmission.
Lecture-2	Definition and examples of agonist, antagonist neurotransmitters and receptors.
Lecture-3	Drugsactingonreceptors:Adrenergic receptors - Introduction and classification. α-Adrenergic-receptor agonists and antagonists
Lecture-4	Synthesis and biological activity ofNor-adrenaline, Methyl L dopa and Tetrazosin.
Lecture-5	β-Adrenergic-receptor-agonistsandantagonists– Synthesisandpharmacologicalactivity of Salbutamol
Lecture-6	Tetrabutalin, Propranolol and Atenolol.
Lecture-7	Cholinergic-receptors: Introduction and classification.Cholinergic-receptor agonists and antagonists
Lecture-8	Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline
Lecture-9	Dopaminereceptors:Introductionandclassification.Dopamine-receptoragonistsand antagonists

Lecture-10	Biosynthesis of Dopamine. Synthesisof L-Dopa and Chlorpromazine.
Lecture-11	Serotoninreceptors:Introductionandclassification.Serotoninreceptoragonistsand antagonists.
Lecture-12	synthesis and pharmacological activity of Serotonin andMetoclopramide.
Lecture-13	Histaminereceptors:Introduction and classification. Histaminereceptoragonistsandantagonists-synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.
Lecture-14	Hormones and their receptors:Introduction to estrogen structural formulae of Tamoxifen.
Lecture-15	Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca^{2+}, Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine.

UNIT- IV : CHIRAL DRUGS

Lecture-1: Introduction to chiral drugs
Lecture-2: Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule.
Lecture-3: Role of chirality on biological activity
Lecture-4: Distomers – a) with no side effects.
Lecture-5: With undesirable side effects.
Lecture-6: Both isomers having independent therapeutic valued combination products having therapeutic advantages.
Lecture-7: Mmetabolic chirality inversion
Lecture-8: Synthesis and pharmacological activity of S-Ibuprofen.
Lecture-9: S- Metaprolol, Ininavir sulfate.
Lecture-10: Levocetrazine, 2S-Verapamil, S,S-Ethambutol.
Lecture-11: (+)Lomefloxacin, Fluvastatin
Lecture-12: Dextropropoxyphen, (+)Ephedrine.
Lecture-13: (+)Griseofulvin, Dexormaplatin, R-Indacrinone.
Lecture-14: Nateglinide, Oxybutynin hydrochloride
Lecture-15: S,S- Captopril and S,S,S- Enalaprilate.

PAPER-III A: ADVANCED HETEROCYCLIC CHEMISTRY

UNIT-I : NONAROMATIC HETEROCYCLICS & AROMATICITY

Lecture-**1.** Different types of strains of nonaromatic heterocycles.
Lecture-2. Interactions and conformational aspects of nonaromatic heterocycles.
Lecture-3. Synthesis, reactivity and importance of the Azirine ring systems
Lecture-4. Synthesis, reactivity and importance of the Aziridines, ring systems
Lecture-5. Synthesis, reactivity and importance of the Oxiranes, ring systems

Lecture-6. Synthesis, reactivity and importance of the Thiiranes, ring systems
Lecture-7. Synthesis, reactivity and importance of the Diazirenes, ring systems
Lecture-8. Synthesis, reactivity and importance of the Diaziridines, ring systems
Lecture-9. Synthesis, reactivity and importance of the Oxaziridines, ring systems
Lecture-10. Synthesis, reactivity and importance of the Azetidines, ring systems
Lecture-11. Synthesis, reactivity and importance of the Oxetanes ring systems
Lecture-12. Synthesis, reactivity and importance of the thietanes ring systems
Lecture-13. Aromaticity: Introduction, Aromatic and anti aromatic compounds. Criteria for aromaticity.
Lecture-14. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. Cyclopropenium ion, cyclopentadienyl ion
Lecture-15. Huckel's 4n+2 electron rule for benzene and non benzenoid aromatic compounds. Eg. cycloheptatrienium ion, azulene and annulenes.

UNIT II: 5- & 6- MEMBERED HETEROCYCLICS WITH TWO HETERO ATOMS

Lecture 1.	Synthesis, reactivity, aromatic character and importance of the Pyrazole
Lecture 2.	Synthesis, reactivity, aromatic character and importance of the Immidazole
Lecture 3.	Synthesis, reactivity, aromatic character and importance of the Oxazole
Lecture 4.	Synthesis, reactivity, aromatic character and importance of the Thiazole
Lecture 5.	Synthesis, reactivity, aromatic character and importance of the Isoxazole,
Lecture 6.	Synthesis, reactivity, aromatic character and importance of the Isothiazole
Lecture 7.	Synthesis, reactivity, aromatic character and importance of the Pyrimidine.
Lecture 8.	Synthesis, reactivity, aromatic character and importance of the Pyridazine
Lecture 9.	Synthesis, reactivity, aromatic character and importance of the Pyrazine
Lecture 10.	Synthesis, reactivity, aromatic character and importance of the Oxazine,
Lecture 11.	Synthesis, reactivity, aromatic character and importance of the thiazine
Lecture 12.	Synthesis, reactivity, aromatic character and importance of the benzimidazole
Lecture 13.	Synthesis, reactivity, aromatic character and importance of the benzoxazole
Lecture 14.	Synthesis, reactivity, aromatic character and importance of the benzthiazole
Lecture 15.	Explained Biological importance compounds

UNIT III: HETEROCYCLICS WITH MORE THAN TWO HETERO ATOMS

Lecture 1.	Synthesis, reactivity, aromatic character and importance of the 1,2,3 triazoies
Lecture 2.	Synthesis, reactivity, aromatic character and importance of the 1,2,4-triazoles
Lecture 3.	Synthesis, reactivity, aromatic character and importance of the Tetrazoles
Lecture 4.	Synthesis, reactivity, aromatic character and importance of the T1,2,4-oxadiazole
Lecture 5.	Synthesis, reactivity, aromatic character and importance of the 1 ,3,4-oxadiazole,
Lecture 6.	Synthesis, reactivity, aromatic character and importance of the1,2,5-oxadiazole,
Lecture 7.	Synthesis, reactivity, aromatic character and importance of the , 1,2,3-thiadiazoles,
Lecture 8.	Synthesis, reactivity, aromatic character and importance of the 1,2,5-thiadiazoles,
Lecture 9.	Synthesis, reactivity, aromatic character and importance of the 1,2,3-triazine,
Lecture 10.	Synthesis, reactivity, aromatic character and importance of the 1,2,4-triazine,
Lecture 11.	Synthesis, reactivity, aromatic character and importance of the 1,2,3,4-tetrazines and 1,2,3,5- tetrazines.
Lecture 12.	Synthesis, reactivity, aromatic character and importance of the 1,2,4,5-tetrazines.
Lecture 13.	Synthesis and importance of purines
Lecture 14.	Synthesis and importance of pteridines
Lecture 15.	Syntheis of Caffeine, theobromine and theophylline

UNIT- IV : LARGER RING AND OTHER HETEROCYCLES

Lecture-**1.** Synthesis, structure, stability and reactivity ofAzepines,
Lecture-2. Synthesis, structure, stability and reactivity of Oxepines
Lecture-3. Synthesis, structure, stability and reactivity of Thiepines.
Lecture-4. Synthesis of Diazepines
Lecture-5. rearrangements of 1,2 - diazepines.
Lecture-6. Synthesis of Benzoazepines,
Lecture-7. Synthesis of Benzodiazepines,
Lecture-8. Synthesis of Benzooxepines,
Lecture-9. Synthesis of Benzothiepines,
Lecture-10. Synthesis of Azocines
Lecture-11. Synthesis of Azonines.
Lecture-12. Synthesis of selenophenes
Lecture-13. Synthesis of Tellerophenes
Lecture-14. Synthesis of Phospholes
Lecture-15. Synthesis of Boroles.

PAPER-III B : POLYMERS, DYES and PIGMENTS

UNIT -I : POLYMERS- I

Lecture 1: Introduction to Organic Polymers.
Lecture 2: Classification of Polymers
Lecture 3: Types of Polymerization Addition polymerization: free radical polymerization
Lecture 4: Types of Polymerization -Condensation polymerization
Lecture 5: Radical and Ionic Polymerization
Lecture 6: Ziegler-Natta Polymerization Applications
Lecture 7: Stereochemistry of Polymers Tacticity, Examples and applications
Lecture 8: Plasticity and Types of Plastics
Lecture 9: Molecular Mass of Polymers,
Lecture 10: Resins and Plastics - Polystyrene and Styrene Copolymers
Lecture 11: Poly(vinyl chloride/vinyl acetate) and Related Polymers
Lecture 12: Acrylic Polymers,: PMMA, Manufacturing processes and uses
Lecture 13: Polyesters and Phenol-Formaldehyde Polymers PET, PBT
Lecture 14: Polyurethanes and Epoxide Polymers uses
Lecture 15: Natural and Synthetic Rubbers natural rubber

UNIT -II : POLYMERS- II

Lecture 1: Introduction to Organic Polymers
Lecture 2: Classification of Polymers
Lecture 3: Types of Polymerization –Addition .free radical polymerization
Lecture 4: Types of Polymerization Condensation polymerization Copolymerization
Lecture 5: Radical and Ionic Polymerization Comparison of radical
Lecture 6: Ziegler-Natta Polymerization Applications and examples (e.g., polypropylene)
Lecture 7: Stereochemistry of Polymers Tacticity: isotactic, syndiotactic, atactic polymers
Lecture 8: Functional Polymers - Electrically Conducting Polymers
Applications in electronics and other fields
Lecture 9: Functional Polymers - Photoconductive and Liquid Crystal Polymers
Lecture 10: Functional Polymers - Smart Materials Examples and applications
Lecture 11: Functional Polymers - Biodegradable Polymers Applications in sustainable materials and medical fields
Lecture 12: Membranes - Filtration and Separation Techniques used in these processes
Lecture 13: Membranes - Liquid Separation Techniques Applications Representative polymers
Lecture 14: Fire Retarding Polymers and Photonic Polymers Applications in optics
Lecture 15: Polymers in Biomedical Applications

UNIT- III : DYES-I

Lecture 1: Introduction to Dyes
Lecture 2: Nomenclature and Classification of Synthetic Dyes
Lecture 3: Color and Constitution.
Lecture 4: Theories of Color and Constitution - Part 1
Lecture 5: Theories of Color and Constitution - Part 2
Lecture 6: Valence Bond Theory and Molecular Orbital Theory

Lecture 7: Triphenyl Methane Dyes - Part 1
Lecture 8: Triphenyl Methane Dyes - Part 2
Lecture 9: Azo Dyes - Types and Synthesis
Lecture 10: Chemistry and Synthesis of Acidic and Basic Azo Dyes
Lecture 11: Cyanine Dyes
Lecture 12: Natural Dyes - Introduction and Importance
Lecture 13: Structure Determination and Synthesis of Alizarin
Lecture 14: Structure Determination and Synthesis of Quinizarin
Lecture 15: Structure Determination and Synthesis of Indigo

UNIT – IV : DYES-II AND PIGMENTS

Lecture 1: Introduction to Fluorescent Dyes
Lecture 2: Interaction of Organic Molecules with Electromagnetic Radiation
Lecture 3: Fluorescence and Delayed Fluorescence Mechanism Factors affecting
Lecture 4: Effect of Molecular Structure on Fluorescence
Lecture 5: General Properties of Fluorescent Dyes
Lecture 6: Synthesis of Fluorescent Aromatic Hydrocarbons
Lecture 7: Synthesis of Fluorescent Heteroaromatic Compounds
Lecture 8: Introduction to Laser Dyes
Lecture 9: Synthesis of Oligophenylenes
Lecture 10: Synthesis of Oxazoles and Benzoxazoles
Lecture 11: Synthesis of Stilbenoid Compounds
Lecture 12: Coumarin and Rhodamine Laser Dyes.
Lecture 13: Introduction to Pigments.
Lecture 14: Structures and Synthesis of Natural Pigments.
Lecture 15: Synthetic Pigments Preparation of phthalocyanines Applications

PAPER-IV A : ADVANCED NATURAL PRODUCTS

UNIT-I : BIOSYNTHESIS OF NATURAL PRODUCT

Lecture-1: Introduction to Biosynthesis of secondary metabolites.
Lecture-2: Introduction, Difference between Laboratory synthesis and biosynthesis.
Lecture-3: Methods for determination of biosynthetic mechanism.
Lecture-4: Isolation andidentification of Biosynthetic precursors.
Lecture-5: Feeding experiments use of radioisotopes.
Lecture-6: Measurement of incorporation absolute incorporation. Specific Incorporation
Lecture-7: Identificationof the position of labels in labeled natural products
by chemical degradation and spectralmethods.
Lecture-8: Identificationof the position of labels in labeled natural products
by chemical degradation and spectralmethods.

