INDRASHIL UNIVERSITY

(Established by an Act under the Gujarat Private Universities Act, 2009)

A Life Sciences University

Sustained Excellence with Relevance

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INDRASHIL UNIVERSITY

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DEPARTMENT OF CHEMISTRY (CHE)

PROGRAM STRUCTURE

M. Sc. (Chemistry) 2019-2021

SEMESTER - I			
Subject code	**Subject Name**	**L-T-P**	**Credits**
CH4 101	Mathematics for Chemists	3-0-0	3
CH4 102	Principles of Organic Chemistry	3-0-0	3
CH4 103	Inorganic Chemistry: Principles, Structure and Reactivity	3-0-0	3
CH4 104	Statistical Thermodynamics and Kinetics	3-0-0	3
CH4 105	Structures and Function of Biomolecules	3-0-0	3
CH4 106	Advanced Organic Chemistry Laboratory	0-0-6	3
CH4 107	Advanced Inorganic Chemistry Laboratory	0-0-6	3
	Total	15L-12P	**21**
SEMESTER -II			
Subject code	**Subject Name**	**L-T-P**	**Credits**
CH4 201	Advanced Organic Chemistry I	3-0-0	3
CH4 202	Advanced Inorganic Chemistry I	3-0-0	3
CH4 203	Advanced Physical Chemistry I	3-0-0	3
CH4 204	Bioinorganic and Bioorganic Chemistry	3-0-0	3
CH4 205	Applications of Spectroscopy I	3-0-0	3
CH4 206	Spectroscopic and Analytical Techniques	3-0-0	3
CH4 207	Advanced Physical Chemistry Lab	0-0-6	3
CH4 208	Biochemical Techniques Laboratory	0-0-6	3
IUM 000	Basic Communication and Soft Skills	1-0-0	0
	Total	19L-12P	**24**

SEMESTER -III			
Subject code	**Subject Name**	**L-T-P**	**Credits**
CH5 101	Advanced Organic Chemistry II	3-1-0	4
CH5 102	Advanced Inorganic Chemistry II	3-0-0	3
CH5 103	Advanced Physical Chemistry II	3-0-0	3
CH5 104	Applications Of Spectroscopy II	3-1-0	4
CH5 105	Analytical Techniques Lab	0-0-6	3
CH5 106	Organic And Medicinal Chemistry Lab	0-0-6	3
	Elective I	2-0-0	2
	Elective II	2-0-0	2
	Total	16L-2T-12P	**24**
SEMESTER -IV			
Subject code	**Subject Name**	**L-T-P**	**Credits**
CH5 201	Research or Industrial Project/Viva	0-0-20	10
CH5 202	Student Seminar (Based on Recent Research Articles)	0-0-2	2
	Elective III	2-0-0	2
	Elective IV	2-0-0	2
	TOTAL	4L-22P	**16**

Credit to Hours calculation:
Lecture: 1h = 1C
Practicals: 2h = 1C
Total credits: 85

LIST OF ELECTIVES

SEMESTER III

List of Available Subjects for Electives I, II

Subject code	Subject Name	L-T-P	Credits
CH5 107	Chemistry of Natural Products	2-0-0	2
CH5 108	Medicinal Chemistry	2-0-0	2
CH5 109	Supramolecular Chemistry	2-0-0	2
CH5 110	Chemistry of Materials	2-0-0	2

SEMESTER IV

List of Available Subjects for Electives III, IV

Subject code	Subject Name	L-T-P	Credits
CH5 203	Pharmaceutical Analysis	2-0-0	2
CH5 204	Chemistry of Nanomaterials	2-0-0	2
CH5 205	Advanced Heterocyclic Chemistry	2-0-0	2
CH5 206	Environmental and Green Chemistry	2-0-0	2

SEMESTER - I

CH 4 101 Mathematics for Chemists (L-T-P-C: 3-0-0-3)

Unit 1: Differential Calculus

Functions of several variables, continuity and differentiability, rules of differentiation, applications of differential calculus including maxima and minima, exact and non-exact differentials, Application of integral calculus, Coordinates transformation (e.g. Cartesian to spherical polar, cylindrical)

Unit 2: Vectors and Matrix Algebra

Gradient, divergence and Vector calculus, Green's theorem, Matrix equations: homogeneous, non-homogeneous linear equations and conditions for the solution, Linear dependence and independence, Eigen values, Eigen vectors

Unit 3: Ordinary Differential Equations

Variables separation method, Homogeneous linear differential equation, and exact first order differential equations, solutions of differential equations by the power series method, second and higher order homogeneous differential equations and their solutions, Complementary function, Particular integral by variation of parameter and method of undetermined coefficient, ODE with variable coefficient: Cauchy-Euler equation, Legendre's equation

Text Books:

1. Bhupendra Singh, "Mathematics for Chemist", 15th edition, Pragati Prakashan, **2015**.

Reference Books:

1. Peter Tebbutt, "Basic Mathematics for Chemists", 2nd edition, Wiley, 1998.
2. George Turrell, "Mathematics for Chemistry and Physics", Academic Press, 2002.

CH4 102 Principles of Organic Chemistry (L-T-P-C: 3-0-0-3)

Unit 1: Structure and Reactivity

Chemical bonding, delocalization, resonance, hyderconjugation, tautomerism, inductive effect, bonds other than covalent like ionic, hydrogen bonds.

Types of reactions, mechanisms, thermodynamic and kinetic requirements, Hammett equation, Hammond's postulate, Curtin-Hammett principle, Potential energy diagram, transition state & intermediate, methods of determining mechanism, isotope effects, solvent effects, substituent effects, Hard and soft acids and bases, Fate of structure on reactivity, resonance and field effects, steric effects, quantitative treatment. Generation, structure, stability and reactivity of organic reactive intermediates, such as carocations, carbanions, free radicals, carbenes and nitrenes.

Retrosynthesis: Introduction, synthons and synthetic equivalents, functional group inter-conversion, Synthesis of amines, region-specific, chemo-specific and stereospecific reactions, umpolung methods. Principles and applications of protective groups in protection of hydroxyl, amino, carbonyl and carboxyl groups, synthetic strategies for cyclic compounds.

Unit2: Organic Reaction Mechanism

Aliphatic nucleophilic substitution, S_N1, S_N2, S_Ni and mixed mechanism, the neighbouring group participation, anchimeric assistance. Classical and nonclassicalcarbocations, and detection by NMR spectroscopy. Reactivity effects of substrate structure, attaching nucleophile, leaving group and reaction medium, phase transfer catalysis, ambidentnucleophilicity. Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon.

Aromatic nucleophilic substitution reactions, S_{NAr}, S_N1, benzyne and $S_{RN}1$ mechanisms, Reactivity – effect of substrate structure, leaving group and attacking nucleophile.

Aromatic electrophilic substitution reactions, arenium ion mechanism, orientation and reactivity, energy profile diagram, the ortho/para ratio, ipso attack, orientation in other ring systems, and reactions thereof.

