Chaudhary Charan Singh University, Meerut

Syllabus of: M.Sc. (Chemistry)

[For fourth and fifth years of Higher education (PG)]

(As per guidelines of U.P. Government according to National Education Policy-2020 w.e.f. the session 2022-2023)

Head
Department of chemistry
Meerut

Sem.	Course Code	Course Title	Duration	Lecture Duration	Lect./Week (Th+Tu+ Pr)	Max. Marks=100 (Ext.+ Int.)	Credits	External Exam duration
I	CH-1507	Inorganic Chemistry I	60 hours	60 minutes	6	40+40	05	3 hours
	CH-1508	Organic Chemistry I	60 hours	60 minutes	6	40+40	05	3 hours
	CH-1509	Physical Chemistry I	60 hours	60 minutes	6	40+40	05	3 hours
	CH-1510	Computer for Chemists	60 hours	60 minutes	6	40+40	05	3 hours
	CH-1511	Qualifying Courses (any one of the following): a) Biology for Chemist (For students with maths in B.Sc.)	30 hours	60 minutes	2	25+25	04	3 hours
	CH-1512	b) Mathematics for Chemist (For students with Biology in B.Sc.)	30 hours	60 minutes	2	25+25	04	3 hours
	As per chosen language)	Core Elective			04	100	04	3 hours
	CH-507	Inorganic Practical	90 Hrs	180 minutes	02	20	08	5 hours
		Organic Practical	90 Hrs	180 minutes	02	20		5 hours
		Physical Practical	90 Hrs	180 minutes	02	20		5 hours
		Computer Practical	90 Hrs	180 minutes	02	20		3 hours
	Max. Marks of Semester-I					**500**		
II	CH-2507	Inorganic Chemistry II	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-2508	Organic Chemistry II	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-2509	Physical Chemistry II	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-2510	Group Theory Spectroscopy &,	60 hours	60 minutes	6	40+40	**5**	3 hours
	CO-6604	Open Elective CBCS (Chemistry in Life-1)	20 hours	60 minutes	4	100	**4**	3 hours
	CH-607	Inorganic Practical	90 Hrs	180 minutes	02	26	**08**	6 hours
		Organic Practical	90 Hrs	180 minutes	02	26		6 hours
		Physical Practical	90 Hrs	180 minutes	02	26		6 hours
	Max. Marks of Semester-II					**500**		

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III	CH-3507	Photochemistry	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-3508	Spectroscopy	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-3509	Analytical Chemistry	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-3510	Any one of the following: a) Bio-Inorganic Chemistry	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-3511	b) Bio-Organic Chemistry	60hours	60 minutes	6	40+40	**5**	3 hours
	CH-3512	c) Bio-Physical Chemistry	60hours	60 minutes	6	40+40	**5**	3 hours
	Code is yet to be allotted	Minor Project				80	**8**	Project Viva
	CO-7604	Open Elective CBCS (Chemistry in Life-2)	20 hours	60 minutes	4	100	**4**	3 hours
	Max. Marks of Semester-III					500		
IV	CH-4507	Environmental Chemistry	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4508	Any three for Inorganic specialization: Inorganic Chemistry Special I	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4509	Inorganic Chemistry Special II	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4510	Inorganic Chemistry Special III (Advanced Inorganic Chemistry)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4511	Inorganic Chemistry Special IV (Advanced Spectral Technique	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4512	Inorganic Chemistry Special V (Chemistry of Materials)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4513	Any three for Organic specialization: Organic Chemistry Special I (Organic Synthesis)	60 hours	60 minutes	6	40+40	**5**	3 hours

	CH-4514	Organic Chemistry Special II (Medicinal Chemistry)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4515	Organic Chemistry Special III (Polymer Chemistry)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4516	Organic Chemistry Special IV (Chemistry of Natural Products)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4517	Organic Chemistry Special V (Heterocyclic Chemistry)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4518	Any three for Physical specialization: Physical Chemistry Special I (Solid State Chemistry)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4519	Physical Chemistry Special II (Advanced Quantum Chemistry)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4520	Physical Chemistry Special III (Liquid State)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4521	Physical Chemistry Special IV (Physical Chemistry of Inorganic Reaction)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-4522	Physical Chemistry Special V (Computational Chemistry)	60 hours	60 minutes	6	40+40	**5**	3 hours
	CH-807	Practical Organic Synthesis	90 hours	180 minutes		80	**08**	12 Hours
	Max. Marks of Semester-IV					500		