Lecture-9: Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds.
Lecture-10:Shikimic acid pathway
Lecture-11:Biosynthesis of essential amino acids phenylalanine, tyrosine and tryptophan.
Lecture-12: Biosynthesis of carboxylic acid derivatives, flavonoids and morphine alkaloids.
Lecture-13:Mevalonic acid pathway.
Lecture-14:Biosynthesis of terpenes mono, sesqui, di,tri (β-amyrin).
Lecture-15:Biosynthesis of carotenoids, steroids – cholesterol

UNIT-II:STRUCTURE DETERMINATION OF NATURALPRODUCTS-I

Lecture 1: Introduction to Chemical Methods in Structure Determination
Lecture 2: Morphine - Initial Structural Insights through Chemical Reactions
Lecture 3: Morphine - Elucidation of Structure
Lecture 4: Morphine - Determination of Stereochemistry&Total synthesis
Lecture 5: Reserpine - Initial Structural Insights through Chemical Reactions
Lecture 6: Reserpine - Elucidation of Structure
Lecture 7: Reserpine - Determination of Stereochemistry &Total synthesis
Lecture 8: Abietic Acid - Initial Structural Insights through Chemical Reaction
Lecture 9: Abietic Acid - Elucidation of Structure &. Total synthesis
Lecture 10: Abietic Acid - Determination of Stereochemistry
Lecture 11: Cholesterol - Initial Structural Insights through Chemical Reactions
Lecture 12: Cholesterol - Determination of Stereochemistry.
Lecture 13;- Total synthesis
Lecture 14: Rotenone - Initial Structural Insights through Chemical Reactions.
Lecture 15: Rotenone - Elucidation of Structure , Stereochemistry Total synthesis

UNIT-III : STRUCTURE DETERMINATION OF NATURALPRODUCTS-II

Lecture-1	Introduction of Spectroscopic techniques IR, UV, ^{1}Hnmr, ^{13}Cnmr.
Lecture-2	Spectroscopic techniques IR, UV, ^{1}Hnmr, ^{13}Cnmr, COSY, HETEROCOSY, NOESY, 2D- INADEQUATE and MS in the structure elucidations of natural products, examples, flavones.
Lecture-3	Biflavones
Lecture-4	Flavanones
Lecture-5	Isoflavones
Lecture-6	Coumarins
Lecture-7	Quinolines
Lecture-8	Isoquinolines.
Lecture-9	**Study of the following solved problems:** Mass, IR, ^{1}H,^{13}C NMR, HOMOCOSY, HECTOR,Geraniol.
Lecture-10	DEPT, 2D-INADEQUATE and NOE of Geraniol
Lecture-11	INEPT of **menthol**

Lecture-12	APT of **appericine**
Lecture-13	Heteronuclear 2D-J resolved spectrum of **stricticine**.
Lecture-14	NOESY of **buxaquamarine**
Lecture-15	HETEROCOSY of **strictanol**, 2D-INADEQUATE of **α-picoline** and **β-methyl tetrahydranfuran**.

UNIT-IV : TOTAL STEREOSELECTIVE SYNTHESIS.

Lecture 1: Retrosynthetic analysis of Dynemicin-A and synthesis of Isobenzofuran.
Lecture 2: Synthesis of Imidoquinone tricyclic system.
Lecture 3: Construction of ring A and C cyclohexenoids.
Lecture 4: Assembling Imidoquinone and Isobenzofuran to Dynemicin-A.
Lecture 5: Biological significance and synthesis of PGE2 and PGF2α.
Lecture 6: Medicinal importance and synthesis of Paeoniflorin.
Lecture 7: Sharpless- Masamune synthesis of four L-hexoses from Threose unit.
Lecture 8: Sharpless- Masamune synthesis of four L-hexoses from Erythrose unit.
Lecture 9: Takasago synthesis of menthol.
Lecture10: Hoffmann-LaRoche synthesis of Biotin.
Lecture11: Synthesis of sulfonyl hydrazine- a source of Ring A skeleton.
Lecture12: Shapiro coupling between organolithium and cyclohexenoid aldehyde.
Lecture13: Attachment of sidearm with β-lactam ring to complete the Taxol synthesis.
Lecture14: Construction of Indolizidine skeleton.
Lecture15: Development of trans-triene fragment.

PAPER-IV B : BIOPHARMACEUTICS AND PHARMACODYNAMICS

UNIT-I : PHARMACOKINETICS

Lecture-1: Introduction and importance of ADME studies of Drugs.
Lecture-2: Routes of Administration
Lecture-3: i)Absorption: Definition, Absorption Of Drugs Across The Membranes.
Lecture-4: Physico Chemical Factors Affecting The Drug Absorption
(Emphasis On Ph Partition Hypothesis and Drug Dissolution).
Lecture-5: Physico Chemical Factors Affecting The Drug Absorption
(Emphasis On Ph Partition Hypothesis And Drug Dissolution).
Lecture-6: Methods Of Determination Of Drug
Absorption.
Lecture-7: Bioavailability. Ii)Distribution: Apparent Volume Of Drug Distribution
Lecture-8: Factors Affecting Distribution.
Lecture-9: Plasma Protein Binding.
Lecture-10: iii) Metabolism: Sites Of Drug Metabolism,
Lecture-11: Metabolic Rate Constant,
Lecture-12: Bioactivation And Biotransformation Of Drugs (Phase I and II Reactions)
Lecture-13: Elimination: Types Of Elimination

Lecture-14: Elimination: Overall Apparent Elimination Rate Constant
Lecture-15: Elimination: Half-Life, Concept Of Clearance

UNIT- II : PHARMACODYNAMICS

Lecture-1: Introduction, Targets For Drug Action,
Lecture-2: Receptor Concept.
Lecture-3: Pharmacological Binding Terms.
Lecture-4: Two- Statereceptor Model,
Lecture-5: Receptor Families- Structure
Lecture-6: Signal Transduction Mechanisms
Lecture-7: Gating Mechanism,
Lecture-8: G-Protein Coupled Receptors
Lecture-9: G-Protein And Their Role
Lecture-10: Targets for G-proteins
Lecture-11: Kinase Linked Receptors
Lecture-12: Receptors That Regulate Gene Transcription.
Lecture-13: Theories Of Concentration
Lecture-14: Response Relationship
Lecture-15: Dose-Response Curve.

UNIT - III : PRINCIPLES OF THERAPEUTICS

Lecture-1: Introduction of Plasma Drug concentration vs Time profile
Lecture-2: Definition and explanation of various terms: MEC, MSC, MTC, AUC(graph).
Lecture-3: Peak Plasma Concentration Therapeutic Range.
Lecture-4: Steady State Concentration, Onset Of Action, Onset Of Time
Lecture-5: Duration Of Action, Intensity Of Action. LD50, ED50.
Lecture-6: Therapeutic objective. Dosage regimen,
Lecture-7: Design of dosage regimes: Dose size, dosing frequency,
Lecture-8: Drug Accumulation during multiple dosing,
Lecture-9: TimeTo Reach Steady-State During Multiple Dosing,
Lecture-10: Average Concentration And Body Content On Multiple Dosing To Steady State,
Lecture-11: Loading Dose, Maintenance Dose, Maintenance Of Drug Within The Therapeutic Range,
Lecture-12: Design Of Dosage Regimen From Plama Concentration. Kinetics Of FixedDose,
Lecture-13: Fixed Time Interval Regimes. Modification To Dosage Regime: Dosing Of Drugs In ObesePatients,
Lecture-14: Dosing Of Drugs In Neonates, Infants & Children, Dosing Of Drugs In Geriatrics (Elderly),
Lecture-15: Dosing Of Drugs In Hepatic Disease, Dosing Of Drugs In Renal Disease

UNIT IV : DRUG INTERACTIONS:

Lecture-1: Introduction, classification, Mechanisms of Drug Interactions.–
Lecture-2: Pharmacokinetic Interactions (alteration of gastrointestinal absorption
Lecture-3: Compexation and Adsorption
Lecture-4: AlterationOf Distribution Alteration Of Metabolism And
Alteration Of Excretion)
Lecture-5: Pharmacodynamic Interactions (Antagonistic Effects,
Lecture-6: Synergistic Effects, Alteration Of Electrolyte Levels
Lecture-7: Interactions Involving Adrenergic System
Lecture-8: Alteration Of Receptor Site Interaction And AntibioticCombinations.
Lecture-9: Influence of alcohol(Anti biotics,
Lecture-10: Anti coagulants, Anti histamines
Lecture-11: Anti psychotic drugs
Lecture-12: Sedatives And Hypnotics), Smoking(Theophylline
Lecture-13: Diazepam, a Tri cyclicantidepressants
Lecture-14: Food (Bronchodaliators, Diuretics
Lecture-15: ACE Inhibitors, Anticoagulants,Tetracyclines) on drug action.

PAPER V : LABORATORY COURSE

SPECTROSCOPIC IDENTIFICATION OF ORGANIC COMPOUNDS & PRACTICE OF CHEMISTRY SOFTWARE PRGRAMMES

Lect-1(lab)	Identification of unknown organic compound **1** and **2** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-2(lab)	Identification of unknown organic compound **3** and **4** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-3(lab)	Identification of unknown organic compound **5** and **6** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-4(lab)	Identification of unknown organic compound **7** and **8** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-5(lab)	Identification of unknown organic compound **9** and **10** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-6(lab)	Identification of unknown organic compound **11** and **12** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .

Lect-7(lab)	Identification of unknown organic compound **13** and **14** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-8(lab)	Identification of unknown organic compound **15** and **16** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-9(lab)	Identification of unknown organic compound **17** and **18** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-10(lab)	Identification of unknown organic compound **19** and **20** by interpretation of IR, UV, ^{1}H -NMR, ^{13}C NMR,and massspectral data .
Lect-11(lab)	Chemistry software programmes: Chem Draw
Lect-12(lab)	Chemistry software programmes: Chem Draw
Lect-13(lab)	Chemistry software programmes: Chem Draw
Lect-14(lab)	analysis of IR and NMR using ACD/Id NMR processor
Lect-15(lab)	EXCEL: Drawing graphs, Molecular docking.