Unit 3: Stereo Chemistry

Stereochemistry: Basic principles, elements of symmetry, chirality, molecules with more than one chiral centre, enantiomers, diastereomers, threo and erythro isomers, groups and faces, absolute configurations at carbon (R, S, E and Z). Stereospecific and stereoselective reactions. Prochiral relationship, optical activity in biphenyls, spiranes, allenes and helical structures.

Stereochemistry of compounds containing Nitrogen, Sulphur and Phosphorous.Conformation and reactivity in acyclic compounds.

Reference Books:

1. Stereochemistry of carbon compounds - E.L. Eliel
2. Stereochemistry of organic compounds – D. Nasipuri
3. Stereochemistry: conformation and mechanism – P.S. Kalsi
4. Reaction mechanisms – Jerry March
5. A guide book to reaction mechanisms in organic chemistry – Peter Sykes
6. Mechanism and structure in organic chemistry - S.M. Mukherji & S.P.Singh
7. Organic Chemistry - L. G. Wade Jr

8. Advanced Organic Chemistry, Part A: Structure and Mechanisms - Francis A. Carey and Richard J. Sundberg
9. Advanced Organic Chemistry: Part B: Reaction and Synthesis - Francis A. Carey and Richard J. Sundberg
10. Organic Chemistry - Greeves, Warren, and Wothers Clayden.

CH4 103 Inorganic Chemistry: Principles, Structure and Reactivity (L-T-P-C: 3-0-0-3)

Unit 1: Principles of Inorganic Chemistry

VSEPR theory - Coordination polyhedra - Enumeration of geometrical and optical isomers

Theory of Acids and Bases: Bronsted and lewis acids and bases, gas phase versus solution acidity- solvent levelling effects, Hardness and softness- Surface acidity.

Oxidation and Reduction: Use of redox potential data - Nernst equation - Influence of complex formation, precipitation, change of pH and concentration on redox potentials - Analysis of redox cycles - Redox stability in water - Disproportionation/Comproportionation - Frost, Latimer and Pourbaix diagrams

Unit 2: Structure

Symmetry and Group Theory: Definitions and theorems of group theory, subgroups, Classes Molecular symmetry and symmetry groups – symmetry elements and operations. Symmetry planes, reflections, inversion centre, proper/ improper axes of rotation, products of symmetry operations, equivalent symmetry elements and atoms, symmetry elements and optical isomerism, symmetry point groups, classes of symmetry operations, classification of molecular point groups. Representations of groups. Great orthogonality theorem, character tables, properties of characters of representations. (No mathematical part.) Group theory and quantum mechanics, wave function as basis for irreducible representations.

Unit 3: Reactivity

Inorganic Reaction Mechanisms: Substitution reactions - Dissociative and associative interchange - trans-effect - Linear free energy relations - Rearrangements - Berry pseudo rotation - Electron transfer reactions - Photo-dissociation, -substitution and - redox reactions, Fluxional molecules.

Reference Books:

1. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Ed., 2009, OUP or D. F. Shriver and P. W. Atkins, ''Inorganic Chemistry'', 3rd Ed, OUP, 1999.
2. C. Housecroft, A. G. Sharpe, ''Inorganic Chemistry'', 3rd Ed., (or 4th Ed. in 2012) Prentice Hall/Pearson, 2008.
3. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Ed., John Wiley, 1988 (or F. A. Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ''Advanced Inorganic Chemistry'', 6th Ed. Wiley, 1999).
4. J. E. Huheey, E. A. Keiter, R. L. Keiter, ''Inorganic Chemistry: Principles of Structure and Reactivity'', 4th Ed., Prentice Hall, 1997.
5. G. L. Miessler, D. A. Tarr, ''Inorganic Chemistry'', 3rd Ed. Pearson Education, 2004.
6. G. Wulfsberg, ''Inorganic Chemistry'', University Science Books, 2000.

CH4 104 Statistical Thermodynamics and Kinetics (L-T-P-C: 3-0-0-3)

Unit 1: Statistical Thermodynamics

Limitations of classical thermodynamics. Introduction to the terms like ensemble, population, equipartition of energy, degeneracy. Boltzmann's distribution law, Evaluation of β, partition function, Distinguishable and indistinguishable particles, molar partition function, Electronic, Translational, Rotational and Vibrational partition functions. Sackur-Tetrode equation. Derivation of Fermi-Dirac statistics and Bose-Einstein statistics distribution law and their application. Applications of statistical thermodynamics- Heat capacity behaviour of solid and calculation of equilibrium constant.

Unit 2: Chemical Kinetics

Complex Reactions: Reactions approaching equilibrium, steady state approximation, Rate laws for consecutive, opposing and parallel reactions, explosive reactions. Chain reactions (formation and decomposition of HBr, HI, phosgene, thermal decomposition of N_2O_5 and C_2H_{10}, oxidation of methane). Comparison between gas phase and solution reactions, factors determining rates in solution. Reaction between ions, reactions involving dipoles, reactions in solution.

Fast reactions: Relaxation, stop flow and flash photolysis. Kinetics of enzyme reactions, Harpoon mechanism (Molecular Beam method).

Activated complex theory: Reaction coordinate and the transition state, potential energy surface, concentration of activated complex and rate constant, experimental observation of activated complex.

Theories of uni-molecular reactions: Lindemann, Hinshelwood, RRK and RRKM

Suggested Books:

1. Statistical Thermodynamics, M.C. Gupta, New Age Int. Ed. (1998)
2. An Introduction to Statistical Thermodynamics, T. L. Hill, Dover Publication (1986)
3. Fundamental of Classical and Statistical thermodynamics, B.N. Roy, Wiley (2002)
4. Chemical Kinetics, K. J. Laidler,(3rd Ed.), Pearson Education, Noida (1987).
5. Molecular reaction Dynamics, R.D. Levine, , Cambridge University Press, NY. (Paperback Edition) (2009)
6. Kinetics and Mechanism of Chemical Transformations, J. Raja Ram and J.C. Kuriacose, MacMillan Indian Ltd. (1993).

CH4 105 Structures and Function of Biomolecules (L-T-P-C: 3-0-0-3)

Unit 1: Amino-acids, Peptides and Proteins

Classification, structure and properties of amino acids and proteins, Synthesis of protein: reactive ester method and Merrifield synthesis.

Primary and Secondary structure of proteins, forces responsible for holding of secondary structures. α-helix, β-sheets, superb secondary structures, triple helix structure of collagen.

Tertiary structure of protein-folding and domain structure, Quaternary structure. Sequence determination; chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytosin and tryptophan releasing hormone (TRH).

Unit 2: Lipids

Classification, Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerol phospholipids, sphingo lipids, cholesterol, bile acids, prostaglandins eicosanoids, leukotriene.

Lipoproteins-composition and function, role in atherosclerosis.

Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological function. Biological membranes. Fluid mosaic model of membrane structure.

Unit 3: Carbohydrates

Classification, Conformation of monosaccharides, structures 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 function of glucosaminoglycans or mucopolysaccharides.

Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition, blood group substances.

Unit 4: Nucleic Acids

Purine and pyrimidine bases of nucleic acids, 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.