Sem	Course Code	Paper Title	Course Outcome
I Sem	CH-1507	Inorganic Chemistry I	To help them to learn the stereochemistry and bonding in main group compounds, metal ligand equilibrium in solution, reaction mechanism of transition metal complexes and metal-ligand bonding.
	CH-1508	Organic Chemistry I	To develop skills in the identification of nature of bonding in organic molecules, stereochemistry, and reaction mechanism: structure and reactivity, aliphatic nucleophilic substitution and aliphatic electrophilic substitution.
	CH-1509	Physical Chemistry I	To help them to learn advance quantum chemistry and thermodynamic.
	CH-1510	Computer for Chemists	To develop the skills in the area of knowledge of introduction to computers and computing, computer programming in FORTRAN/C/BASIC
	CH-1511	Qualifying Courses (any one of the following): a) Biology for Chemist (For students with maths in B.Sc.)	To help them to learn the cell structure and functions, carbohydrates, lipids, amino acids, peptides and proteins and nucleic acids. OR To develop the skills in vectors and matrix algebra analysis
	CH-1512	b) Mathematics for Chemist (For students with Biology in B.Sc.)	
	CH-507	Inorganic Practical	Students gain expertise in gravimetric analysis, preparation of inorganic complexes and analysis of their properties.
		Organic Practical	Gain expertise on basic laboratory procedures involved in purification, identification and preparation of organic compounds.
		Physical Practical	It helps them to learn the practical aspects of thermochemistry.
		Computer Practical	Students gain knowledge about Basic Know how of computers and C language.

II Sem	CH-2507	Inorganic Chemistry II	To develop the knowledge about electronic spectra and magnetic properties of transition metal complexes, metal pi complexes, metal clusters, and nuclear chemistry.
	CH-2508	Organic Chemistry II	To develop the knowledge about aromatic electrophilic substitution, aromatic nucleophilic substitution, free radical reactions, addition to carbon carbon multiple bonds, addition to carbon hetero multiple bonds, elimination reactions and pericyclic reactions.
	CH-2509	Physical Chemistry II	To develop the knowledge about chemical thermodynamics, surface chemistry and electrochemistry
	CH-2510	Group Theory, Spectroscopy & Diffraction Methods & Solid State	To develop the knowledge about symmetry and group theory in chemistry, unifying principles, vibrational spectroscopy, electronic spectroscopy, X-ray diffraction and magnetic resonance spectroscopy.
	CO-6604	Open Elective CBCS (Chemistry in Life-1)	To develop the knowledge about general introduction of materials in daily life, pharmaceutical chemistry and in cosmetics and personal care products.
	CH-607	Inorganic Practical	Students gain knowledge in the practical field of acidimetric titrations, oxidation reduction titrations, estimate copper nickel in the given solution etc.
		Organic Practical	Students gain knowledge in the analysis of binary organic mixture and two step preparations.
		Physical Practical	To develop practical skills in the determination of surface tension.
III Sem	CH-3507	Photochemistry	To help the students gain knowledge in the field of photochemical reactions.
	CH-3508	Spectroscopy	To develop the knowledge about inorganic spectroscopy and organic spectroscopy.
	CH-3509	Analytical Chemistry	To develop the knowledge about classification of analytical methods, errors and evaluation, radiochemical methods, thermal methods of analysis, chromatographic techniques, electro analytical techniques and atomic adsorption spectroscopy and flame photometry.
		Any one of the following:	

	CH-3510	a) Bio-Inorganic Chemistry	To develop the knowledge about bio-inorganic compounds and chemistry
	CH-3511	b) Bio-Organic Chemistry	To develop the knowledge about bioorganic compounds and chemistry
	CH-3512	c) Bio-Physical Chemistry	To develop the knowledge about biophysical compounds and chemistry.
		Practical a) Analytical b) Biochemistry	To gain the knowledge in the practical field of lamberts beers law, determination of concentration, scan the U.V. visible spectra of unknown compound, viscosity, separation of amino acids etc. To gain knowledge about qualitative tests, determination of acid values, saponification, iodine no. etc.
	CO-7604	Open Elective CBCS (Chemistry in Life-2)	To develop the knowledge about greenhouse effects, pesticides, cleansing agents and enzymes.
IV Sem	CH-4507	Environmental Chemistry	To develop the knowledge about environment, hydrosphere, soils, atmosphere, industrial pollution and environmental toxicology.
	CH-4513	Any three for Organic specialization: Organic Chemistry Special I (Organic Synthesis)	To develop the knowledge about organometallic reagents, oxidation, reduction, rearrangements and metallocenes, nonbenzenoid aromatic and polycyclic aromatic compounds.
	CH-4514	Organic Chemistry Special II (Medicinal Chemistry)	To help the students to know about medicinal chemistry, drug design, combinatorial chemistry, computational approaches, biodisposition and implications, neuroactive agents, cardiovascular agents, antineoplastic agents and local anti-infective design.
	CH-4515	Organic Chemistry Special III (Polymer Chemistry)	To help the students know about basics of polymer, characterization, structure and properties of polymer, polymer processing, and properties of commercial polymers.