PAPER VI : LABORATORY COURSE

SYNTHESIS AND ANALYSIS OF DRUGS

Lecture 1: Synthesis of Paracetamol and purification by recrysatallization.
Lecture 2: Synthesis of Phenytoin and purification by recrysatallization.
Lecture 3: Synthesis of Benzocaine(Step 1) and purification by recrysatallization.
Lecture 4: Synthesis of Benzocaine(Step 2) and purification by recrysatallization.
Lecture 5: Synthesis of 6-Methyluracil and purification by recrysatallization.
Lecture 6: Synthesis of Chloritone and purification by recrysatallization.
Lecture 7: Synthesis of FIuorescein and purification by recrysatallization.
Lecture 8: Estimation of ascorbic acid by titrimetry.
Lecture 9: Estimation of Riboflavin by colorimetry
Lecture10: Estimation of Aspirin by titremetry.
Lecture11: Estimation of Ibuprofen by titrimetry.,
Lecture12: Estimation of Chloride in Ringer's lactate by argentometry.
Lecture13: Estimation of Ca^{+2} ions in Calcium gluconate injection by complexometry.
Lecture14: Synthesis of 4-Aminobenzene sulphonamide(Step1 &2
Lecture 15: Synthesis of 4-Aminobenzene sulphonamide(Step3 &4)

M.Sc (Physical Chemistry): Semester-III (2017-18)

Teaching Plans

1. **PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY**
2. **PAPER – II CH (PC) 302T: SPECTROSCOPY AND LASERS**
3. **PAPER III- ELECTIVE 3A-CH (PC) 303T(CB1): APPLIED CHEMISTRY, MATERIAL SCIENCE AND RADIATION EFFECTS**
4. **PAPER-IV-ELECTIVE 4A-CH(PC) 304T(CB3): POLYMER CHEMISTRY**

M.Sc. CHEMISTRY (PHYSICAL CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters

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

[Under CBCS Scheme]

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

Semester - III (Physical Chemistry)

PAPER –CH(PC) 301T: QUANTUM CHEMISTRY AND GROUP THEORY (15 h)

PC - 09: Applications of Schrödinger equation

Lecture-1: **Simple Potential Barrier-**Introduction to systems with discontinuous potential fields, concept of a simple potential barrier, mathematical formulation and boundary conditions.

Lecture-2: **Potential Barrier with Finite Thickness-**Analysis of a potential barrier with finite thickness, transmission and reflection coefficients, quantum mechanical tunneling through a barrier.

Lecture-3: **Quantum Mechanical Tunneling-**Examples of quantum tunneling: α-particle emission, Inversion of NH_3 molecule

Lecture-4: **Quantum Mechanical Tunneling-** Hydrogen transfer reactions in chemical processes.

Lecture-5: **The Harmonic Oscillator-**Detailed Treatment, Schrödinger equation for the harmonic oscillator, Solutions for wave functions and energy levels, Quantum harmonic oscillator model for diatomic molecule vibrations.

Lecture-6: **The Rigid Rotator-**Detailed Treatment, Schrödinger equation for the rigid rotator, Solutions for wave functions and energy levels.

Lecture-7: **Introduction to spherical harmonics**- Rigid rotator model for rotating diatomic molecules.

Lecture-8: **The Hydrogen Atom-Detailed** Treatment of Schrödinger equation for the hydrogen atom, Separation into radial and angular parts.

Lecture-9: **Solutions for angular and radial functions-**Representation and interpretation of atomic orbitals, Ground-state energy and its measurability.

Lecture-10: **Orthonormal nature of hydrogen-like wave functions-** Probability density calculations and visualizations

Lecture-11: **Atomic and Molecular Term Symbols-** Introduction to term symbols for atomic and molecular states.

Lecture-12: **Term Symbols-** Explanation and examples of term symbols.

Lecture-13: **Zeeman Effect-**Introduction to the Zeeman effect and its significance.

Lecture-14: **Analysis of the normal and anomalous Zeeman effect-** Impact of external magnetic fields on atomic energy levels and term symbols.

Lecture-15: **Summary**-summary of the topic, problem solving, assignment of questions, problems for submission.

PC - 10: **Angular momentum & approximate methods (15 h)**

Lecture-1: **Angular Momentum Operators-**Introduction to angular momentum in quantum mechanics, Definition and properties of angular momentum operators

Lecture-2: **Commutation Relations of Angular Momentum Operators-**Commutation relations, consequences of commutation relations in quantum mechanics.

Lecture-3: **Eigen Functions-** Eigen functions of L^2 and L_z and the eigen values

Lecture-9: **Magnitude and orientation of angular momentum vectors**-Explanation and significance.

Lecture-10: **Electron Spin-**Introduction to electron spin and its significance, Spin operators and their properties, Explanation of the Pauli principle, Pauli exclusion principle and its implications for electron configurations.

Lecture-11: **Approximate Methods-**The Variation Method, introduction to the variation method in quantum mechanics, construction of variation functions using linear combinations,

Lecture-12: **Application to Hydrogen and Helium Atoms-**Variation method applied to the hydrogen atom, variation method applied to the helium atom.

Lecture-13: **Perturbation Theory (First Order and Non-Degenerate)-** Introduction to perturbation theory, First-order perturbation theory for non-degenerate states, calculating wave function &energy corrections using perturbation theory, Application of perturbation theory to helium atom, energy and wave function corrections for helium.

Lecture-14: **Time-Dependent Perturbation Theory**-Introduction to time-dependent perturbation theory, Interaction of radiation with matter: basic principles, explanation of allowed and forbidden transitions, selection rules for quantum transitions.

Lecture-15: **Multielectron Atoms and Hartree-Fock Method-** Introduction to multielectron atoms, Hartree-Fock self-consistent field method, Basis functions

in quantum mechanics, Slater-type orbitals (STOs) and their applications in the Hartree-Fock method, brief summary of the topic, allocation of Assignments.

PC - 11: Bonding in molecules (15 h)

Lecture-1: **Born-Oppenheimer Approximation**-Introduction to the Born-Oppenheimer approximation, separation of nuclear and electronic motion, implications and applications in molecular quantum mechanics.

Lecture-2: **MO Theory of H_2^+ion**-Introduction to molecular orbital (MO) theory, Construction and calculation of MOs for the H_2^+ ion, calculation of MO energies and evaluation of the overlap integral.

Lecture-3: **Probability Curves and Energy Diagrams**-Understanding probability curves for molecular orbitals, constructing and interpreting energy diagrams for H_2^+.

Lecture-4: **MO Theory of H_2 Molecule**-Applying MO theory to H_2 molecule, calculation of bonding and antibonding molecular orbitals, energy calculations for H_2.

Lecture-5: **MO Theory of Polyatomic Molecules**-General ideas of MO theory applied to polyatomic molecules, Introduction to symmetry-adapted linear combinations (SALCs), MO treatment of the H_2O molecule.

Lecture-6: **MOs of H_2O**-Constructing MOs H_2O, Symmetry considerations in MO formation for H_2O.

Lecture-7: **Concept of Hybridization**-Introduction to the concept of hybridization, sp, sp^2, sp^3 hybrid orbitals, examples and applications of hybridization in molecular structure.

Lecture-8: **Semiempirical MO Methods**-Introduction to semiempirical MO methods, Huckel theory of conjugated systems.

Lecture-9: **HMO Calculations on Ethylene and Allyl System**-HMO calculations for ethylene, HMO calculations for the allyl system.

Lecture-10: **HMO Calculations on Butadiene, Cyclopropenyl System, and Benzene**-HMO calculations for butadiene, HMO calculations for the cyclopropenyl system, HMO calculations for benzene.

Lecture-11: **π-Electron Charges and Bond Orders**-Calculation of π-electron charges and bond orders using HMO theory, simplification of secular determinants for symmetric systems.

Lecture-12: **Simplification of Secular Determinants**-Simplifying secular determinants of the cyclopropenyl system, simplifying secular determinants of cyclobutadiene and benzene using molecular symmetry.

Lecture-13: **Extended Huckel Theory-**Introduction to extended Huckel theory, Extension of Huckel's approach to molecules containing heteroatoms.

Lecture-14: **Orbital Symmetry and Reactivity-**Orbital symmetry and chemical reactivity, $H_2+F_2 \rightarrow 2HF$reaction.

Lecture-15: **Reaction Mechanisms-**Detailed study of the $2NO \rightarrow N_2+O_2$ reaction, applications of MO theory in understanding reaction mechanisms.

PC - 12: **Group theory (15 h)**

Lecture-1: **Matrices-**Introduction to matrices: definitions and types, Addition and multiplication of matrices: rules and examples.

Lecture-2: **Special Matrices-**Diagonal matrix and unit matrix: definitions and properties, Transpose of a matrix: definition and examples.

Lecture-3: **Adjoint and Inverse of a Matrix-**Adjoint of a matrix: definition and computation, Inverse of a matrix: methods to find the inverse.

Lecture-4: **Determinants-**Definition and properties of determinants, expansion of a determinant: cofactor expansion,

Lecture-5: **Properties of Determinants-**Important properties of determinants: theorems and proofs, Applications of determinant properties in solving linear equations.

Lecture-6: **Symmetry Operations and Groups-**Introduction to symmetry operations: definition and examples, symmetry operations forming a group: group properties.

Lecture-7: **Classes of Symmetry Operations-**Classification of symmetry operations: examples from molecular symmetry, matrix representation of symmetry operations: basic concepts.

Lecture-8: **Point Groups and Representations-**Introduction to point groups in chemistry, Matrix representations of point groups, process of generating representations for point groups, examples and applications in molecular symmetry.

Lecture-9: **Reducible and Irreducible Representations-**Definitions and differences between reducible and irreducible representations, methods to reduce representations.

Lecture-10: **Great Orthogonality Theorem-**Statement of the Great Orthogonality Theorem, consequences and applications of the theorem in group theory.

Lecture-11: **Character tables-**Construction of character tables for C_{2h} C_{2v} and C_{3v} groups.

Lecture-12: Construction of character tables for C_{2v} and C_{3v} groups.

Lecture-13: Quantum Mechanics and Group Theory-Introduction to the intersection of quantum mechanics and group theory, wave functions as bases for irreducible representations.

Lecture-14: Quantum mechanics and group theory-Wave functions as bases for irreducible representations, the direct product – vanishing of integrals, projection operators.

Lecture-15: Symmetries of vibrations- IR and Raman activity, summary of the topic, giving assignments

PAPER – II CH (PC) 302T: SPECTROSCOPY AND LASERS (15 h)

PC- 13: Physical Principles of Spectroscopy and Vibrational Spectroscopy

Lecture-1: Interaction of Electromagnetic Radiation with Matter - Define absorption and emission of radiation, explain induced absorption, spontaneous emission, and stimulated emission.

Lecture-2: Oscillator Strength and Transition Moment Integral-Define oscillator strength and transition moment integral, allowed and forbidden transitions.

Lecture-3: Selection Rules - Discuss selection rules with the spectrum of formaldehyde as an example.

Lecture-4: Spectral Lines-Factors affecting the width and intensity of spectral lines, explain line width, natural line broadening, and Doppler broadening

Lecture-5: Infrared Spectroscopy-Discuss the anharmonic oscillator and Morse potential energy diagram, selection rules.

Lecture-6: Vibration-Rotational Spectroscopy- explain vibration-rotation spectroscopy, selection rules and the P, Q, R branches.

Lecture-7: Polyatomic Molecules-Classification of types of molecules as linear, symmetric top, and asymmetric top molecules, examples.

Lecture-8: Vibration-Rotation Spectra of Polyatomic Molecules- Discuss the spectra of linear, symmetric top, and asymmetric top molecules, examples and selection rules.

Lecture-9: FTIR- Principles of FTIR (Fourier Transform Infrared Spectroscopy), Instrumentation, advantages over conventional IR spectroscopy.

Lecture-10: **Raman Spectroscopy-**Explain the classical and quantum theories of the Raman effect.

Lecture-11: **Raman Spectra -** Discuss pure rotational, vibrational, and vibrational-rotational Raman spectra, examples.

Lecture-12: **Selection Rules and Depolarization Factors-**Selection rules for Raman spectroscopy, discuss the depolarization factors of Raman lines and their relevance.

Lecture-13: **Raman Spectroscopy Instrumentation-**Overview of Raman spectroscopy instrumentation.

Lecture-14: **Applications-**Typical applications, including structure determination of XY_4 molecules and phase transitions.

Lecture-15: **Summary –** Summarize the topics, give questions & problems as assignment.

PC- 14: NMR, NQR and Mossbauer Spectroscopy (15 h)

Lecture-1: **Principles of NMR-**Introduction to Nuclear Magnetic Resonance (NMR) spectroscopy, Basic principles and theory behind NMR, Derivation of $h\nu=g\beta H$.