Chemical synthesis of mono and trinucleoside.

The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code.

Text Books:

1. Satyanarayana U, ChakrapaniU.,2014, Essentials of Biochemistry, Elsevier Health Sciences.
2. Robert K. Murray, Victor W. Rodwell, David Bender, Kathleen M. Botham, P. Anthony Weil, Peter J. Kennelly, 2009,Harper's Illustrated Biochemistry, 28th Edition, McGraw Hill Professional.

Reference Books:

1. Albert L. Lehninger, David L. Nelson, Michael M. Cox, 2005, *Lehninger, Principles of Biochemistry* W. H. Freeman, University Michael M Cox.

2. Donald Voet, Judith G. Voet, 2011, Biochemistry, 4th Ed. Hoboken, NJ: John Wiley & Sons.
3. Berg JM, Tymoczko JL, Stryer L., 2010, Biochemistry, 7th Ed. W.H. Freeman and Company.
4. James D. Watson, Andrew Berry, 2003, DNA: The Secret Life, Alfred A Knopf.
5. Keith Wilson, John Walker, 2010, Principles and Techniques of Biochemistry and Molecular Biology, Cambridge University Press.

CH4 106 Advanced Organic Chemistry Laboratory (L-T-P-C: 0-0-6-3)

Unit 1: Qualitative Analysis

Separation, Purification, drying of organic solvents and identification of three components mixture of Three organic compounds(three solids or two liquids and one solid or two solids and one liquid) using TLC for checking purity, Separating techniques, Introduction of IR, PMR and Mass Spectral data.

Unit 2: Purification Techniques

TLC, Rf values, Column Chromatography, Distillation, Vacuum Distillation, Steam Distillation.

Unit 3: Multistep Organic Synthesis

1. Preparation of m-dinitrobenzene.
2. Preparation of Tribromo aniline.
3. Preparation of Benzanilide
4. Methyl orange preparation.
5. Preparation of 2,4-dihydroxyacetophenone.
6. Preparation of Dibezalacetone

Suggested Books:

1. Vogel's textbook of practical organic chemistry – Arthur Israel Vogel, B. S. Furniss
2. Practical Organic Chemistry - Frederick George Mann and Bernard Charles Saunders
3. Advanced Practical Organic Chemistry - N K Vishnoi
4. Laboratory Manual of Organic Chemistry - R. K. Bansal

CH4 107 Advanced Inorganic Chemistry Laboratory (L-T-P-C: 0-0-6-3)

Unit 1: Quantitative Analysis
Statistical analysis of data sampling methods. Redox titrations (permanganometry, dichromatometry, iodometry). Complexometric titrations using EDTA (estimation of some metal ions, hardness of water).Quantitative separation of metal ions from a binary mixture (e.g. Cu2+/Fe3+). Gravimetric analysis (e.g. estimation of Ni2+).Analysis of ores and minerals (e. g. Iron ore, Potassium alum).Ion exchange separation of metal ions (e.g. Zn2+/Mg2+).

Unit 2: Synthesis
Synthesis of a variety of Inorganic Compounds/Complexes of 3d metal ions, main group elements and rare earths by using common experimental techniques.

Unit 3: Instrumental Methods
Introduction to various physical measurements (IR, UV-vis, mass, NMR, magnetic susceptibility, EPR and X-ray diffraction) for characterization of the compounds. Analysis and interpretation of the physical data of the compounds to determine their structures.

Suggested Books:
1. Vogel's Textbook of Quantitative Chemical Analysis, 5th Edn, Orient Longman, 1989.
2. Vogel's Textbook of Macro and Semimicro Qualitative Inorganic Analysis, 5th Ed., Orient Longman, 1982.

SEMESTER II

CH4 201 Advanced Organic Chemistry I (L-T-P-C: 3-0-0-3)

Unit 1: Organic Reaction Mechanism

Reactions of multiple bonds, mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio- and chemoselectivity. Addition to carbon-heteroatom multiple bonds. Addition of organometallic reagents containing lithium, magnesium, copper, zinc, mercury and cadmium. Ylides and Wittig reaction, mechanism of alkylation and condensation reactions involving enolates.

Elimination reactions. E_2, E_1 and E_{1cB} mechanism, orientation of the double bond.

Oxidation reactions, application using Cr, Mn, Ce, Pb, Pd, Pt, Os based reagents, m-CPBA, O_3, $NaIO_4$, etc. Reduction reactions involving hydrogen and metal catalysts, and dissolving metals, R_3SnH, Wilkinson catalyst, borane and reagents thereof, $LiAlH_4$ and Dibal-H.

Unit 2: Reactions and Rearrangement Reactions

Molecular Rearrangements. Mechanism of molecular rearrangements involving nucleophilic, electrophilic and free radical. Carbon-carbon rearrangements: Wagner–Meerwein, Tiffeneau–Demyanov, Favorskii, Wolff, Benzil–Benzilic acid, Neber, Benzidine rearrangements, Carbon–nitrogen rearrangements: Hoffmann, Curtius, Lossen Schmidt and Beckmann rearrangements. Carbon–oxygen rearrangements: Bayer–Villiger, Dakin and Wittig rearrangements. Fries, Claisen, Cope reactions. Reactions involving P, N and S Ylides.

Unit 3: Introduction to Hetero cyclic chemistry

Heterocyclic chemistry: Nomenclature, Hantzsch-Widman rules for fused and bridge ring systems. Heterocycles containing 3, 4, 5, 6-member rings and their reactivity, synthesis and applications in drug molecules. Fused heterocycles.

Suggested Books:

1. Guide book to organic synthesis- R. K. Meckie, D. M. Smith, R. A. Atken
2. Organic synthesis -O. House
3. Organic synthesis- M. B. Smith
4. Advanced organic chemistry. Part A Structure & Mechanism -Francis A.
5. Coreyan. Richard J. Sundberg Heterocycles by R.K. Bansal
6. An introduction to chemistry of heterocyclic compounds – R.M. Acheson
7. Heterocyclic chemistry – John A. Joule and Keith Mills
8. Heterocyclic Chemistry - Thomas. L. Gilchrist

CH4 202 Advanced Inorganic Chemistry I (L-T-P-C: 3-0-0-3)

Unit 1: Main Group Chemistry

Perspectives, periodicity & periodic anomalies – Relativistic effects on chemical properties.

Hydrogen and its compounds: H-bond and its influence on the structure and properties of crystals Hydrides→classification: electron deficient, electron precise and electron rich hydrides.

Alkali and alkaline earth metals: Solutions in liquid ammonia - Synthesis, properties, uses and structures of crown ether complexes, cryptands and organometallic compounds.

Group 13 elements: Borides, borates, boron halides, boranes, carboranes and metallocarboranes, BN compounds, transition-metal stabilized borylene and boryllithium, organoaluminum compounds, Lewis Base adducts of AlR_3 compounds, Subvalentorgano-Al compounds, Organo-gallium, -indium, and –thallium compounds.