	CH-4516	Organic Chemistry Special IV (Chemistry of Natural Products)	To help students know about natural products and their applications.
	CH-4517	Organic Chemistry Special V (Heterocyclic Chemistry)	To provide detailed knowledge of heterocyclic compounds, their synthesis, properties and applications.
	CH-807	Practical	To gain the practical aspects of analysis of ternary organic mixture, three step organic preparation, determine the strength of given aniline solution and determine the percentage of sulphur in the given organic compound.

FIRST SEMESTER

CH-1507 COURSE- I 60 Hrs

INORGANIC CHEMISTRY-I

1. **Stereochemistry and Bonding in Main Group Compounds 06 Hrs**
   VSEPR, Walsh diagrams (tri atomic molecules), d π - P π bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.
2. **Metal-ligand equilibrium in solution 08 Hrs**
   Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constant by pH-metry and spectrophotometry.
3. **Reactions mechanism of Transition Metal complexes 12 Hrs**
   Energy profile of a reaction, the reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories. Kinetics of Substitution Reactions -Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidence in favor of conjugate mechanism. Anation reaction, reactions without Metal-Ligand bond cleavage. Substitution reactions in square planer complexes, the trans effect, mechanism of substitution reactions.
   Redox reactions (electron transfer reactions) - Mechanism of one electron reactions [such as Henry Taube's classical reaction of $(NH_3)5Co^{3+}$- Cr^{2+}], Inner sphere type Reactions, Outer-sphere type Reactions (cross-reactions) and Marcus-Hush theory (No mathematical treatment)
4. **Metal -ligand Bonding 16 Hrs**
   Adjusted CFT, Limitations of crystal field theory, Octahedral, tetrahedral and square planar complexes.
5. **Electronic spectra and magnetic properties of transition metal compounds 18 Hrs**
   Spectroscopic ground states, correlation, orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 states), calculation of Dq, B, and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

CH-1508 **COURSE - II**

ORGANIC CHEMISTRY - I **60 Hrs**

1. **Aromaticity** **10Hrs**

   Aromaticity- Huckel's rule, PMO approach, antiaromaticity, homo-aromaticity, Aromaticity in benzenoid and non-benzenoid compounds, annulenes. General considerations, synthesis and reactions of Ferrocene, Chrysene, Azulene.

   Bonds weaker than covalent-addition compounds, crown ether complexes, cryptands, inclusion compounds, cyclodextrins.

2. **Stereochemistry** **15 Hrs**

   Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, Enantiotopic, and diastereotopic atoms, groups, and faces. Stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes, and spiranes), chirality due to helical shape.

3. **Reaction Mechanism: Structure and Reactivity** **15 Hrs**

   Types of mechanism, types of reactions, thermodynamics and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagram, transition states, and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability, and reactivity of carbocations, carbanions, free radicals carbenes, and nitrenes. Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment of the effect of structure on reactivity- Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

4. **Aliphatic Nucleophilic Substitution** **15 Hrs**

   SN1, SN2, Mixed SN1 & SN2 & SET mechanism. Neighbouring group mechanism, neighboring group participation by π and σ bonds, anchimeric assistance. Classical and nonclassical carbocations, Phenonium ions, nonbornyl system. Common carbocation rearrangements, Application of NMR spectroscopy in the detection of the carbocation.

   SNi mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal, and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. Phase transfer catalysis, ambident nucleophile, regioselectivity.

5. **Aliphatic Electrophilic Substitution** **5 Hrs**

   Bimolecular mechanism-SE2 & SE1. SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group, and solvent polarity on the reactivity.

CH-1509 **COURSE - III**

PHYSICAL CHEMISTRY-I **60 Hrs**

1. Chemical Dynamics

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady-state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme, reactions, general features of fast reactions, study of fast reactions by flow method: relaxation method, flash photolysis, and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

2. Surface Chemistry

A. Adsorption Surface tension, capillary action, the pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Elementary treatment of BET equation, catalytic activity at surfaces.

B. Micelles Surface active agents, classification of surface-active agents, micellization. hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization. solubilization, micro emulsion, reverse micelles.

3. Electrochemistry

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy -Chapman, Stern. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces - theory of double-layer at Semiconductor, electrolyte solution interfaces, structure of double layer interfaces.

CH-1510 **COURSE - V**

COMPUTERS FOR CHEMISTS **60 Hrs**

This is a theory cum laboratory course with more emphasis on laboratory work.

1. **Introduction to computers and computing**

   Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices, secondary storage. Computer languages. Operating system with DOS as an example. introduction to Unix and windows. Data Processing. Principles of programming. Algorithms and flowcharts.

2. **Computer programming in FORTRAN/C/BASIC**

   The language feature are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C and the feature to be replaced appropriately. Elements of the computer language. Constants and variables. Operations and symbols. Expression. Arithmetic assignment statement input and output. Format statement. Termination statements. Branching statements such as IF or GO TO statement.

   LOGICAL variables, Double Precision variables. Subscripted variables, and DIMENSIONS. DO statements. FUNCTION and SUBROUTINE. COMMON and DATA statements.