Lecture-2: **Larmor Precessional Frequency-**Explanation of Larmor precessional frequency, Spin-spin splitting (AX system), Quantitative treatment of spin-spin splitting.

Lecture-3: **Instrumentation of NMR-**Continuous Wave (CW) NMR instruments, Fourier Transform (FT) NMR instruments.

Lecture-4: **Two-Dimensional NMR Spectroscopy**-Principles of 2D NMR spectroscopy, Graphical representation of 2D NMR spectra.

Lecture-5: **Homonuclear ^{1}H J, δ Spectroscopy**-Homonuclear ^{1}H J, δ spectroscopy, Application for mixture analysis (e.g., n-butyl bromide and n-butyl iodide).

Lecture-6: **The COSY Experiment-**Introduction to the COSY experiment, Two-dimensional ^{1}H, ^{1}H shift correlations, COSY spectra of an AX system and o-nitroaniline.

Lecture-7: **COSY Spectra of Amino Acids-**Analysis of COSY spectra for alanine, glutamic acid, arginine.

Lecture-8: **Nuclear Overhauser Effect (NOE)-**Explanation of the Nuclear Overhauser Effect (NOE), Principles of two-dimensional nuclear Overhauser spectroscopy (NOESY)

Lecture-9: **Nuclear Quadrupole Resonance-**Introduction to Nuclear Quadrupole Resonance (NQR), Quadrupole nuclei and quadrupole moments, Prolate and oblate nuclear charge distributions.

Lecture-10: **Energies of Quadrupolar Transitions-**Energies of quadrupolar transitions, Electric field gradient, coupling constants, and splitting.

Lecture-11: **Introduction to Mossbauer Spectroscopy-**Introduction to Mossbauer spectroscopy, explanation of the Mossbauer effect and recoil energy.

Lecture-12: **Mossbauer Spectrum and Isomer Shift-**Typical Mossbauer spectrum, understanding isomer shift in Mossbauer spectra.

Lecture-13: **Quadrupole Splitting and Magnetic Hyperfine Interaction-**Explanation of quadrupole splitting, Magnetic hyperfine interaction in Mossbauer spectroscopy.

Lecture-14: **^{57}Fe Mossbauer Spectra-**Analysis of ^{57}Fe Mossbauer spectra, spectra of Fe^{2+} and Fe^{3+} (paramagnetic) compounds.

Lecture-15: **Mossbauer Spectra of Magnetic Compounds-**Analysis of Fe^{3+} (magnetic) compounds, summary and applications of Mossbauer spectroscopy in various compounds. Allotment of assignment questions & problems.

PC- 15: **X-ray Spectroscopy & Diffraction Techniques (15 h)**

Lecture-1: **Introduction-**Introducing briefly various X-ray techniques and their importance. Generation of X-rays and the labelling of X-rays emitting from various principal energy levels.

Lecture-2: **XRF-** Principle, overview of the setup, process and procedure for XRF analysis and limitations.

Lecture-3: **XRF spectra & Interpretation-**K-emission Spectrum of Tin, L-emission Spectrum of Gold.

Lecture-4: **X-ray Absorption Techniques-**Methods used to measure X-ray absorption, Principle of Absorption Edge Fine Structure (AEFS) and Extended X-ray Absorption Fine Structure (EXAFS): Explanation of AEFS and EXAFS spectra, and their significance. Examples.

Lecture-5: **X-ray Diffraction-Bragg Condition:** Derivation and explanation of Bragg's Law equation and its application in X-ray diffraction.

Lecture-6: **Miller Indices and d-spacing Formula -** Definition and use in identifying lattice planes.

Lecture-7: **Numericals-**Numerical problems on Miller indices, Bragg's law

Lecture-8: **Experimental Methods-**Laue method and Debye-Scherrer method for X-ray diffraction.

Lecture-9: **Unit Cells-**Differences between primitive and nonprimitive unit cells, and indexing reflections.

Lecture-10: **Systematic absences in diffraction pattern-**

Lecture-11: **Structure Factor-**Its relation to intensity and electron density.

Lecture-12: **X-ray Structure Analysis-**Step-by-step procedure with typical examples.

Lecture-13: **Electron Diffraction-**Scattering Intensity vs. Scattering Angle: Analysis using the Wierl equation.

Lecture-14: **Instrumentation -** Measurement Technique, Description of the setup and process.

Lecture-15: **Structure Elucidation:** Determining structures of simple gas-phase molecules using electron diffraction, summary of the topic and assignment of questions and problems for submission.

PC- 16: Lasers in Chemistry (15 h)

Lecture-1: **Introduction of LASERs-** Introduction to LASERs, General Principles of Laser Action, stimulated Emission, rates of absorption and emission-governed by Einstein coefficients (A and B coefficients).

Lecture-2: **Population Inversion-**Lasing action

Lecture-3: **Laser Systems –** Lasing Action in Three-Level System, Four-Level System, examples.

Lecture-4: **Pumping and Laser Cavity-**Explanation of pumping action, working principle and importance of Laser cavity in Lasing Process.

Lecture-5: **Characteristics of Laser Light-**Coherence, Monochromaticity, Directionality

Lecture-6: **Laser Pulses-** Pulse length, Pulse interval, frequency, Q-Switching, Mode-Locking

Lecture-7: **Practical Lasers-**Types of Lasers, Solid-State Lasers: e.g., Ruby laser, Nd laser.

Lecture-8: **Gas Lasers-**He-Ne laser, CO_2 laser etc.. Chemical and Excimer Lasers: e.g., Excimer lasers for UV light.

Lecture-9: **Applications in Chemistry- Femtochemistry**: Study of chemical reactions on extremely short timescales.

Lecture-10: **Pump-Probe Technique-**Working principle, application in Femtochemistry

Lecture-11: **Time-Resolved Spectroscopy-** Principle, Studies the dynamics of chemical processes.

Lecture-12: **Applications of Femtochemistry -** Photodissociation of ICN, CO-Hemoglobin Complex: Formation and dissociation studied using lasers

Lecture-13: **Laser Induced Reactions-**Ethylene to Cyclobutane Conversion, Bond Selectivity: E.g., Reaction between H atoms and HDO molecules.

Lecture-14: **Multiphoton Spectroscopy**-Two-Photon Spectra: Example: Diphenyloctatetraene.

Lecture-15: **Applications of Lasers -** Fluorescence and Raman Spectroscopy: Lasers used for excitation and analysis, summary of the topic, give Assignment questions.

ELECTIVE 3A

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

PC(CB1)-1: **Applied Kinetics (15 h)**

Lecture-1: **Introduction to Reactor Design-**Overview of the basic objectives in the design of a chemical reactor, key parameters affecting reactor performance.

Lecture-2: **Balance Equations for Reactor Design-**Understanding balance equations for reactor design, application of balance equations in various reactor models.

Lecture-3: **Single Ideal Reactor Models-**Introduction to single ideal reactor models, Comparison of different ideal reactor models.

Lecture-4: **Batch Reactors (BR): General Features-** General features and characteristics of batch reactors, advantages and limitations of batch reactors.

Lecture-5: **Design Equations for Batch Reactors-**Development and application of design equations for batch reactors, case studies and practical applications, performing material and energy balances for batch reactors, examples of material and energy balance calculations.

Lecture-6: **Isothermal Operation and Constant-**Density Systems in BR, Design considerations for isothermal operation in batch reactors, analyzing constant-density systems in batch reactors.

Lecture-7: **Continuous Stirred-Tank Reactors (CSTR):** General Features, General features and operational principles of CSTRs, comparison with other reactor types, developing and applying design equations for CSTRs, case studies and practical applications.

Lecture-8: **Material and Energy Balances in CSTR-**Performing material and energy balances for CSTRs, examples of material and energy balance calculations, Design considerations for steady-state operation in CSTRs, analysis of constant-density systems in CSTRs.

Lecture-9: **Damkohler Number and Numerical Problems in CSTR-**Understanding the Damkohler number and its significance, solving numerical problems involving the Damkohler number.

Lecture-10: **Plug-Flow Reactors (PFR)-**General Features, General features and characteristics of plug-flow reactors, comparison with other reactor types, Developing and applying design equations for PFRs.

Lecture-11: **Material and Energy Balances in PFR-**Performing material and energy balances for PFRs, examples of material and energy balance calculations.

Lecture-12: **Comparisons of Ideal Reactors for a Single Reaction-** Comparative analysis of different ideal reactors for a single reaction, understanding the performance metrics of each reactor type.

Lecture-13: **Single-Vessel Comparisons: BR and CSTR-**Comparative study of batch reactors and CSTRs, analyzing the advantages and limitations of each.

Lecture-14: **Single-Vessel Comparisons: BR and PFR-**Comparative study of batch reactors a nd plug-flow reactors, analyzing the advantages and limitations of each.

Lecture-15: **Numerical Examples of Reactor Comparisons-**Solving numerical examples Involving comparisons of different reactors, practical applications, summarizing the topic, assignment questions.

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

Lecture-1: **Battery Parameters-**Introduction to key battery parameters, Definitions and significance of energy density and power density.

Lecture-2: **Ragone Plot-**Understanding the Ragone plot and its implications, How to use the Ragone plot to compare battery performance.

Lecture-3: **Measures of Battery Performance-**Key performance measures: capacity, efficiency, and cycle life. Factors affecting battery performance.

Lecture-4: **Primary and Secondary Batteries-**Differences between primary and secondary batteries, examples and applications of each type.

Lecture-5: **Zn/MnO_2, Lead-Acid, and Ni-Cd Batteries-**Overview of Zn/MnO2 batteries: construction, chemistry, and uses, detailed study of lead-acid and Ni-Cd batteries: operation, advantages, and limitations.

Lecture-6: **Lithium Cells and Batteries-**Introduction to lithium cells: chemistry and types, Focus on lithium-thionyl chloride cells and lithium-ion batteries.

Lecture-7: **Fuel Cells: General Chemistry-**Basic chemistry of fuel cells, Electrochemical reactions and principles of operation.

Lecture-8: **Types of Fuel Cells-**H_2/O_2 fuel cells: design, operation, and applications, Methanol/O_2 fuel cells: design, operation, and applications.

Lecture-9: **Factors influencing the efficiency of fuel cells-**Porous Electrodes in Fuel Cells, role and advantages of using porous electrodes in fuel cells, impact on efficiency and performance, detailed analysis of the benefits and challenges of fuel cells, factors influencing the efficiency of fuel cells.

Lecture-10: **Photovoltaic Cells-**Semiconductor-Based Photoelectrochemical Cells-Introduction to semiconductor-based photovoltaic cells, mechanisms of converting solar energy into electrochemical energy.

Lecture-11: **Electrochemical Energy from Solar Energy-**Principles of electrochemical energy generation from solar energy, applications and future prospects of solar energy in electrochemistry.

Lecture-12: **Anodic Oxidation of Metals-**Process and principles of anodic oxidation, characteristics and formation of anodic oxide films, various industrial uses of anodic oxide films, benefits and examples of applications in different industries.

Lecture-13: **Electroplating: Technical Importance and Mechanism-**Importance and technical aspects of electroplating, mechanism of electroplating, including alkaline and acid plating of copper and nickel.

Lecture-14: **Electro-Organic Synthesis-**Introduction to electro-organic synthesis and its importance, detailed examples: reduction of carboxylic acids and polymerization of acrylonitrile to adiponitrile for nylon synthesis.

Lecture-15: **Reduction of Nitro Compounds-**Process and principles of reducing nitro compounds in electro-organic synthesis, industrial applications and significance of these reductions, summary of the topic, Assignments.

PC(CB1)-3: Types of materials, conducting organics and NLO materials (15 h)

Lecture-1: **Classification of Materials**-Introduction to the classification of materials, overview of metals: properties, applications, and examples.