Group 14 elements: Allotropes of Carbon- C60 and its compounds (fullerenes) - carbon nanotubes: synthesis and properties -Intercalation compounds of graphite - Pure Silicon, silica and silicates, Silicones - Low coordinated and hypervalent Silicon compounds - Brief survey of Ge, Sn, and Pb chemistry- Organo-germanium, -tin, and -lead compounds.

Group 15 elements: P(V) compounds (structure, bonding, reactivity) - P(III) compounds: diphosphenes, phosphaalkenes, iminophosphanes - P-containing ring systems (phosphabenzene, phosphole), phosphazenes, P-S compounds.

Group 16 elements: Sulfur polycationic and anionic species - SN compounds.

Unit 2: Halogens and Nobel Gases

Group 17 elements: Charge-transfer complexes of halogens, inter-halogen compounds, halogen oxides and oxygen fluorides, pseudo halogens.

Group 18 elements: Noble gas clathrates and compounds.

Unit 3: Inner Transition Elements

Inner transition elements: Chemistry of f-block elements - Binary compounds – Organometallic compounds - Relation to p-block and d-block chemistry – Tran'sactinides (super-heavy elements).

Suggested Books:

1. A G. Massey, "Main group chemistry", Wiley, 2000.
2. N. N. Greenwood and A. Earnshaw, "Chemistry of the Elements", Pergamon Press, 1989.
3. P. Atkins, T. Overton, J. Rourke, M. Weller, F. Armstrong: Shriver and Atkins' Inorganic Chemistry, Fifth Edition, 2009, OUP or D. F. Shriver and P. W. Atkins, ''Inorganic Chemistry'', 3rd Ed., OUP, 1999.
4. C. Housecroft, A. G. Sharpe, ''Inorganic Chemistry'', 3rd Ed. (or 4th Ed. in 2012) Prentice Hall/Pearson, 2008.
5. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 5th Ed., John Wiley, 1988
6. A.Cotton , C. A. Murillo, M. Bochmann and R. N. Grimes, ''Advanced Inorganic Chemistry'', 6th Edn Wiley, 1999).
7. J. E. Huheey, E. A. Keiter, R. L. Keiter, ''Inorganic Chemistry: Principles of Structure and Reactivity'', 4th Ed., Prentice Hall, 1997.

CH4 203 Advanced Physical Chemistry I (L-T-P-C: 3-0-0-3)

Unit 1: Surface Sciences

Adsorption – surface tension, capillary action pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon), Catalytic activity at surfaces.

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-phase separation, solubilisation, micro emulsion, reverse micelles

Unit 2: Electrochemistry

Electrochemistry of solutions. Debye-Hückel-Onsager treatment and its extension, ion-solvent interactions, Debye-Hückel-Jerummodel. Thermodynamics of electrified interface equations, derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces- Guoy-Chappman, Stern, Graham-Devanathan-Mottwatts models.

Polarography theory- Ilkovic equation, half-wave potential and its significance.

Introduction to corrosion, homogeneous theory, forms of corrosion monitoring and prevention methods.

Suggested Books:

1. Non-ionic surfactants, M. J. Schick, Surfactant Science Series, (1985)
2. Colloids and Interface Science, P. Ghosh, PHI learning Pvt. Ltd. New Delhi (2009).
3. Surfactants and Interfacial Phenomena, M. J. Rosen, John Wiley, New Jersey (2004).
4. Handbook of surfactants, M. R. Porter, Chapman and Hall, London (1994).
5. Physical Chemistry of Surface, A.W. Adamson, John Wiley (1997).
6. Textbook of Polymer Chemistry , F.W. Billmeyer Jr., John Wiley (1994)
7. Introduction to Polymer Chemistry , R.B. Seymour, McGraw Hill (1971)
8. Physical chemistry of Polymer , A Tager, Mir Pub (1978)
9. Polymer Science ,V.R. Gowarikar, N.V. Viswanathan & J. Sreedhar, New Age Int. Ed. (1986)
10. Polymeric Multicomponent Materials, L.H. Sperling, John Wiley (1997)
11. Physical Chemistry of Electrolytic Solution, H.S. Harned& B.B. Owen, Reinhold (1950)

CH4 204 Bioinorganic and Bioorganic Chemistry (L-T-P-C: 3-0-0-3)

Unit 1: Bio Inorganic Chemistry

Essential and trace metals, Na^+/ K^+ pump, Role of metal ions in biological processes, DNA Polymerization, Glucose Storage, metal complexes in transmission of energy Chlorophylls, Photo system I and Photo system II in cleavage of water.

Model systems, Heme proteins and Oxygen uptake, spectrum and function of hemoglobin, myoglobin, hemocyanins, and hemeerythrin, model synthetic complexes of Iron, Cobalt and Copper.

Structure and function of metallo proteins in electron transport process cytochromes and ion sulphur proteins. Synthetic models, Biological nitrogen Fixation, Molybdenum nitrogenase, Spectroscopic and other evidences.

Unit 2: Bio Organic Chemistry

Basic considerations, Proximity effects and molecular adaptation, Introduction and historical perspective, chemical and biological analysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification, Fisher's Lock and key theory, induced fit theory.

Hypothesis, Concept and identification of actives site using inhibitors, affinity labelling and enzyme modification by site directed mutagenesis. Enzyme kinetics, Michaelis-Menten and line weaver, Burk plots, reversible and irreversible inhibition.

Suggested Books:

1. Principles of Biochemistry A. L. Lehninger, Worth publishers.
2. Biochemistry by L. Stryer, W. H. Freeman.
3. Biochemistry by Voet and Voet, Wiley.
4. Biochemistry by J. David and Rawn, Neil Patterson.
5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, John Wiley.
6. Understanding Enzymes by Trevor palmer, Prentice Hall.
7. Enzyme chemistry: Impact and applications Ed. Collins, J. Suckling, Chapman and Hall.
8. Enzyme mechanisms Ed., M. I. Page and A. Williams, RSC.
9. Fundamentals of Enzymology N. C. Price and L. Stevens, Oxford.
10. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D.

CH4 205 Applications of Spectroscopy I (L-T-P-C: 3-0-0-3)

Unit 1: Vibrational, UV and IR Spectroscopy

Vibrational Spectroscopy Rotational and vibrational spectra. Moment of inertia and rotational spectra of rigid and non rigid diatomic molecules. Vibrational excitation effect. Rotational spectra of symmetric - top molecules. Strakeffect. Vibrational energy of diatomic molecules.Anharmonic oscillator, overtones and hot bands. Diatomic vibrator rotator (P, Q and R branches of diatomic vibrator rotator). Rotational vibrational spectra of symmetric top molecules.

UV Spectroscopy Origin of electronic spectra, Lambert-Beer's absorption law, Types of electronic transitions. Effect of solvent, substituent, conjugation on electronic transitions.Benzene and its substituted derivatives. Applications of UV visible spectroscopy in analysis (qualitative/quantitative) of polyenes/aromatic (hetero & homo) systems, geometrical isomers, keto-enoltautomers, components of a mixture, ionization constants of acids and bases. Woodward-Fieser rules for calculating absorption maximum in dienes, trienes and α, β-unsaturated carbonyl compounds.