   Decision control structure, case for control structure, functions, introduction to arrays, programs based on above.

3. **Programming in Chemistry**

   Development of small computer course involving simple formulas in chemistry such as Vander Waal's equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equation with in the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc of molecules extracted from a database such as Cambridge database.

4. **Use of Computer Programs**

   Execution of linear regression, X-V plot, Numerical integration and differentiation as well as differential equation solution programmes. Monte-Carlo and Molecular dynamics. Introduction to MS Office (MS Word, MS Excel, MS PowerPoint). Lab sessions based on MS Office Package. Introduction to Internet Explorer.

CH-1511 **COURSE- IV**

BIOLOGY FOR CHEMISTS **60 Hrs**

1. **Cell structure and functions**

   Structure of prokaryotes cells, intracellular organelles, and their functions, comparison of plant and animal cells, Overview of metabolic processes- Catabolism, anabolism. ATP-biological energy currency.

2. **Carbohydrates** **08 Hrs**

   Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol amino sugars, N-acetylmuramic acid, sialic acid, disaccharides, and polysaccharides. Structural polysaccharides- Cellulose and chitin. Storage polysaccharides- starch and glycogen, Structure and biological functions of glycosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition, ascorbic acid.

   Carbohydrate metabolism-Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

3. **Lipids** **06Hrs**

   Fatty acids, essential fatty acids, structure, and function of triacylglycerols, glycerophospholipids, sphingolipids cholesterol, bile acids, prostaglandins, lipoproteins-composition and function, role in artherosclerosis.

   Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes, fluid mosaic model of membrane structure. Lipid metabolism- β oxidation of fatty acids.

4. **Amino acids- Peptides and proteins** **06Hrs**

   Chemical and enzymatic hydrolysis of proteins to peptides, secondary structure of proteins, forces responsible for holding of secondary structure, α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein- folding and domain structure. Quaternary structure.

   Amino acid metabolism- degradation and biosynthesis of amino acids, sequence determination: chemically/enzymatic/mass spectral, racemization/detection.

5. **Nucleic acids** **05Hrs**

   Purine and pyrimidine bases of nucleic acid and their synthesis base-pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double-helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, and an overview of replication of DNA. Transcription, translation, and genetic code. Chemical synthesis of mono and trinucleoside.

CH-1512 **COURSE- IV**

MATHEMATICS FOR CHEMISTS **60 Hrs**

I. Vectors and Matrix Algebra **10Hrs**

A- Vectors

Vectors, dot, cross and triple products etc. The gradient, divergence and curl. Vector calculus, Gauss theory, divergence theorem etc.

B- Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogenous, non-homogenous linear equations and conditions for the solution., linear dependence and independence.

Introduction to vector spaces, matrix eigen values and eigen vectors, diagonalization, determinants (examples from Huckel theory).

Introduction to tensors; polarizability and magnetic susceptibility as examples.

II. Differential Calculus **10Hrs**

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.) exact and inexact differentials with their applications to thermodynamic properties.

Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. cartesian to spherical polar), curve sketching.

III. Elementary differential equations **7Hrs**

Variables-separable and exact first-order differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differential equations by the power series method. Fourier series solutions of harmonic oscillator and Legendre equation etc., spherical harmonics, second order differential equations and their solutions.

IV. Permutation and Probability **3Hrs**

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least square fit etc.) with a general polynomial fit.

CH-507 **Practical Syllabus I semester**

Physical Practical

1. To find out the strength of the given HCl solution by titrating it against N/10 NaOH using a pH meter.
2. To find out the strength of the given CH_3COOH solution by titrating it against NaOH using a pH meter.
3. To find out the strength of HCl and CH_3COOH in a mixture of both by titrating it against N/10 NaOH using a pH meter.
4. To determine the solubility of a given salt at room temperature and also draw its solubility curve.
5. To find out the heat of solution of oxalic acid by solubility method.
6. To standardize the given KMnO4 solution by titrating it against standard Ferrous Ammonium Sulphate solution.
7. To determine the critical solution temperature of the phenol water system.
8. To determine the viscosity of a given sample of oil at different temperature using a Red Wood Viscometer.

Inorganic Practical

1. To analyze the mixture of two components.
2. To analyze the mixture of three components.
3. To prepare Hexa-ammine(II) chloride.
4. To prepare Potassium dioxalato curate (II) dihydrate.
5. To prepare Potassium trioxalato chromate (III).
6. To prepare Tetrammine cupric sulfate.
7. To prepare Sodium ferric oxalate.
8. To prepare crystals of potassium tris oxalate aluminate (III).

Organic Practical

1. To identify the given organic compound and prepare its derivatives.
2. To analyze the given organic mixture (water separation).
3. Single-step preparation

a) Hydrolysis
b) Bromination
c) Nitration
d) Oxime formation
e) Reduction
f) Hoffmann bromide reaction
g) Benzoin condensation reaction etc

4. To determine the iodine value of the given fat sample.
5. To determine the saponification value of the given fat sample.