Lecture-2: **Ceramics**-Introduction to ceramics: properties, applications, and examples, criteria for determining the crystal structure of ceramic materials, examples of ceramic materials and their crystal structures, numerical problems.

Lecture-3: **Polymers**-Introduction to polymers: properties, applications, and examples, different types of polymers and their uses.

Lecture-4: **Composites**-Introduction to composites: definition and types, particle reinforced composites: properties and applications, Fibre reinforced composites: properties and applications.

Lecture-5: **Semiconductors & Biomaterials**-Introduction to semiconductors: properties, applications, and examples, Role of semiconductors in electronic devices, introduction to biomaterials: definition, properties, and applications, examples of biomaterials and their use in medical applications.

Lecture-6: **Glassy State**-Understanding the glassy state and its characteristics, glass transition temperature, glass formers and glass modifiers, examples, applications of glassy materials.

Lecture-7: **Preparative Methods of Solid Materials**-Ceramic method (Solid State method): principles and process.

Lecture-8: Co-precipitation-Co-precipitation method for synthesis of solids, steps involved, various parameters that effect the characteristics of resulting solid formed in co-precipitation.

Lecture-9: **Solution and Gel Methods**-Solution methods and gels for material preparation, Zeolite synthesis: principles and applications.

Lecture-10: **Vapour Phase Transport Method**-Principles and applications of vapour phase transport method, Modification of existing structures by ion-exchange and interaction reactions.

Lecture-11: **Techniques of Single Crystal Growth**-Growth from solutions: principles and techniques, Growth from melts: principles and techniques, Growth from vapour: principles and techniques.

Lecture-12: **Crystallization from Melts**-Czochralski method for crystal growth, Kyropolous method for crystal growth.

Lecture-13: **Non-Linear Optical (NLO) Behavior**-Basic concepts of non-linear optical behavior, second and third harmonic generation.

Lecture-14: **Examples of NLO Materials-**Organic NLO materials: properties and applications, Inorganic NLO materials: properties and applications, Polymer NLO materials: properties and applications.

Lecture-15: **Conducting Organics-**Introduction to conducting organics: properties and examples, Fullerenes and their role in conducting organics, Alkali metal-doped fullerides and fullerenes as superconductors, summary of the topic, Assignments allotment.

PC(CB1)-4: Radiation effects (15 h)

Lecture-1: **Introduction to Radiation Hazards-**Overview of radiation hazards, Types of high-energy radiation and high-energy particles, Sources of radiation and their impacts.

Lecture-2: **Radiation Effects on Biological Systems-**Biological effects of radiation exposure, Acute and chronic effects on human health, Radiation sickness and long-term health risks.

Lecture-3: **Radiation Protecting Materials-** Materials used for radiation protection, Mechanisms of radiation shielding, Examples and applications of radiation shielding materials.

Lecture-4: **Radiation Chemistry of Liquid Water-**Radiation interaction with liquid water, Formation of reactive species in water, Chemical yields and their significance.

Lecture-5: **Dosimetry: Measurement of Radiation-**Introduction to dosimetry and its importance, Types of dosimeters and their applications, Principles and uses of the Fricke dosimeter.

Lecture-6: **Thiocyanate Dosimeter-**Detailed study of the thiocyanate dosimeter, Mechanism and applications, Comparison with other dosimetry methods.

Lecture-7: **Effect of Radiation on DNA-**Direct effects of radiation on DNA, Indirect effects via reactive species, Mechanisms of DNA damage by radiation.

Lecture-8: **Reaction of OH Radicals with DNA Constituents-**Interaction of OH radicals with DNA, Specific reactions and resulting damage, Role of OH radicals in strand break formation.

Lecture-9: **General Mechanism of Strand Break Formation-**Mechanisms of strand breaks in DNA, Role of radiation-induced reactive species, Biological consequences of DNA strand breaks.

Lecture-10: **Radioactive Waste Management-**Introduction to radioactive waste management, Classification of radioactive waste, Principles and methods of radioactive waste treatment.

Lecture-11: **Radioactive Waste Disposal**-Techniques for radioactive waste disposal, Safety measures and regulations, Long-term storage and environmental impact.

Lecture-12: **Applications of Radioisotopes in Nuclear Medicine**-General applications of radioisotopes in medicine, Use of radiopharmaceuticals in diagnostics and treatment, Safety considerations in medical applications.

Lecture-13: **In Vivo Diagnostic Procedures**-Principles of in vivo diagnostic testing with radioisotopes, Common diagnostic procedures and their applications, Advantages and limitations.

Lecture-14: **In Vitro Diagnostic Testing**-Use of radioisotopes in in vitro diagnostics, Techniques and applications in laboratory testing, Comparison with other diagnostic methods.

Lecture-15: **Therapeutic Use of Radiations and Other Applications**-Therapeutic applications of radiation in medicine, Use of radiation for food preservation and sterilization, Benefits and safety measures in these applications.

ELECTIVE 4A

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

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

Lecture-1: **Introduction**-Introduction to polymers and classification of polymers based on origin, structure and method of polymerization, examples.

Lecture-2: **Types of Polymerization**-Addition Polymerization, examples

Lecture-3: **Other type of polymerization**-Condensation Polymerization, examples

Lecture-4: **Free Radical Polymerization**-Kinetics and Mechanism

Lecture-5: **Degree of Polymerization**-Kinetic Chain Length and Chain Transfer Coefficient, Trommsdorff Effect.

Lecture-6: **Effect of Pressure and Temperature**-Effect of T & P on polymerization kinetics.

Lecture-7: **Other Polymerization** - Kinetics and mechanism of cationic, anionic polymerization

Lecture-8: **More types of polymerization**- Kinetics and mechanism of coordination polymerization, linear stepwise polymerization.

Lecture-9: **Copolymerization**-copolymer composition, reactivity ratios and their determination

Lecture-10: **Copolymer composition**-Alfrey and Price Q-e scheme for monomer and radical reactivity

Lecture-11: **Co-polymers**-Block and graft copolymers.

Lecture-12: **Polymerization in various systems**- Polymerization in homogeneous and heterogeneous systems

Lecture-13: **Techniques of Polymerization**-Details of Bulk & solution polymerization

Lecture-14: **Other Polymerization Techniques**-Description of suspension and emulsion polymerizations

Lecture-15: **Summary, Q&A**-Summarize the topic, clarifications, giving assignment questions & Problems.

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

Lecture-1: **The Process of Polymer Dissolution**-Introduction to polymer dissolution, Steps involved in the dissolution process, Factors affecting polymer dissolution.

Lecture-2: **Thermodynamics of Polymer Dissolution**-Basic thermodynamic principles, Entropy, heat, and free energy of mixing, Application to polymer solutions.

Lecture-3: **Conformations of Dissolved Polymer Chains**-Introduction to polymer chain conformations, the freely jointed chain model, examples of short-range and long-range interactions.

Lecture-4: **The Flory-Huggins Theory of Polymer Solutions**-Introduction to the Flory-Huggins theory, mathematical formulation and assumptions, significance and applications of the theory.

Lecture-5: **Dilute Polymer Solutions and Flory-Krigbaum Theory**-Properties of dilute polymer solutions, Overview of the Flory-Krigbaum theory, Comparison with the Flory-Huggins theory.

Lecture-6: **Mechanical Properties of Polymers**:**The Elastic State**- Introduction to the elastic state of polymers, rubber-like elasticity, examples and applications in materials science.

Lecture-7: **Viscoelasticity in Polymers**-Definition and significance of viscoelasticity, Newtonian and non-Newtonian behaviour, Real-world examples and applications.

Lecture-8: **Models of Viscoelastic Behaviour**-Introduction to the Maxwell model, Introduction to the Voigt-Kelvin model, Comparison and applications of both models.

Lecture-9: **Crystal Structure of Polymers**-Overview of polymer crystal structures, Morphology of crystalline polymers, Techniques for studying polymer crystallinity.

Lecture-10: **Crystallization and Melting of Polymers**-Process of polymer crystallization, Factors influencing crystallization, Determination of the melting temperature (T_m).

Lecture-11: **Thermodynamics of Crystalline Melting**-Basic thermodynamic principles of melting, Heats and entropies of fusion, Degree of crystallinity and its significance.

Lecture-12: **Factors Affecting Crystallization in Polymers**-Internal and external factors affecting crystallization, Influence of polymer structure and processing conditions, Examples and case studies.

Lecture-13: **The Glassy State and Glass Transition Temperature (T_g)-**Definition and significance of the glassy state, Factors influencing T_g, Relationship between Tg and melting point.

Lecture-14: **Measurement of Molecular Weights**-Techniques for measuring molecular weights, End group analysis and osmometry, Gel permeation chromatography (GPC) and its applications.

Lecture-15: **Molecular Weight Distribution in Polymers**-Importance of molecular weight distribution, Methods for analyzing molecular weight distribution, Applications in polymer science and industry.

PC(CB3)-11: Processing of Polymers (15 h)

Lecture-1: **General Applications of Polymers-**Overview of the diverse applications of polymers in various industries, Key properties that make polymers versatile.

Lecture-2: **Fillers in Polymers**-Role and types of fillers used in polymer formulations**,**

Lecture-3: **Plasticizers in Polymers**-Function and examples of plasticizers enhancing polymer flexibility.

Lecture-4: **Lubricants in Polymers-**Importance and types of lubricants in polymer processing.

Lecture-5: **Catalysts in Polymerization-**Types and roles of catalysts in polymerization processes.

Lecture-6: **Stabilizers in Polymers-**Different stabilizers and their significance in polymer longevity.

Lecture-7: **Colorants in Polymers-**Use of colorants to modify the appearance and properties of polymers.

Lecture-8: **Antioxidants & Flame Retardants in Polymers-**Mechanisms and types of antioxidants protecting polymers from degradation, Importance and examples of flame retardants enhancing polymer safety.

Lecture-9: **One-Dimensional Coating Techniques-**Techniques and applications of adhesives and lamination in polymers.

Lecture-10: **Extrusion, Calendering, and Thermoforming-**Processes and benefits of extrusion, calendering, and thermoforming.

Lecture-11: **Compression and Injection Molding-**Detailed processes, advantages, and limitations of compression and injection molding.

Lecture-12: **Extrusion and Blow Molding-**Overview of extrusion and blow molding processes and their applications.

Lecture-13: **Casting Techniques-**Different casting techniques including vacuum casting, potting, and encapsulation.

Lecture-14: **Fibre Reinforced Plastics and Synthetic Fibres-**Preparation and properties of fiber reinforced plastics and synthetic fibers like rayons, nylons, and Dacron.

Lecture-15: **Processing of Fiber Reinforced Composites-**Introduction to pultrusion technique, prepreg production, and filament winding, summary, assignments.

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

Lecture-1: **Introduction to Smart Materials-**Overview of smart materials and their characteristics.

Lecture-2: **Uses of Smart Materials in Sensing Devices-**Applications of smart materials in various sensing devices.

Lecture-3: **Smart Materials in Communication Networks-**Role and benefits of smart materials in communication networks.

Lecture-4: **Electrically Conducting Polymers: Introduction and Principles-**Introduction to electrically conducting polymers and their basic principles**.,** Diverse applications of electrically conducting polymers in industry.

Lecture-5: **Specific Conducting Polymers: Polyanilines and Polypyrrole-**Overview and applications of polyanilines and polypyrrole.

Lecture-6: **Specific Conducting Polymers: Polyacetylene and Polythiophene-**Overview and applications of polyacetylene and polythiophene.

Lecture-7: **Photoconductive Polymers-**Properties and applications of photoconductive polymers.

Lecture-8: **Liquid Crystal Polymers:Smectic, Nematic, and Cholesteric Structures-** Structures and properties of smectic, nematic, and cholesteric liquid crystal polymers.

Lecture-9: **Ionic Exchange Polymers: Cationic and Anionic-** Introduction and uses of cationic and anionic exchange polymers.