R Spectroscopy Vibrational energy of a diatomic molecule-and harmonic oscillator, Selection rules- Overtones-hot bands. Zero-point energy-Calculation of force. Constant of diatomic molecules. Rotational –Vibrational spectra of diatomic molecules- P,Q,R branches. Instrumentation sources sampling techniques. Characteristic vibrational frequencies of alkanes, alkenes, 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, overtones, combination bands and Fermiresonance. FTIR. Rofgaseous, solids and polymeric materials.

Unit 2: Raman and Mossbauer Spectroscopy

Raman spectroscopy Quantum theory of Raman effect, Classical theory of Raman effect, Pure rotational Raman spectra, Raman activity of vibrations, Vibrational Raman spectra, polarization of light and Raman effect, applications., Mutual exclusion principle and Raman spectra of Hg_2^{2}+, NO_3-, ClO^{3-}, N_2O, CO_2 and CH_4.

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 detection of oxidation state and in equivalent MB atoms.

Unit 3: Chromatography, GC and HPLC techniques

Chromatographic and Electrophoretic methods of separation, Principles and applications of Paper, Thin layer & HPTLC, Gas, Gas-liquid, Liquid chromatography, HPLC and FPLC; Paper and gel electrophoresis.

Suggested Books:

1. Instrumental methods of Analysis- Willard, Dean & Settle.
2. Principles of Instrumental Analysis - Skoog, Holler and Wieman
3. Introduction to photoelectron spectroscopy - P. K. Ghosh
4. Applications of Mössbauer Spectroscopy - Green Wood
5. Structural inorganic chemistry-Mössbauer spectroscopy – Bhide

6. Spectroscopic identification of organic compounds- Silverstein, Basseler and Morril
7. Application of absorption spectroscopy - John R. Dyer
8. NMR in chemistry -A multinuclear introduction - Willam Kemp
9. Organic Spectroscopy - William Kemp
10. Spectroscopic methods in Organic chemistry - DH Williams and I Fleming
11. Modern NMR techniques for chemistry research - Andrew B Derome
12. Introduction to organic spectroscopy - Pavia
13. Carbon-13 NMR for organic chemists - GC Levy and O L Nelson
14. Nuclear Magnetic Resonance Basic principles - Atta-Ur-Rahman
15. Applications of Mössbauer spectroscopy -N.N. Greenwood and T.C. Gibb, Chapman & Hall
16. Principles of Mössbauer spectroscopy-T.C. Gibb, Chapman & Hall.
17. Physical methods for chemists- R.S. Drago, 2nd ed. (Saunders College Publishers)
18. Spectroscopy of organic compounds- P. S. Kalsi.

CH4 206 Spectroscopic and Analytical Techniques (L-T-P-C: 3-0-0-3)

Unit 1: NMR Spectroscopy

Introduction, Defination, Chemical shift, spin spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic andaromatic) and other nuclei (alcohols, phenols, enols, carboxylicacids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (firstorderspectra), virtualcoupling.

Stereochemistry, hindered rotation, Karpluscurve variation of coupling constant with dihedral angle.

Simplification of complex spectra nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Over Hause effect (NOE). Resonanceofother nuclei-F.P.

Applications of spin-spin coupling in determination of structure and stereochemistry of Organic molecules, NOE and its applications.

Electron Spin Resonance Spectroscopy Hyper 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.

Unit 2: Mass Spectroscopy

Origin of mass spectrum, principles of EI mass spectrometer- Instrumentation. Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule, Nitrogen rule, isotopic peaks, metastable ion peaks, determination of molecular formula and High-resolution mass spectrometry.

Salient features of fragmentation pattern of organic compounds- α-cleavage, β-cleavage, McLafferty rearrangement, Retro-Diels-Alder fragmentation and ortho effect.

Fragmentation pattern of individual heterocyclic systems viz., Furan, Pyrrole, Thiophene and Pyridine. Preliminary account of chemical ionization.

Unit 3: Hands on Examples Based on Above Techniques

Combined application of UV, IR, 1 H-NMR, 13C -NMR and Mass spectra: Introduction to the analytical approach towards the structure elucidation of simple organic molecules by combined application of UV, IR, 1 H-NMR 13C-NMR and Mass spectra.

Suggested Books:

1. Physical Methods for Chemistry, R. S. Drago, Saunders Company.
2. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
3. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
4. Progress in Inorganic Chemistry vol.,8, ed., F.A. Cotton, Vol., 15, ed.S.J. Lippard, Wiley.
5. NMR, NOR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
6. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J.IV Brtin, Heyden.
7. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and, T.C. Morrill, John Wiley.

8. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
9. Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
10. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.

CH4 207 Advanced Physical Chemistry Lab (L-T-P-C: 0-0-6-3)

1. To determine the percentage composition of strong acid and weak acid in given mixture using conductometric method.
2. To determine the rate constant and energy of activation of hydrolysis of methyl acetate at two different temperature.
3. To determine the relative strengths of the given strong acids by studying the kinetics of inversion of cane sugar using polarimeteric method.
4. To determine the Critical Micelle Concentration of given surfactant (SDS) by conductometric method.
5. To determine the viscosity average molecular weight of a given polymer sample using Ostwald's viscometer.
6. To determine the Redox potential of Fe^{2+}/ Fe^{3+} system by potentiometric method.
7. To determine the strength of given unknown $AgNO_3$ using potentiometric method.
8. To determine the dissociation constants (pK_1 and pK_2) of given dibasic acid using pH-metric method.
9. To determine the K_{sp} of Barium Sulphate, Silver Chloride and Silver Chromate using conductometric method.
10. To determine the dissociation constant of monobasic acids (acetic acid, benzoic acid and Salicylic acid) by potentiometric method.

CH4 208 Biochemical Techniques Laboratory (L-T-P-C: 0-0-6-3)

1. Determination of pI of Amino acid by titration method.
2. Identification of monosacharides and di-sacharides by recrystalization.
3. Separation of amino acids by TLC.
4. Estimation of total sugar by Anthrone method.
5. Estimation of amino acid by Anthrone method.
6. Estimation of protein by Lowery's method.
7. Determination of a) Iodine number b) Acetyl number of a Lipid.
8. Separation of amino acids by paper chromatography.

Suggested Books:

1. Analytical techniques in Biochemistry and Molecular Biology by Katoch, R, Springer (2011).
2. Basic methods for the Biochemical Lab; Martin H, Springer (2007).
3. Principles and Techniques in Biochemistry and Molecular Biology 7th Ed. Wilson. K., Walker. J, Cambridge University Press (2010)
4. Biochemistry Lab fax Ed. J.A.A. Chambers and D. Rickwood, Blackwell Science, (1993).
5. Laboratory Techniques in Biochemistry and molecular biology, Work and Work Vol. I & II.