SECOND SEMESTER

CH-2507 **COURSE-I**

INORGANIC CHEMISTRY-II **60 Hrs**

1. **Metal π complexes**
   Metal carbonyls, structure, and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding. Structure and important reactions of transition metal nitrosyl, dinitrogen, dioxygen complexes, tertiary phosphine as ligand.
2. **Metal clusters**
   Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.
3. **Nuclear chemistry**
   Radioactive decay and equilibrium. Nuclear reactions, Q-value cross-sections, types of reactions, chemical effects of nuclear transformations, Fission & fusion, fission products and fission yields. Radioactive techniques, tracer techniques. Radiation hazards and therepeutics
4. **Electronic spectroscopy**

A. **Atomic spectroscopy** Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

B. **Molecular spectroscopy** Energy levels, molecular orbitals, vibronic transition, vibrational progressions and geometry of the excited states, Frank-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radioactive and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

C. **Photoelectron spectroscopy** Basic principles; photo-electric effect, ionization process, Koopman's theorem, Photoelectron spectra of simple molecules, ESCA chemical information from ESCA, Auger electron spectroscopy- basic idea.

CH-2508 **COURSE-II**

ORGANIC CHEMISTRY

1. **Aromatic electrophilic substitution**
   The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.
2. **Aromatic Nucleophilic Substitution**
   The SNAr, SN 1, benzyne and SRN 1 mechanism. Reactivity- effect of substrate structure, leaving group and attacking nucleophile. Von Richter, Sommelet-Hauser and Smiles rearrangements.
3. **Free radical reactions**
   Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.
4. **Addition to Carbon-Carbon Multiple bonds**
   Mechanism and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.
5. **Addition to Carbon-Hetero Multiple Bonds**
   Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters, and nitriles. Additian of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig Reaction. Mechanism of condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.
6. **Elimination Reactions**
   The E2, El, and E1 CB mechanisms and their spectrum. Orientation of the double bond. Reactivity- effects of substrates structures, attacking base, the leaving group, and the medium. Mechanism and orientation in pyrolytic elimination.
7. **Pericyclic Reactions**
   Molecular orbital symmetry. Frontier orbitals of ethylene, 1, 3- butadiene, 1, 3, 5 hexatriene and allyl system. Classification of pericyclic reactions. Wodward- Hoffmann correlation diagrams. FMO and PMO approach. Electrolytic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl system.

Cycloadditions- antarafacial and Suprafacial additions, 4n and 4n+ 2 system, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements - suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moeties, 3,3- and 5, 5- sigmatropic rearrangements. Claisen, Cope, Sommlet Hauser rearrangement, Ene reaction.

CH-2509 **COURSE-III**

PHYSICAL CHEMISTRY- II **60 Hrs**

I. Quantum chemistry **40Hrs**

1. **Introduction to Exact Quantum Mechanical Results-** The Schrodinger equation and postulates of quantum mechanics. Discussion of solution of the Schrodinger equation to some model systems viz, particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.
2. **Approximate methods-** The variation theorem, linear variation principle. Perturbation theory (first order and nondegenerate). Application of variation method and perturbation theory to the helium atom.
3. **Angular Momentum-** Ordinary angular momentum, generalized angular momentum, eigenfunction for angular momentum, eigenvalues of angular momentum, an operator using ladder operators, the addition of angular momenta, spin, anti-symmetry, and Pauli's exclusion principle.
4. **Electronic structure of atoms-** Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the pn configuration, term separation energies of the dn configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.
5. **Molecular Orbital Theory –** Huckel Theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel Theory.

II. Thermodynamics **20 Hrs**

Statistical Thermodynamics- Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers).

Partition functions- translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions.

Heat capacity behaviour of solids- chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics- distribution law and application to helium.

CH-2510 COURSE-IV

GROUP THEORY, SPECTROSCOPY AND DIFFRACTION METHODS, AND SOLID STATE 60 Hrs

1. **Symmetry and Group Theory in chemistry**
   Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup, Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of group by matrics, representations of group by matrices (representation for the Cn, Cnv, Cnh, Dnh etc groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use in spectroscopy.
2. **Unifying principles**
   Electromagnetic radiation, interaction of electromagnetic radiation with matter absorption. emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.
3. **Vibrational spectroscopy**
   A. **Infrared spectroscopy** Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths, anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, p,a,R branches. Breakdown of Oppenheimer approximation; vibration of poly atomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.
   B. **Raman spectroscopy** classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, Coherent Anti Stokes Raman spectroscopy (CARS).
4. **Magnetic Resonance Spectroscopy**
   A. **Nuclear Magnetic Resonance Spectroscopy** Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin- spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc), spin decoupling, basic ideas about instrument, NMR studies of nuclei other than proton – 13 C.
   B. **Electron Spin Resonance Spectroscopy** Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