Lecture 10: **Biodegradable Polymers:** Definition, Classification, and and various applications of biodegradable polymers

Lecture 11: **Specific Biodegradable Polymers: Polyhydroxyalkanoates and Polycaprolactone-** Detailed description of polyhydroxyalkanoates and polycaprolactone, Detailed description of polyacetic acid and polyvinylalcohol

Lecture 12: **Polymers in Membrane Separation: Filtration Techniques &Separation of Gases -**Applications of polymers in micro, ultra, and nanofiltration techniques, Permeselectivity and gas permeability of representative polymers.

Lecture 13: **Liquid Separation Techniques**: Dialysis, Electro-Osmosis, and Reverse Osmosis,

Lecture -14: **Fire Retarding Polymers-**Properties and applications of fire-retarding polymers.

Lectur-15: **Photonic Polymers & Polymers in Biomedical Applications-** Overview and applications of photonic polymers, Use of polymers in artificial organs and controlled drug delivery systems.

M.Sc (Physical Chemistry): Semester-IV (2017-18)

Teaching Plans

1. **PAPER–I CH(PC) 401T: THERMODYNAMICS, CHEMICAL KINETICS AND ELECTROCHEMISTRY**
2. **PAPER – II CH (PC) 402T: SUPRAMOLECULAR CHEMISTRY, PHOTO CHEMISTRY AND COMPUTATIONAL CHEMISTRY**
3. **PAPER III-ELECTIVE 3A-CH(PC) 403T(CB1): CATALYSIS**
4. **PAPER-IV-ELECTIVE–4A-CH(PC) 404T(CB3): COMPUTATIONAL CHEMISTRY AND IT'S APPLICATIONS**

PAPER-I CH(PC) 401T(CB1): THERMODYNAMICS, CHEMICAL KINETICS AND ELECTROCHEMISTRY

PC- 17: Statistical Thermodynamics (15 h)

Lecture-1: **Introduction to Distribution and Probability**-Basic concepts of distribution and probability.

Lecture-2: **Estimation of Probability**-Methods for estimating probability and the concept of the most probable distribution.

Lecture-3: **Systems Composed of Non-Interacting Particles & Interacting Particles** - Analysis of systems with non-interacting particles, Characteristics and analysis of systems with interacting particles.

Lecture-4: **Boltzmann Distribution Law**-Derivation and significance of the Boltzmann distribution law.

Lecture-5: **Molecular Partition Function-**Introduction to the molecular partition function and its importance.

Lecture-6: **Concept of Ensemble and Canonical Ensemble & Canonical Partition Function-**Definition and importance of ensembles, with a focus on the canonical ensemble, Relationship between canonical partition function and molecular partition function.

Lecture-7: **Factorization of Molecular Partition Function-**Breaking down the molecular partition function into translational, rotational, vibrational, and electronic components, Derivation and applications of the translational partition function.

Lecture-8: **Rotational and Vibrational Partition Functions-** Derivation of rotational (diatomic) and vibrational partition functions.

Lecture-9: **Partition Functions and Thermodynamic Functions-** Relationship between partition functions and thermodynamic functions.

Lecture-10: **Law of Equipartition Energy-** Explanation and implications of the law of equipartition energy.

Lecture-11: **Specific Heats of Solids-** Einstein equation of heat capacity of solids and its derivation.

Lecture-12: **Explanation of heat capacity at very low and very high temperatures-** Dulong and Petit's Law, Debye theory, Heat Capacity at Different Temperatures

Lecture-13: **Entropy of a Monoatomic Ideal Gas-** Understanding and deriving the entropy of a monoatomic ideal gas. Sackur-Tetrode Equation- Derivation and significance of the Sackur-Tetrode equation.

Lecture-14: **Mean Translational and Vibrational Energies-** Calculation and significance of mean translational and vibrational energies, Equilibrium Constant and Partition Function-Derivation of the relationship between equilibrium constant and partition function.

Lecture-15: **Introduction to Bose-Einstein Statistics & Fermi-Dirac Statistic**s **-** Basic concepts and applications of Bose-Einstein statistics, Basic concepts and applications of Fermi-Dirac statistics. Comparison with Maxwell-Boltzmann Statistics, Comparing Bose-Einstein, Fermi-Dirac, and Maxwell-Boltzmann statistics.

PC- 18: Non-equilibrium Thermodynamics (15 h)

Lecture-1: **Thermodynamic Criteria for Non-Equilibrium States-**Introduction to thermodynamic criteria for identifying non-equilibrium states.

Lecture-2: **Entropy Production in Irreversible Processes-**Concept and calculation of entropy production in irreversible processes.

Lecture-3: **Entropy Production in Heat Flow-**Detailed analysis of entropy production in heat flow.

Lecture- 4: **Entropy Production in Material Flow-**Examination of entropy production in material flow.

Lecture-5: **Fluxes and Forces in Irreversible Processes-**Introduction to fluxes and forces in thermodynamics.

Lecture-6: **Linear Flux-Force Relations-**Understanding linear relations between fluxes and forces.

Lecture-7: **Phenomenological Equations and Coefficients-**Formulation and significance of phenomenological equations and coefficients.

Lecture-8: **Microscopic Reversibility and Onsager Reciprocal Relations-**Concepts of microscopic reversibility and Onsager reciprocal relations.

Lecture-9: **Application of Onsager Relations to Electrokinetic Phenomena-**Applying Onsager relations to electroosmotic pressure and streaming current.

Lecture-10: **Onsager Relations and Detailed Balance-**Principle of detailed balance in the context of Onsager relations.

Lecture-11: **Liquid Junction Potentials-**Derivation of equation for liquid junction potential using transport numbers and Onsager relations.

Lecture-12: **Steady States in Thermodynamics-**Concept and analysis of steady states in thermodynamic systems.

Lecture-13: **Principle of Minimum Entropy Production-**Explanation and applications of the principle of minimum entropy production.

Lecture-14: **Irreversible Thermodynamics in Biological Systems-**Examples and applications of irreversible thermodynamics in biological systems.

Lecture 15: **Application to Thermoelectric Circuits-**Thermoelectric effects, including the Seebeck and Peltier effects, and their applications.

PC- 19: Chemical Kinetics-II (15 h)

Lecture-1: **Factors Affecting Reaction Rates in Solution-**Overview of factors influencing reaction rates in solution.

Lecture-2: **Effect of Pressure on Rate of Reaction-**Examination of how pressure impacts reaction rates.

Lecture-3: **Diffusion Controlled Reactions-**Understanding diffusion-controlled reactions and their characteristics.

Lecture-4: **Influence of Dielectric Constant and Ionic Strength-**Effect of dielectric constant and ionic strength on ion-ion, ion-dipole, and dipole-dipole reactions.

Lecture- 5: **Primary and Secondary Salt Effects-**Detailed analysis of primary and secondary salt effects on reaction rates.

Lecture-6: **Kinetic Isotope Effects: Primary and Secondary-**Exploration of primary and secondary kinetic isotope effects.

Lecture-7: **Solvent Isotope Effects-**Discussion on the impact of solvent isotope effects on reaction kinetics.

Lecture-8: **Fast Reactions: Flow Methods and Stopped-Flow Technique**-Introduction to flow methods and the stopped-flow technique for studying fast reactions, Fluorescence Technique and Shock Tube Method-Application of the fluorescence technique and shock tube method in fast reaction studies.

Lecture-9: **Relaxation Methods: T-jump and P-jump-**Understanding T-jump and P-jump relaxation methods, **Kinetic Equations for Chemical Relaxation-**Derivation and application of kinetic equations for chemical relaxation

Lecture-10: **Enzyme Kinetics: Michaelis-Menten Mechanism-**Introduction to Michaelis-Menten mechanisms for enzyme-catalyzed reactions involving one intermediate.

Lecture-11: . **Michaelis-Menten Mechanism with Two Intermediates-**Detailed study of Michaelis-Menten mechanisms for reactions with two intermediates.

Lecture-12: **Steady-State Approximation and Kinetic Equations-**Application of the steady-state approximation and derivation of kinetic equations, methods for evaluating kinetic parameters in enzyme kinetics.

Lecture-13: **Enzyme-Substrate Complex: Fischer's Lock and Key Hypothesis-**Explanation of Fischer's lock and key hypothesis for enzyme-substrate interaction. Koshland's Induced Fit Hypothesis-Discussion of Koshland's induced fit hypothesis and its implications

Lecture-14: **Specificity of Enzyme-Catalyzed Reactions-**Factors determining the specificity of enzyme-catalyzed reactions, Forces Involved in Enzyme-Substrate Complex Formation-Various types of forces involved in the formation of enzyme-substrate complexes

Lecture-15: pH Dependence of Enzyme-Catalyzed Reactions-Kinetics and equations related to the pH dependence of enzyme-catalyzed reactions, Summary, Assignments.

PC- 20: **Electrochemistry –II (15 h)**

Lecture-1: **The Electrical Double Layer-**Introduction to the electrical double layer at the electrode-electrolyte interface.

Lecture-2: **Helmholtz-Perrin Parallel-Plate Model-**Detailed explanation of the Helmholtz-Perrin parallel-plate model.

Lecture-3: **Gouy-Chapman Diffuse-Charge Model-**Understanding the Gouy-Chapman diffuse-charge model and its implications.

Lecture-4: **Stern Model-**Analysis of the Stern model combining Helmholtz and Gouy-Chapman models.

Lecture-5: **Quantum Aspects of Charge Transfer-**Quantum aspects of charge transfer at the electrode-electrolyte interface, including tunneling.

Lecture-6: **Charge Transfer Reactions at the Interface-**Examination of charge transfer reactions at the electrode-electrolyte interface.

Lecture-7: **Exchange Current Density and Overpotential-**Introduction to exchange current density and overpotential.

Lecture- 8: **Derivation of the Butler-Volmer Equation-**Detailed derivation of the Butler-Volmer equation for electrode kinetics.

Lecture- 9: **High Field Approximation and Tafel Equation-**Understanding high field approximation and the derivation of the Tafel equation.

Lecture-10: **Equilibrium and Nernst Equation-**Analysis of equilibrium conditions and derivation of the Nernst equation.

Lecture-11: **Symmetry Factor and Its Significance-**Explanation of the symmetry factor in electrochemical reactions and its importance.

Lecture-12: **Electrochemical Corrosion-**Introduction to electrochemical corrosion processes and short-circuited energy producing cells.

Lecture-13: **Corrosion Current and Corrosion Potential-**Definition and derivation of corrosion current and corrosion potential.

Lecture-14: **Evans Diagrams and Pourbaix Diagrams-**Analysis and interpretation of Evans diagrams and Pourbaix diagrams for iron.

Lecture-15: **Corrosion Protection and Inhibition-**Techniques for protecting against corrosion and inhibition using organic molecules, Summary, Assignments.

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

PC-21: **Supramolecular Chemistry (15 h)**

Lecture-1: **Concepts of Molecules, Supermolecules, and Supramolecules-**Introduction to molecules, supermolecules, and supramolecules.

Lecture-2: **Nature of Supramolecular Interactions-**Overview of the types and nature of supramolecular interactions.

Lecture-3: **Molecular Recognition – Factors Involved-**Key factors involved in molecular recognition processes.

Lecture-4: **Ionophores-**Understanding ionophores and their role in molecular recognition.

Lecture-5: **Molecular Receptors – Design Principles-**Principles for designing molecular receptors.

Lecture-6: **Molecular Receptors for Alkali Metal Ions-**Design and function of molecular receptors for alkali metal ions.

Lecture-7: **Molecular Receptors for Ammonium Ions, Anions, and Neutral Molecules-**Specific receptors for ammonium ions, anions, and neutral molecules.

Lecture-8: **Crown Ethers, Cryptands, Spherands-**Overview and selectivity of crown ethers, cryptands, and spherands.

Lecture-9: **Calixarenes and Cyclodextrins-**Structure, function, and selectivity of calixarenes and cyclodextrins.

Lecture-10: **Fullerenes as Supramolecules-**Examination of fullerenes as supramolecular entities.