IUM 000 Basic Communication and Soft Skills (L-T-P-C: 1-0-0-0)

Unit 1: Fundamentals of Communication
- Importance of Communication
- Importance of Interpersonal Communication
- Process of Communication
- Flows and Types of Communication

Unit 2: Barriers to Communication
- Definition
- Types of Barriers

Unit 3: Listening
- Hearing & Listening
- Types of Listening
- Do's and Don'ts of Effective Listening

Unit 4: Effective Presentation
- Patterns & Methods of Presentation, Oral Presentation
- How to prepare presentation
- Effective ways to deliver the presentation
- How to prepare multi-media presentation
- Difference between C.V & Resume, types of resume

Unit 5: Corporate Etiquettes
- Non-verbal Communication
- E-mail etiquette, telephone etiquette, dining etiquette
- Office meeting etiquettes, dress etiquette

Text Books:
1. Soft Skills for Everyone by Jeff Butterfield, Cengage publication
2. Technical Communication; Principles and Practice" by Meenakshi Raman & Sangita Sharma (Oxford University Press)
3. "Communication Skills" by Dr. Sanjay Kumar and Dr. Pushp Lata, Oxford University Press

Reference Books:
1. Personality Development and Soft Skills by Barun K Mitra
2. Business Correspondence and Report writing"- R C Sharma and Krishna Mohan, Tata McGraw Hill, 8th Ed.2015

SEMESTER - III

CH5 101 Advanced Organic Chemistry II (L-T-P-C: 3-1-0-4)

Unit 1: Free Radicals, Photochemistry and Pericyclic Reactions

Formation, stability and detection of short and long lived free radicals, homolysis, addition and rearrangements and cyclization of free radicals and their applications.

Basics of photochemical reactions, photochemistry of olefins, carbonyl compounds and aromatic compounds (Isomerization, Norrish Type I and II, photoreduction, Patterno-Buchireaction, cycloaddition, rearrangement and aromatic substitution reactions. Barton reaction, reactions of singlet oxygen. Applications of photochemical reactions in organic synthesis and natural product synthesis.

Orbitals, molecular orbital symmetry, molecular orbital of ethylene, 1,3-butadiene, 1,3,5–hexatriene and allyl systems, concerted reactions, classification of pericyclic reactions, derivation of selection rules through construction of correlation diagrams for cycloaddition reactions and for electrocyclic reactions with 4n and 4n+2 π electrons, conrotatory and disrotatory motions for electrocyclic ring opening and ring closure. FMO approach for derivation of Woodward-Hoffman selection rules for cyclo addition and electrocyclic reactions, suprafacial and antarafacialcyclo additions. Secondary effects and stereochemistry of cyclo additions; 2s+2a cyclo addition of ketenes. The Cope and the Claisen rearrangements, theene reaction.

Unit 2: Organic Synthesis

Transitional metals complexes in organic synthesis and Boron, Si, Sn Chemistry, Transition metal complexes in organic synthesis-Introduction-oxidation states of transitionmetals, 16-18 rule, dissociation, association, insertion, oxidative addition, reductive eliminationof transition metalOrganopalladium in organic synthesis- Heck arylation, allylic activation, carbonylation, wackeroxidation, isomarization formation N-aryl and N-alkyl bond transmetalation, allyldeprotectioninpeptides, coupling reactions: Stille coupling, Sonogashira and Suzuki coupling reactions andtheir importance

Reactions Iron carbonyls, ferrocenes, Fe-cyclopentadiene complex, protection of dienes, Isomerization.Wilkinson, Noyori, Knowls catalyst of Ruthenium and Rhodium – synthesis and uses its use inhydrogenation reactions-deallylation, C-C, C-O, C-N bond cleavages, Synthesis and uses of organosilane and organo tin compounds, Olefin metathesis by Ist, and IIndgeneration catalyst, reaction mechanism and application in the synthesis of homo and heterocyclic compounds

Unit 3: Assymetric synthesis

Recapitulation of Stereochemical concepts- enantiomers, diastereomers, homotopic and heterotopic ligands, stereoselective and stereospecific reactions, prochirality, Chemo-, regio-,diastereo- and enantio-controlled approaches; Chirality transfer, Asymmetric inductions; Chiralpools, Chiral auxiliaries, chiral reagents and catalysts, and templates;Asymmetricallylation, Asymmetriccycloaddition reactions. Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, FelkinAnh rule, Houk model, Cram's chelate model. Asymmetric synthesis use of chiral auxiliaries, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation.

Asymmetric reduction reactions: Reduction of ketones, imines and olefins(use of BINOLS) Asymmetric C-C bond forming reaction: Simmon-Smith reaction, aldol reaction and alkylation based on Organo catalytic methods, Mukayamaaldol reaction, Shibasaki bi-metallic catalyst system; RAMP-SAMP based alkylation strategy, Meyers oxazoline and bis-lactam based methods.

Suggested Books:

1. Molecular reactions and photochemistry -C. Dupey & O. L. Chapman
2. Molecular photochemistry -Turro
3. Molecular Photochemistry - Gilbert & Baggo
4. Organic Photochemistry - D Coyle
5. Molecular Reactions and Photochemistry – Depuy and Chapman
6. Photochemistry - C W J Wells
7. Some modern methods of organic synthesis -W. Carruthers
8. Guide book to organic synthesis- R. K. Meckie, D. M. Smith, R. A. Atken
9. Organic synthesis -O. House
10. Organic synthesis- M. B. Smith
11. Advanced organic chemistry. Part A Structure & Mechanism -Francis A.
1. Coreyand Richard J. Sundberg
12. March's Advanced Organic Chemistry -Michael B. Smith
13. Conservation of Orbital Symmetry -Woodward and Hoffmann
14. Organic Reactions and Orbital Symmetry, -Gilchrist and Storr
15. Pericyclic Reactions — a problem solving approach- Lehr and Merchand
16. Pericyclic Reactions - A Textbook: Reactions, Applications and Theory- S. Sankararaman, Roald Hoffmann
17. Pericyclic Reactions - Mukherjee S M

CH5 102 Advanced Inorganic Chemistry II (L-T-P-C: 3-0-0-3)

Unit 1: Organometallic Chemistry and Catalysis

Organometallic Chemistry: Complexes with pi-acceptor and sigma-donor ligands - 16 electron and 18 electron rules – Stability and Reactivity - Isolobal analogy - Structure and bonding - Agnostic interaction.

D bock carbonyl, σ-Organyls, Metal carbenes and metal carbynes, Ferrocene.

Homogeneous and Heterogeneous Catalysis: Hydrogenation, carbonylation, polymerization, Wacker oxidation and other reactions catalyzed by transition metal complexes.

Metal Cluster Compounds: Metal-metal bond - Carbonyl and non-carbonyl clusters - Structure and bonding - Low-dimensional solids - Clusters in catalysis.

Unit 2: Properties of Solids

Thermal Properties: Lattice vibrations - phonon spectrum; Lattice heat capacity; Thermal expansion; Thermal conductivity. Electrical Properties: Free electron theory - electrical conductivity and Ohm's law - Hall effect; Band theory - band gap - metals and semiconductors - intrinsic and extrinsic semiconductors; Hopping semiconductors; Semiconductor/metal transition; p-n junctions; Superconductors - Meissner effect - type I and II superconductors - isotope effect - basic concepts of BCS theory - manifestations of the energy gap - Josephson devices. Magnetic Properties: Classification of magnetic materials; Langevin diamagnetism; Quantum theory of paramagnetism; Cooperative phenomena - ferro, antiferro and ferrimagnetism - magnetic domains and hysteresis; Super paramagnetism.