5. X-ray Diffraction

Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

CH-607 PRACTICAL SYLLABUS II SEMESTER

PHYSICAL CHEMISTRY

1. To find out the surface tension of the given liquid by drop weight method at room temperature.
2. To determine the parachor value of given liquid.
3. To find out the surface tension of CH_3COOH, C_2H_5OH, n-hexane at room temperature and hence calculate the atomic parachors of C, H and O.
4. To compare the cleaning powers of two samples of detergents supplied to you.
5. To determine the critical micelle concentration of soap.
6. To find out the strength of HCl solution by titrating it against N/10 NaOH using Conductometer.
7. To find out the strength of given NH_4OH by titration it against HCl solution using conductometer.
8. To find out the velocity constant of the hydrolysis of methyl acetate catalyzed by
   a) HCl b) H_2SO_4

9. Determine the relative strengths of two acids i.e. HCl and H_2SO_4 by studying the hydrolysis of methyl acetate.

INORGANIC PRACTICAL

1. Acidimetry alkalimetry titration
2. Oxidation reduction titration
3. Silver nitrate titration
4. Complexometric-EDTA titration
5. To estimate copper and nickel in the given solution.
6. To estimate iron and nickel in a given solution.
7. Preparation of Ferrocene
8. Instrumental methods of analysis utilizing flame photometer, atomic absorption spectrophotometer, pHmeter, separation of mixture of metals ions by chromatography.
9. Synthesis of Inorganic complexes/compounds and their characterization by various physiochemical method, viz.IR, UV, visible, NMR, etc. Complexes of Cr, Mn ,Cu, Ni, Fe, Co like Nickel DMG, Prussian blue, Turnsbull's blue, Potassium ferrioxalate, Dichloro pyridine, Ferroferrioxalate.

ORGANIC PRACTICAL

1. Analysis of binary organic mixtures
    a) Separation with $NaHCO_3$
    b) Separation with NaOH
    c) Separation with HCl

2. Two step preparations

a) To prepare anthranilic acid from phthalic anhydride
b) To prepare o-Chlorobenzoic acid from phthalamide
c) To prepare benzil from benzaldehyde.
d) To prepare benzanilide from benzophenone.

THIRD SEMESTER

CH-3507 PAPER-I PHOTOCHEMISTRY 60 Hrs

(COMPULSROY FOR ALL BRANCHES)

1. Basic of Photochemistry

Absorption, excitation, photochemical laws, quantum yield, electronically excited states- life times. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck Condon principle, photochemical stages-primary and secondary processes. Bimolecular deactivation quenching.

2. Photochemical Reactions

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

3. Determination of Reaction Mechanism

Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical-photo-dissociation, gas-phase photolysis.

4. Photochemistry of Alkenes

Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4 and 1,5-dienes.

5. Photochemistry of Carbonyl compounds

Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, β, γ unsaturated and α, β unsaturated compounds, Cyclohexadienones. Intermolecular Paterno-Buchi Reaction.

6. Photochemistry of Aromatic Compounds

Isomerisations, additions and substitutions.

7. Miscellaneous Photochemical Reactions

Photo Fries rearrangement, Photo-Fries reactions of anilides. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photo degradation of polymers, Photochemistry of vision.

CH-3508 PAPER-II SPECTROSCOPY 60 Hrs

(COMPULSORY FOR ALL BRANCHES)

1. Ultraviolet Visible Spectroscopy

Various electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

2. Infrared Spectroscopy Instrumentation and sample handling

Characteristic vibrational frequencies of alkanes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of Vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds), Effect of hydrogen bonding and solvent effect on vibrational frequencies. Symmetry and shapes of AB, A_2, AB_2, AB_3, AB_4, AB_5, and AB_6, mode of bonding of ambidentate ligand, ethylenediamine and diketonato complexes, application of resonance.

3. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

Definition, deduction of absolute configuration, octant rule for ketones.

4. Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism, of measurement chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), Intensity of NMR signals, chemical exchange effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra) virtual coupling, stereochemistry hindered rotation, karlus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transforms technique, Nuclear Overhauser Effect (NOE) Resonance of other nuclei-F, P. Some applications including biochemical systems.

5. Carbon-13 NMR Spectroscopy

General Considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants, Introduction to 2 D NMR.

6. Electron Spin Resonance Spectroscopy

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as PH_4, F_2^-, and BH_3.

7. Mossbauer spectroscopy

Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, (2) Sn^{2+} and Sn^{4+} compounds- nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

CH-3509 PAPER-III ANALYTICAL CHEMISTRY 60 Hrs
(COMPULSORY FOR ALL BRANCHES)

1. Introduction

Classification of analytical methods- classical and instrumental, types of instrumental analysis, selecting an analytical method.