Lecture-11: **Rotaxanes and Catenanes-**Creation and significance of rotaxanes and catenanes.

Lecture-12: **Thermodynamics of Host-Guest Complexation-**Thermodynamic principles of host-guest complexation.

Lecture-13: **Enthalpy and Entropy Contributions-**Analysis of enthalpy and entropy contributions in complexation.

Lecture-14: **Supramolecular Catalysis-**Role of crownether-supported alkaline earth metal ions, cyclodextrins, and calixarenes as catalysts.

Lecture-15: **Molecular Electronic Devices-**Introduction to molecular wires, molecular switches, and molecular machines Summary, Assignments

PC-22: **Photochemistry-II (15 h)**

Lecture-1: **Formation of Excimers and Exciplexes-**Understanding the formation of excimers and exciplexes, PE diagram, and quantum yields.

Lecture-2: **Energy Transfer Mechanism for Bimolecular Quenching-**Detailed analysis of energy transfer mechanisms involved in bimolecular quenching.

Lecture-3: **Long-Range Coulombic Energy Transfer-**Explanation of long-range Coulombic energy transfer and critical transfer distance.

Lecture-4: **Short-Range Electron Exchange Energy Transfer-**Mechanisms and principles of short-range electron exchange energy transfer.

Lecture-5: **Triplet-Triplet Energy Transfer and Sensitization-**Understanding triplet-triplet energy transfer and sensitization processes.

Lecture-6: **P-Type Delayed Fluorescence-**Exploring the concept and mechanisms of P-type delayed fluorescence.

Lecture-7: **Experimental Study of Photochemical Reactions**-Overview of experimental techniques used to study photochemical reactions.

Lecture-8: **Product Analysis in Photochemical Reactions**-Methods and importance of product analysis in photochemical studies.

Lecture-9: **Chemical Methods in the Study of Intermediates**-Chemical techniques used to identify and study reaction intermediates.

Lecture-10: **Spectroscopic Methods in Photochemical Studies**-Application of various spectroscopic methods in studying photochemical reactions.

Lecture-11: **ESR and CIDNP in Photochemical Studies**-Use of ESR (Electron Spin Resonance) and CIDNP (Chemically Induced Dynamic Nuclear Polarization) in photochemistry.

Lecture-12: **Rate Coefficients for Photochemical Processes**-Determination and significance of rate coefficients in photochemical reactions.

Lecture-13: **Identification of Excited States**-Techniques for identifying excited states in photochemical processes.

Lecture-14: **Electronic Transitions in Transition Metal Complexes**-Understanding electronic transitions in transition metal complexes, Analysis of ligand field (LF) and charge transfer (CT) electronic states.

Lecture-15: **$Ru(bpy)_3^{2+}$ as Sensitizer for Photoredox Reactions**- Study of Ru(bpy)32+ complex as a sensitizer in photoredox reactions, with examples, Mechanisms and significance of photochemical cleavage of water, Summary, Assignments.

PC-23: Computational Chemistry (15 h)

Lecture-1: **Introduction to Multi-Electron Atoms**-Overview of the complexity and challenges in studying multi-electron atoms compared to single-electron atoms.

Lecture-2: **The Antisymmetry Principle and Slater Determinant**-Explanation of the antisymmetry principle and construction of the Slater determinant.

Lecture-3: **The Hartree-Fock Method**-Introduction and significance of the Hartree-Fock method in quantum chemistry.

Lecture-4: **The Hartree-Fock Equations and Fock Operator**-Presentation of the Hartree-Fock equations (no derivation) and explanation of the Fock operator.

Lecture-5: **Core Hamiltonian, Coulomb, and Exchange Operators**-Detailed analysis of the core Hamiltonian, Coulomb operator, and exchange operator.

Lecture-6: **Slater-Type Orbitals (STOs) as Basis Functions-**Discussion on the use and importance of Slater-type orbitals (STOs) as basis functions.

Lecture-7: **Orbital Energies, Total Energy, and Koopman's Theorem-**Understanding orbital energies, total energy in Hartree-Fock, and Koopman's theorem with a helium atom example.

Lecture-8: **Hund's Rules and Aufbau Principle-**Explanation of Hund's rules and the theoretical basis of the Aufbau principle.

Lecture-9: **Electron Correlation Energy-**Introduction to electron correlation energy and its importance in accurate quantum chemical calculations.

Lecture-10: **Hartree-Fock Method for Molecules-**Application of the Hartree-Fock method to molecules, including restricted and unrestricted HF calculations.

Lecture-11: **The Roothan Equations and Fock Matrix-**Explanation of the Roothan equations and the construction and significance of the Fock matrix.

Lecture-12: **Basis Sets: Minimal and GTOs-**Discussion of different types of basis sets, including minimal basis sets and Gaussian-type orbitals (GTOs).

Lecture-13: **Model HF Calculations on H_2 and Simple Molecules-**Performing and discussing Hartree-Fock calculations on H_2 and simple molecules like H_2O and NH_3.

Lecture-14: **Introduction to Configuration Interaction-**Overview of configuration interaction and its role in improving Hartree-Fock results.

Lecture-15: **Density Functional Theory (DFT) and Kohn-Sham Equations-**Introduction to DFT, the Hohenberg-Kohn theorem, Kohn-Sham (KS) formulation, KS equations, and exchange-correlation energy and potential, Summary, Allotment of Assignment questions.

PC-24: **Theoretical treatment of bio polymers (15 h)**

Lecture-1: **Types of Biopolymers-**Overview of different types of biopolymers.

Lecture-2: **Methods of Determining Size and Shape: Mean Molecular Masses-**Techniques to determine mean molecular masses of biopolymers.

Lecture-3: **Colligative Properties and Sedimentation-**Use of colligative properties and sedimentation methods for biopolymer analysis.

Lecture-4: **Viscosity and Light Scattering Methods-**Analysis of biopolymer size and shape using viscosity and light scattering methods.

Lecture-5: **Chain Conformation and Configuration of Polypeptides-**Understanding the chain conformation and configuration of polypeptides.

Lecture-6: **Random Coils and Measures of Size-**Measures of size in random coils: contour length, rms separation, radius of gyration, constrained chains.

Lecture-7: **Secondary Structures of Proteins: Helices and Sheets-**Introduction to the secondary structures of proteins, including helices and sheets.

Lecture 8: **Corey-Pauling Rules-**Explanation and significance of the Corey-Pauling rules for protein structures.

Lecture-9: **Conformational Energy of a Polypeptide: Bonding and Nonbonding Potentials-**Analysis of bonding and nonbonding potentials in polypeptide conformational energy.

Lecture-10: **Electrostatic Interactions and Dipole-Dipole Interactions-**Role of electrostatic and dipole-dipole interactions in polypeptide conformational energy.

Lecture-11: **van der Waals Interactions and Hydrogen Bonds-**Understanding van der Waals interactions and hydrogen bonds in protein structure.

Lecture-12: **Molecular Mechanics for Polypeptide Potential Energy-**Principles of molecular mechanics to calculate the potential energy of a polypeptide.

Lecture-13: **Ramachandran Plots of α-Helix and β-Sheet-**Use and interpretation of Ramachandran plots for α-helix and β-sheet structures.

Lecture-14: **Conformational Entropy-**Introduction to conformational entropy in protein folding.

Lecture -15: **Protein Folding Problem-**Overview and introductory treatment of the protein folding problem, summary, Assignments.

ELECTIVE –3A:

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

PC(CB1)-17: Homogeneous catalysis (15 h)

Lecture-1: **Introduction to Catalysis-**Definition and Importance: Catalysis accelerates chemical reactions, vital for industrial, environmental, and biological processes.

Lecture-2: **Types of Catalysis-**Types of Catalysis: Homogeneous (same phase), Heterogeneous (different phase), and Enzyme (biological).

Lecture- 3: **Characteristics of Catalysts-**Characteristics of Catalysts: Activity, selectivity, stability, reusability, and specificity.

Lecture-4: **Catalyst Supports-**Catalyst Supports: Increase surface area and active site dispersion (e.g., silica, alumina).

Lecture-5: **Promoters-**Promoters: Enhance catalyst performance (e.g., potassium in ammonia synthesis).

Lecture-6: **General Mechanism of Catalysis-**General Mechanism: Adsorption, reaction, desorption; lowers activation energy.

Lecture-7: **Equilibrium Treatment-**Equilibrium Treatment: Catalysts speed up reaching equilibrium without changing its position.

Lecture-8: **Steady State Treatment-**Steady State: Approximation for analyzing catalytic cycles and reaction rates.

Lecture-9: **Activation Energies-**Activation Energies: Comparison between catalyzed and non-catalyzed reactions.

Lecture-10: **Acid-Base Catalysis-**Acid-Base Catalysis: Specific vs. general, involving proton transfer.

Lecture-11: **Mechanism of Acid-Base Catalysis-**Mechanism of Acid-Base Catalysis: Role of conjugate acid-base pairs in catalysis.

Lecture-12: **Bronsted Relationships-**Bronsted Relationships: Correlation between catalytic activity and acid/base strength.

Lecture-13: **Acidity Functions-**Acidity Functions: Hammett function (H_o), its measurement, and application.

Lecture-14: **Zucker-Hammett Hypothesis and Bunnett-Olson Criteria-**Zucker-Hammett Hypothesis: Describes acid-base catalysis, complemented by Bunnett-Olson criteria.

Lecture-15: **Transition Metal Catalysis-**Transition Metal Catalysis: Role in reactions like hydrogenation, oxidation, isomerization. Use of Ziegler-Natta/metallocene catalysts for olefin polymerization and asymmetric catalysis (e.g., L-Menthol, epoxidation), Summary of the topic & giving Assignments.

PC-(CB1)-18: Surface Chemistry and Micellar catalysis (15 h)

Lecture-1: **Surface Tension and Curved Interfaces-**Surface Tension: Definition, significance, and applications, Curved Interfaces: Impact on pressure differences and stability.

Lecture-2: **The Laplace Equation and Capillary Action-**The Laplace Equation: Derivation and applications, Capillary Action: Mechanism, examples, and practical implications.

Lecture-3: **Thermodynamics of Surface Layers-**Gibbs Isotherm: Thermodynamics of surface layers and Gibbs adsorption isotherm.

Lecture-4: **Adsorption Basics-**Adsorption: Types, factors affecting adsorption, and basic principles.

Lecture-5: **Chemistry and Thermodynamics of Adsorption-**Chemistry and Thermodynamics: Understanding adsorption processes.

Lecture-6: **Heats and Entropies of Adsorption-**Determination: Methods for measuring heats and entropies of adsorption.

Lecture-7: **Surface versus Bulk Structures-**Comparison: Structural differences and implications on properties.

Lecture-8: **Adsorbate-Induced Restructuring-**Restructuring: How adsorbates alter surface structures.

Lecture-9: **Thermal Activation on Surfaces-**Bond Breaking: Thermal activation mechanisms on surfaces.

Lecture-10: **Co-Adsorption and Chemisorption Isotherms-**Co-Adsorption: Interaction of multiple adsorbates, Chemisorption Isotherms: Models and applications, Kinetics: Reaction rates and mechanisms of chemisorption.

Lecture-11: **Surface Films and Monometallic/Bimetallic Surfaces-**Surface Films: Formation and properties, Monometallic/Bimetallic Surfaces: Characteristics and uses.

Lecture-12: **Experimental Techniques for Monolayer Films-**Techniques: Methods for studying monolayer films

Lecture-13: **Reactions in Monomolecular Films-**States and Reactions: Mechanisms in monomolecular films, NH_3 Synthesis: Surface-catalyzed reaction of H_2 and N_2.

Lecture-14: **Micelles and Their Applications-**Micelles: Classification, structure, and critical micellar concentration (CMC), Micellar Interactions: Factors affecting CMC and applications in catalysis,

Lecture-15: **Thermodynamics and Models-**Micellization, phase separation, and solubilization models, Summary, Assignments.