Optical Properties: Optical reflectance - plasmon frequency; Raman scattering in crystals; Photoconduction; Photo and electroluminescence; Lasers; Photovoltaic and photo electro chemical effects.

Suggested Books:

1. H. V. Keer, Principles of the Solid State (541.0421 K25P)
2. L. E. Smart and E. A. Moore, Solid State Chemistry: an Introduction (541.0421 Sm295)
3. M. T. Weller, Inorganic Materials Chemistry (546 W45I)
4. K. J. Klabunde, Nanoscale Materials in Chemistry (660 K66N)
5. W. D. Callister, Materials Science and Engineering, An Introduction (620.11 C13M)
6. C. Kittel, Introduction to Solid State Physics (530.41 K65I)

CH5 103 Advanced Physical Chemistry II (L-T-P-C: 3-0-0-3)

Unit 1: Catalysis I

Heterogeneous catalysis: Kinetics and Mechanism of surface reactions. Surface heterogeneity, activity and selectivity, deactivation and regeneration. Theories of promotion and poisoning of catalysts. Catalyst Synthesis: supports and supported catalysts. Zeolites and zeolite-like materials, precipitation and impregnation methods. Characterization of catalysts: Surface area, pore size distribution (mercury porosimetry) Thermal methods (DTA, TG, TPD and TPR), Surface acidity, Photoelectron spectroscopy (XPS, AES, XRF),LEED, Mossbauer spectroscopy, IR, SIMS, Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM).

Unit 2: Catalysis II

Theories of catalysis by metals, semiconductors and supported catalysts. Geometric and electronic factors. Important applications of heterogeneous catalysis in petroleum, petrochemicals and fine chemicals, catalysis in pollution control. Homogeneous catalysis: Reactions involving carbocations, transition metal complexes as catalysts, Olefin hydrogenation with Wilkinson's catalyst and methanol carbonylation. Important industrial applications.

Unit 3: Solid State Chemistry

Crystallography- Recapitulation, diffraction properties of crystals. symmetry elements, space groups. Ionic crystals. Determination of crystal structure. Imperfection in crystals- point defects (Thermodynamic treatment) and line defects. Crystal growth, Crystal engineering and polymorphism.

Electronic properties and band theory-Metal, insulators and semiconductors, electronic structure of solid- band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors. Optical properties and magnetic properties.

Suggested Books:

1. Catalytic Chemistry, B.C. Gates, John Wiley (1992)
2. Principles and Practice of Heterogeneous Catalysis, J.M. Thomas & W.J. Thomas, Weinheim NY (1997)
3. Spectroscopic Characterization of Heterogeneous Catalysis, J.L.G. Fierro, Elsevier (1990)
4. Adsorption and Catalysis, D.K.Chakrabarty, New Age International Pvt. Ltd. Tailored Metal Complexes, Y. Ivasawa, D.Reidel Co. (1986).
5. Solid State Chemistry and its Applications, A. R. West, John Wiley (2014).
6. Solid State Chemistry, D. K. Chakrabarty, New Age Int., New Delhi, (2009).
7. Atomic Structure & Chemical Bond, Manas Chandra, Tata McGraw Hill (1995).
8. Treatise on Solid State Chemistry VolI , VII , B.N. Hannay, Plenum Press (1975).
9. Introduction to Solids, L. V. Azaroff, McGraw Hill (1960).
10. The Crystal as A Supramolecular Entity: Perspectives in Supramolecular.
11. Chemistry, G.R. Desiraju, Wiley-VCH (1996)

CH5 104 Application of Spectroscopy II (L-T-P-C: 3-1-0-4)

Unit 1: NMR Spectroscopy

Second order effects, examples of AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, use of chemical shift reagents for stereochemical assignments. ^{13}C NMR, introduction to FT technique, relaxation phenomena, NOE effects, 1H and 13C chemical shifts to structure correlations. Editing techniques: INEPT and DEPT methods Study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (bullvalene and related systems). 2D NMR spectroscopy, COSY, HMBC, HMQC, NOESY. Time scale- Multinuclear and Organometallic NMR spectroscopy -More common spin-1/2 nuclei, ^{19}F, ^{31}P, with few examples.

Unit 2: ORD and CD, Polarimetry

Basic concepts of optical rotatory dispersion (ORD) and circular dichroism (CD), Deduction of absolute configuration–Cotton effect–Octant rule for ketones. Applications of ORD and CD spectroscopy.

Unit 3: Problem Solving

Examples of structure elucidation using UV, IR, NMR and Mass techniques. Hands on training with experiments on above techniques

Suggested Readings:

1. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J.IV Brtin, Heyden.
2. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
3. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.

CH5 105 Analytical Techniques Lab (L-T-P-C: 0-0-6-3)

1. Determination Bathochromic shift in alkaline medium of p-Nitro phenol Compared to p Nitro phenol.
2. Determination Hypsochromic shift in acidic medium of Aniline compared to Aniline.
3. Recording the I.R Spectrum Different Organic compounds
   a) Aliphatic and aromatic alcohols. b) Aliphatic and aromatic carbonyl compounds (aldehydes, ketones, esters and acids etc.) c) Aromatic and aliphatic Nitro, Amines, Nitriles, alkenes, alkynes and Amides.
4. Use of Computer techniques
   a) Chem Draw, Chem Sketch, ISIS Draw, Pymol calculations, Mestrec Softwares operations. b) Draw the Structure of Simple aliphatic, aromatic and heterocyclic compounds in Chem Draw with different substituent. Get the correct IUPAC Name and predict the IH-NMR Spectra.

Suggested Books:

1. Practical Organic Chemistry, R. K. Bansal.
2. Organic Structures from Spectra, 4th Edition, L. D. Field, S. Sternhell, J. R. Kalman, Wiley & Sons, Ltd.
3. Practical Organic Chemistry by Mann & Saunders.
4. Kemp, W (1994): Organic Spectroscopy, 3rd Ed., MacMillan
5. Kalsi,P.S (2007): Spectroscopy of Organic Compounds, 6th Edition, New age international publishers.
6. Sharma Y.R (1992): Elementary Organic Spectroscopy – Principles and Chemical applications, S.Chand

CH5 106 Organic and Medicinal Chemistry Lab (L-T-P-C: 0-0-6-3)

1) Multistep synthesis:
i) Benzanilide by Beckmann's rearrangement:
(a) Preparation of benzophenoneoxime (b) Beckmann's rearrangement to benzanilide
ii) Benzilic acid from benzoin:
(a) Benzil from benzoin (b)Benzilic acid from benzil
iii) Anthranilic acid from phthalic anhydride:
(a) Phthalimide from Phthalic anhydride (b) Hoffmann's rearrangement to anthranilic acid.
2) Monitorization of Each step with HPLC, I. R and NMR. 3) Calculation of Opticatical rotation value of Glucose and Sucrose. 4) Isolation of Piperine from black pepper.