2. Errors and Evaluation:

Definition of terms of mean and median, precision-standard deviation, relative standard deviation, accuracy, absolute error. Types of error in experimental data-determination (systematic), intermediate (random) and gross. Sources of errors and the effect upon the analytical results methods for reporting analytical data. Statistical evaluation of data indeterminate errors. The use of statistics.

3. Radiochemical methods:

Elementary working, Principles of Geiger Muller, Ionization, proportional and γ-ray counters. Neutron radiation sources, radio tracer techniques. Neutron Activation Analysis (NAA): Principle, Techniques and applications in preparation of some commonly used radioactive isotopes. Use of radioactive isotopes in analytical and physiochemical problems, Isotopic Dilution Analysis (IDA), substoichiometric IDA, advantages and limitations of IDA and comparison of IDA with NAA. Principle of Radiometric Titrations, Types, Experimental techniques and its applications.

4. Thermal methods of Analysis:

Introduction of different thermal methods, Thermogravimetry- TGA & DTA, static thermogravimetry, quasi-thermogravimetry and dynamic thermogravimetry, Instrumental and balances, X-Y recorder, thermogram, factors affecting thermograms. Application of thermogravimetry.

Differential Scanning Calorimetry (DSC): Introduction, instrumentation, DSC curves, factors affecting DSC curves and applications.

Thermometric Titrations: Introduction, Instrumentation, apparatus, theory and applications.

5. Chromatographic Techniques:

Adsorption and Partition Chromatography, Paper Chromatography, Thin Layer chromatography, lon exchange and Gas chromatography, HPLC, Size Exclusion Chromatography, their principles, techniques and important applications.

6. Electroanalytical Techniques:

A.Voltammetry: General introduction, Principle, Instrumentation, types of Voltammetry Polarography (Principle & Instrumentation), Cyclic Voltammetry, Pulse Methods.

Stripping Technique: Anodic and Cathodic Stripping Voltammetry and their applications in the trace determination of metal ions and biologically important compounds.

B. Ion Selective Electrodes: Electrical Properties of membrane, Glass electrode with special reference to H^+, Na+, K+ ions, operation of solid membrane electrode, operation of liquid membrane electrode, coated type ion electrode. Applications of ion selective electrode in determination of some toxic metal and some anions (F^-, Cl^-, Br^-, I^-, and NO_3^-).

CH-3511 PAPER-IV BIOORGANIC CHEMISTRY ELECTIVE 1 60 Hrs

1. Introduction:

Chemistry of amino acids proteins and their derivatives; methods of isolation and identification; Primary, secondary, tertiary and quaternary structures of proteins; determination and biochemical applications of the structures proteins; Nomenclature of nucleosides and nucleotides; Effects of acid and alkali on hydrolysis of nucleic acids; Structure of DNA and RNA; prokaryotic versus eukaryotic organisms.

2. Enzymes:

Introduction and historical perspective, Chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fisher's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis Menten and Lineweaver-Burk Plots, reversible and irreversitble inhibition.

3. Mechanism of Enzyme Action

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

4. Kinds of Reactions Catalysed by Enzymes

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reactions, enolic intermediates, intermediates in isomerization reactions, cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

5. Co-Enzyme Chemistry

Co-Factors as derived from vitamins, co-enzymes, prosthetic groups, apoenzymes. Structure and biological functions of co-enzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, vitamin B-12. Mechanisms of reactions catalyzed by the above co-factors.

6. Enzyme Models

Host-guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality. Biomimetic chemistry, crown ethers. Cryptates. Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzyme of synzymes.

7. Biotechnological Applications of Enzymes

Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese-making, syrups from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy. enzymes and recombinant DNA technology. Application of enzymes in organic synthesis.

MINOR PROJECT

Evaluation to be done by external examiner through Viva-voce examination.

FOURTH SEMESTER

CH-4507 ENVIRONMENTAL CHEMISTRY 60 Hrs

1. Environment

Introduction. Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Biodistribution of elements.

2. Hydrosphere

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle. Aquatic pollution - inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards.

Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand. Purification and treatment of water.

3. Soils

Composition, micro and macro nutrients, Pollution - fertilizers, pesticides, plastics and metals: Waste treatment.

4. Atmosphere

Chemical composition of atmosphere-particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry.

Analytical methods for measuring air pollutants. Continuous monitoring instruments.

5. Industrial Pollution

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

6. Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three Mile Island, Sewal D and Minamata disasters.

10. Green Chemistry

Basics & Introduction, 12 Principles of Green Chemistry, Less Hazardous Chemicals, Ionic Liquids, Some Examples of Green Chemistry: Caprolactum, Ibuprofen.

CH-4513 ORGANIC CHEMISTRY SPECIAL I 60 Hrs

(Organic Synthesis)

1. Organometallic Reagents:

Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details:

Group I & II metal organic compounds

Li, Mg, Hg, Cd, Zn and Ce Compounds

Transition metals

Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti Compounds

Other elements

S, Si, B and I compounds.

2. Oxidation:

Introduction. Different oxidative processes.

Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated).

Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.

Amines, Hydrazines and sulphides.

Oxidation with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) Nitrate.

3. Reduction:

Introduction. Different reductive processes.

Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings.

Carbonyl Compounds- aldehydes, ketones, acids and their derivatives.

Epoxides, nitro, nitroso, azo and oxime groups.

4. Rearrangements:

General mechanistic considerations- nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements: Pinacol-Pinnacolone, Wagner Meerwin, Demjanov, Benzyl-Benzilic acid, Favorskii, Arndt-Eistern synthesis, Neber, Beckmann, Hoffman, Curtius, Schmidt, Baeyer Villiger, Shaprio reaction. Barton, Chichibaben, Hoffman-Lofler Freytag reaction.

CH-4514 ORGANIC CHEMISTRY SPECIAL II 60 Hrs

(Medicinal Chemistry)

1. Introduction to Medicinal Chemistry:

Introduction to important functional groups in medicinal chemistry, a century of drug research.

2. Drug design:

Strategies for drug research including various targets, lead generation/ sources for drugs, receptor and drug receptor interactions: enzymes and design of inhibitors, concept of Prodrugs, hard and soft drugs.

3. Combinatorial Chemistry:

Introduction, solid support and linkers; combinatorial synthesis of compounds on solid phase, split and mix method, premix method, spatially addressable parallel chemical synthesis, multiple synthesis, Identification of active compounds from combinatorial libraries; Analytical methods for characterization of combinatorial libraries; Application of combinatorial libraries using solid phase chemistry.

4. Computational approaches:

Structure activity relationship, concept of QSAR, physicochemical parameters- lipophilicity, partition coefficient, electronic-ionization constants, H-bonding, steric parameters, Hammett equation. Isosterism, bioisosterism.

5. Biodisposition and implications:

Pharmacokinetics, concepts including absorption, distribution, metabolism and excretion of the drug, pharmacokinetic parameters, drug metabolism including phase I and phase II biotransformations; mention of the uses of pharmacokinetics in drug development process. Molecular toxicology, avoidance of toxic intermediates.

6. Neuroactive agents:

The chemotherapy of the mind: Introduction, neurotransmitters, CNS depressant, General anaesthetics, mode of action of hypnotics, sedatives, antianxiety agents, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs the neuroleptics, antidepressants, butyrophenone, serendipity and drug development, stereochemical aspects of neuroactive drugs. Synthesis of Diazepam, Oxazepam, Chlorazepam, barbiturates.

7. Cardiovascular agents:

Introduction, cardiovascular diseases, drug inhibitors of the peripheral sympathetic function, central intervention of the cardiovascular output, direct acting arteriolar dilators, synthesis of amyl nitrate, sorbitrate, diltiazam, quinidine, verapamil, methyldopa, atenolol, oxeprenolol.

8. Antineoplastic agents:

Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in the treatement of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors; synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, 6-mercaptopurine. Recent development in cancer chemotherapy, the hormones and natural products.

9. Local anti-infective drugs:

Introduction and general mode of action, synthesis of sulphonamide, furazolidone, naxilidic acid, eiprofloxacin, dapsone, aminosalicylic acid, isoniazid, ethionamide, ethambutol, fluconazole, econozole, gresiofulvin, chloroquin, primaquin.

CH-4515 ORGANIC CHEMISTRY SPECIAL III 60 Hrs
(Polymers)

1. Basics

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reaction. Polymerization in homogeneous and heterogeneous systems.

2. Polymer characterization

Polydispersion-average molecular weight concept. Number, Weight and Viscosity average molecular weight. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight- End group, viscosity light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers and chemical analysis of polymers, spectroscopic methods, physical testing- tensile strength, fatigue, impact. Tear resistance. Hardness and abrasion resistance.

3. Structure and Properties

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties- crystalline melting point Tm-melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature Tg, relationship between Tm & Tg. effects of molecular weight, diluents. chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

4. Polymer Processing

Plastics, elastomers and fibers. Compounding, Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fiber spinning.

5. Properties of Commercial Polymers

Polyethylene, Polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicon polymers. Functional Polymers- Fire retarding polymers and electrically conducting polymers. Biomedical polymers-contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

CH-807 PRACTICAL ORGANIC SYNTHESIS

1. Analysis of ternary organic mixtures
   - Separation with $NaHCO_3$ and water
   - Separation with NaOH and water
   - Separation with HCl and water
   - Separation with organic solvents
2. Three step organic preparations
   - To prepare o-chlorobenzoic acid from phthalic anhydride
   - To prepare benzilic acid from benzaldehyde
   - To prepare dibenzil from benzaldehyde
   - To prepare benzoic acid from benzophenone
3. To determine the strength of given aniline solution (estimation of aniline)
4. To determine the percentage of sulphur in the given organic compound by messenger's method.

Chairman
Department of Chemistry