PC-(CB1)-19: Heterogeneous catalysis (15 h)

Lecture-1: **Introduction to Heterogeneous Catalysis**-Heterogeneous Catalysis: Definition and importance.

Lecture-2: **Categories of Catalysts-**Broad Categories: Metals, bimetals, semiconductors, insulators, zeolites, oxides, nanomaterials.

Lecture-3: **Preparation of Metal Catalysts-**Preparation Methods: Supported metal catalysts and non-metallic catalysts.

Lecture-4: **Co-Precipitation and Impregnation-**Methods: Co-precipitation, impregnation techniques.

Lecture-5: **Sol-Gel and Deposition-Precipitation-**Methods: Sol-gel method, deposition-precipitation.

Lecture-6: **Hydrothermal and other Methods-**Methods: Hydrothermal synthesis, pulsed laser methods, Plasma chemical methods, chemical vapor deposition (CVD).

Lecture-7: **Steps in Catalyzed Reactions-** Reaction Steps: Diffusion and adsorption, adsorption-chemisorption isotherms.

Lecture-8: **Kinetics and Thermodynamics**-Catalyzed reaction dynamics, Mechanism of Surface-Catalyzed Reactions- Langmuir Hinshelwood model, Rideal-Eley mechanism.

Lecture-9: **Catalytic Activity**-turn over number, turn over frequency & rate, Determining Factors: Structure-sensitive and structure-insensitive catalysts.

Lecture-10: **Characterization of Catalysts-** Characterization: Surface area (BET method), pore volume and pore size distribution (BJH method), numerical problems.

Lecture-11: **Surface Acidity and Specificity-**Surface Acidity: Determination by indicator method, IR spectroscopy, TPD methods.

Lecture-12: **Advanced Surface Characterization Techniques-**XRD, LEED, XPS, AES.

Lecture-13: **Surface morphological techniques**-SEM, TEM, AFM

Lecture-14: **Applications of Catalysis-** Environmental catalysis-Auto exhaust emissions

Lecture-15: **Industrial applications-**catalytic hydrogenation and oxidation, cracking and reforming, Fischer-Tropsch synthesis of methanol. Summary of the topic, allotment of assignment questions & problems.

PC-(CB1)-20: Phase transfer, Anchored and Photo catalysis (15 h)

Lecture-1: **Principles of Phase-Transfer Catalysis-**PTC Principles: Overview of phase-transfer catalysis

Lecture-2: **Classification of Phase-Transfer Catalysis-**PTC Classification: Types and categories of PTC.

Lecture-3: **Role of Water in PTC Reactions-**Water's Role: Importance in phase-transfer catalyzed reactions.

Lecture-4: **Factors Influencing PTC Reaction Rates-**Influencing Factors: Key factors affecting the rate of PTC reactions.

Lecture-5: **Inverse Phase Transfer Catalysis-**Inverse PTC: Mechanism and applications.

Lecture-6: **Mechanism of Nucleophilic Displacement Reactions-**Nucleophilic Displacement: Detailed reaction mechanism.

Lecture-7: **Crown Ethers as PTC-**Crown Ethers: Role in phase-transfer catalysis, especially with alkyl halides and superoxide.

Lecture-8: **Permanganate Oxidation with PTC-**Permanganate Oxidation: Oxidation of alkenes and phenols using quaternary ammonium salts and crown ethers.

Lecture-9: **Anchored Catalysis Definition and Examples-**Anchored Catalysis: Definition and examples with organic polymers, inorganic oxides, and clays.

Lecture-10: **Structure of Montmorillonite Anchored Catalysts-**Montmorillonite Structure: HEW and EF structures of anchored catalysts.

Lecture-11: **Applications of Intercalated Clay Catalysts-**Intercalated Clays: Use in hydrogenation reactions.

Lecture-12: **Photocatalysis Basics-**Photocatalysis: Basic principles and photocatalytic effects.

Lecture-13: **Metal Semiconductor Systems as Photocatalysts-**Metal Semiconductor Systems: Nature, loading, and doping of metals and semiconductors.

Lecture-14: **Applications of Photocatalysis-**Applications: Water splitting, pollutant removal, and organic compound oxidation/reduction.

Lecture-15: **Advanced Applications of Photocatalysis-**Advanced Photocatalysis: Further applications in environmental and chemical processes.

ELECTIVE–4B (ID PAPER)

PAPER-IV CH(PC) 404T(CB4): ENGINEERING CHEMISTRY

PC(CB4) -29: Water and Waste Water Treatment (15 h)

Lecture-1: **Review of Hardness-**Causes of Hardness: Sources and impact on water quality.

Lecture-2: **Measurement of Hardness-**Measurement Techniques: Methods and units of hardness.

Lecture-3: **Types of Hardness-**Temporary and Permanent Hardness: Definitions and differences.

Lecture-4: **Estimation of Hardness-**Estimation Methods: Techniques for measuring temporary and permanent hardness.

Lecture-5: **Numerical Problems on Hardness-**Numerical Problems: Calculations involving water hardness.

Lecture-6: **Boiler Troubles - Scales and Sludge-**Scales and Sludge Formation: Causes and effects in boilers.

Lecture-7: **Boiler Troubles - Caustic Embrittlement-**Caustic Embrittlement: Mechanism and prevention.

Lecture-8: **Boiler Troubles - Priming and Foaming-**Priming and Foaming: Causes and control methods.

Lecture- 9: **Boiler Water Treatment - Soda-Lime Process-**Soda-Lime Process: Method and applications.

Lecture 10: **Boiler Water Treatment** - Zeolite Process-Zeolite Process: Method and applications.

Lecture-11: **Boiler Water Treatment - Ion Exchange Process-**Ion Exchange Process: Method and applications.

Lecture-12: **Treating Saline Water-**Saline Water Treatment: Distillation, electrodialysis, reverse osmosis.

Lecture -13: **Municipal Water Supply-**Municipal Supply Methods: Sedimentation, filtration, sterilization.

Lecture-14: **Waste Water Treatment-**Waste Water Treatment: Physical, chemical, and biological methods.

Lecture-15: **Sewage Water, COD and BOD-**Sewage Treatment: COD and BOD concepts and numerical problems, summary of the topic and assignment questions & problems.

PC(CB4) -30: Corrosion and Its Control (15 h)

Lecture-1: **Magnitude of the Problem-**Magnitude of the Problem: Overview of corrosion issues and their impact.

Lecture-2: **Theories of Corrosion-**Corrosion Theories: Chemical and electrochemical mechanisms.

Lecture-3: **Chemical and Electrochemical Corrosion-**Corrosion Reactions: Chemical and electrochemical corrosion processes.

Lecture-4: **Factors Affecting Corrosion - Nature of Metal-**Nature and Purity of Metal: Influence on corrosion rates.

Lecture-5: **Electrochemical Series and Over Voltage-**Electrochemical Series: Impact on corrosion potential and over voltage.

Lecture-6: **Nature of Oxide Film and Corrosion Product-**Oxide Film and Corrosion Product: Their roles in corrosion.

Lecture-7: **Environmental Factors - Nature of Environment-**Environmental Influence: Effect of temperature, pH, oxidants, and humidity.

Lecture-8: **Corrosion Control - Design and Material Selection-**Design and Material Selection: Strategies to prevent corrosion.

Lecture-9: **Corrosion Control - Cathodic Protection-**Cathodic Protection: Methods including sacrificial anode and impressed current.

Lecture-10: **Surface Coating Methods - Surface Preparation-**Surface Preparation: Techniques for preparing surfaces for coating.

Lecture-11: **Metallic Coatings - Application Methods-**Metal Coatings: Hot dipping, galvanizing, tinning, cladding, electroplating.

Lecture-12: **Chemical Conversion Coatings-**Chemical Coatings: Types and applications.

Lecture-13: **Organic Surface Coatings – Paints-**Paints: Constituents, functions, and application methods.

Lecture-14: **Failure of Paint Films-**Paint Failures: Causes and prevention.

Lecture-15: **Varnishes, Enamels, and Lacquers-**Organic Coatings: Types including varnishes, enamels, and lacquers.

PC(CB4) -31: Energy Sources (15 h)

Lecture-1: **Introduction to conventional energy resources-**Chemical fuels: overview and classification (solid, liquid, gaseous).

Lecture-2: **Solid fuels – coal-**Coal: types, proximate and ultimate analysis, and their significance.

Lecture 3: **Liquid fuels – petroleum-**Petroleum: refining processes, including cracking and reforming.

Lecture-4: **Synthetic Petrol-**Synthetic petrol: Bergius and Fischer-Tropsch processes.

Lecture-5: **Fuel quality – Knocking-**Knocking: anti-knocking agents, octane number, and cetane number.

Lecture-6: **Other liquid fuels**-Other liquid fuels: lpg, biodiesel, kerosene, fuel oil, benzol, tar, power alcohol.

Lecture- 7: **Gaseous Fuels**-Gaseous fuels: natural gas, coal gas, producer gas, oil gas, water gas, biogas.

Lecture-8: **Combustion Fundamentals-**Combustion: calorific value, bomb calorimeter, HCV, and LCV values.

Lecture -9: **Flue Gas Analysis**-Flue gas analysis: orsat's method and its applications,

Lecture-10: **Rocket Fuels**-Rocket fuels: solid propellants, liquid propellants, monopropellants, bipropellants.

Lecture-11: **Introduction to non-conventional energy resources**-Non-Conventional energy: overview of alternative energy sources.

Lecture- 12: **Nuclear fuels-**Nuclear fuels: nuclear reactors, fission, fusion, fuel sources, waste disposal, and reprocessing.

Lecture-13: **Solar energy-**Solar energy: methods and technologies for harnessing solar power.

Lecture-14: **Hydro and Wind Energy**-Hydro and wind energy: principles and applications.

Lecture-15: **Tidal, Biofuels, and Hydrogen-**Tidal, biofuels, and hydrogen: energy from tidal movements, biofuels, and hydrogen as a non-polluting fuel.

PC(CB4)- 32: Engineering Materials (15 h)

Lecture-1: **Portland Cement-**Composition and Analysis: Portland cement composition and its analysis.

Lecture-2: **Setting and Hardening of Cement-**Reactions: Processes of setting and hardening of Portland cement.

Lecture-3: **Decay and Types of Cement-**Decay and Lime: Decay of cement concrete, types and manufacture of lime, plaster of Paris.

Lecture-4: **Lubricants – Introduction-**Lubricants: Criteria of a good lubricant, and classification (petroleum oils, fixed oils, synthetic lubricants, semisolid, solid lubricants).

Lecture-5: **Properties of Lubricants-**Properties: Cloud point, pour point, flash and fire point, viscosity.

Lecture-6: **Refractories – Introduction-**Refractories: Classification and characteristics of good refractory.

Lecture-7: **Refractories** – Failure-Failure: Reasons for failure of refractories.

Lecture-8: **Glass-**Glass: Glass making oxides, their functions, and the manufacturing process.

Lecture-9: **Porcelain, Enamels, and Abrasives-**Porcelain and Enamels: Characteristics and uses of porcelain, enamels, and abrasives.

Lecture-10: **Conductors and Insulators – Introduction-**Conductors and Insulators: Classification and characteristics of thermal and electrical insulators.

Lecture-11: **Superconductors-**Superconductors: Properties and applications (Nb-Sn alloy, $YBa_2Cu_3O_{7-x}$).

Lecture-12: **Composite Materials – Introduction-**Composites: Advantageous properties and classification.

Lecture-13: **Strengthening and Hardening-**Mechanisms: Mechanisms of strengthening and hardening of particle reinforcement.

Lecture-14: **Fabrication of Composites-**Fabrication: Techniques used in the fabrication of composite materials.

Lecture-15: **Liquid Crystals-**Liquid Crystals: Characteristics, physical properties, classification, types of mesophases, chemical nature, applications, and future trends.

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