Recommended Books:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner,
4. Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin
5. Practical organic chemistry by Mann & Saunders
6. Spectroscopic identification of organic compounds by R M Silverstein and F X

ELECTIVES: SEMESTER - III

CH5107 Chemistry of Natural Products (L-T-P-C: 2-0-0-2)

Unit 1: Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprenerule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Menthol, Santonin, and B-Carotene.

Unit 2: Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloid sin plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine,(+)-Nicotine and Morphine.

Unit 3: Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bileacids, Estrone,. Biosynthesis of steroids.

Unit 4: Prostaglandins

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGF_2a. Synthesis and reactions of Pyrethroids and Rotenones.

(Forstructure elucidation, emphasis to be placed on the use of spectral parameters wherever possible).

Suggested Books:

1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs,
2. OrganicChemistry,Vol2,I.L.Finar,ELBS.
3. Stereo selective Synthesis: A Practica lApproach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed.S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plantsfrom the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
7. New Trends in Natural Product Chemistry, Atta-ur-Rahmanand M.l. Choudhary, Harwood Academic Publishers.
8. Insectcides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

CH5 108 Medicinal Chemistry (L-T-P-C: 2-0-0-2)

Unit 1: Drug Design

Development of new drugs, procedures followed in Drug design, Concepts of Lead compound and Lead modification, Concepts of Pro drugs and Soft drugs, Structure and activity relationship (SAR), factors effecting the bioactivity, resonance inductive effect, isosterism, Bio isosterism, spatial considerations. Theories of drug activity, occupancy theory, rate theory, induced fit theory, Quantitative structure activity relationship. History and development of QSAR, Concepts of drug receptors, Elementary treatment of drug receptor interaction. Physico chemical parameters, lipophilicity, partition coefficient, electron ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free Wilson analysis, Hansch analysis, relationships between Wilson and Hansch analysis. LD 50, ED-50 (Mathematical derivation of equations excluded). Introduction to adsorption, disposition, elimination using pharmaco kinetics, Important Pharmacokinetic parameters in defining drug disposition and in therapeutics, mention of uses of pharmacokinetics in drug development process. Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, Sulphonamides, membrane active drugs, Drug metabolism, Xenobiotics, Biotranformation, Significance of drug metabolism in medicinal chemistry.

Unit 2: Anti neo Plastic Agents, Cardio Vascular, Anti Infective Drugs

Anti neoplastic agents: Introduction, cancer chemotherapy, special problems, role of alkylating agents and anti metabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

Cardiovascular Drugs and anti-infective drugs:

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular rout put. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine,

Local Antiinfective Drugs:

Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixicacid,ciprofloxacin, norfloxacin, dapsone, amino salicylicacid, isoniazid, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloro quinine and primaquinone.

Unit 3: Antimalarial and Antituberculosis and Anti Biotic Drugs

Antimalarials: Modern chemotherapy of malaria, 4-amino and 8-amino quinolins, 9-amino acridine. Synthesis of mefloquines, chloroquine, primaquine and daraprim Mode of action of antimalarial agents SAR of antimalarial agents Anti tuberculosis: Synthesis of only the following drugs: Isoniazid (INH), Ethionamide, Ethambutol, DDS (Dapsone)

Antibiotics: Cell wall biosynthesis, inhibitors, 13-lactamrings, antibiotics inhibiting proteins synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Suggested Books:

1. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH.
2. Wilson and Gisvolds Text book of Organic Medicinal and Pharmaceutical Chemistry
3. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-1(Chapter-9 and Ch14), Ed. M.E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
6. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

CH5 109 Supramolecular Chemistry (L-T-P-C: 2-0-0-2)

Unit 1:
Definition of supramolecular chemistry, Hydrogen bonding and nature of supramolecular interactions: ion-ion, ion-dipole, dipole-dipole, cation-π, anion-π, π-πand Van der Waals interactions.

Unit 2:
Receptors, host-guest interactions, lock and key analogy, pre-organization and complimentarity, binding of cationic, anionic, ion pair and neutral guest molecules, selectivity and solution behaviour of crown ethers, complexation of organic cations, siderophores, biological anion receptors, cnticrowns and coordination interactions.

Unit 3:
Self-Assembly Self-assembly of molecules: Design, synthesis and properties of the molecules, self-assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots, examples of recent developments in supramolecular chemistry.

Unit 4:
Crystal engineering Crystal engineering: role of H-bonding, halogen bonding and other weak interactions, co-crystals, salts, polymorphs and their physico-chemical properties, coordination polymers, metal organic frameworks and their properties.

Text Books:

1. J.M. Lehn, Supramolecular Chemistry-Concepts and Perspectives, Wiley-VCH, 1995.
2. P. D. Beer, P. A. Gale and D. K. Smith, Supramolecular Chemistry, Oxford University Press, 1999.
3. J. W. Steed and J. L. Atwood, Supramolecular Chemistry, 1st Ed., Wiley, 2000.
4. J.W. Steed, Core Concepts in Supramolecular Chemistry and Nanochemistry,1st Ed., John Wiley & Sons, 2007.
5. J.D. Seader, I. W. Hamley, Introduction to soft mater Synthetic and Biological self 49M.Sc. (Chemistry) 2017-18 assembly materials, Separation process principles, 2nd Ed., Wiley, 2010.
6. G. R. Desiraju, J. J. Vittal and A. Ramanan, Crystal Engineering: A Textbook, World Scientific, 2011.

CH5 110 Chemistry of Materials (L-T-P-C: 2-0-0-2)

Unit 1: Multiphase Materials

Ferrous Alloys, Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

Glasses, Ceramics, Composites and Nanomaterials: Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products, Refractories- characterization, properties and applications.Microscopic composites: dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Thin films and Langmuir-Blodgett Films: Preparation techniques, evaporation/sputtering, chemical processes, MOCVD sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Unit 2: Liquid Crystals

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smecticmesophases; smectic- nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and Smectic C phases, optical properties of liquid crystals, Dilectricsuspceptibility and dielectric cosntants. Lyotropic phases and their description of ordering in liquid crystals.

Polymeric materials: Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric polymers.

Unit 3: Ionic Conductors

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors. High T_c Materials: Defect provskites, high T_c superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties, anisotropy, temperature dependence of electrical resistance, optical phonon modes, superconducting state, heat capacity, coherence length, elastic constants, positron lifetimes, microwave absorption-pairing and multigap structure in high T_c materials, applications of high T_c materials.

Materials for Solid state devices: Rectifiers, transistors, capacitors IV-V compounds, low dimensional quantum structures, optical properties.

Suggested Books:

1. Solid State Physics, N.W.Ashcroft and N.D. Mermiin, Saunders College.
2. Materials Science and Engineering, An introduction, W.D. Callister, Wiley.
3. Principles of the Solid state, H. V. Keer, Wiley Eastern.
4. Materials Science, J.C. Anderson, K. D. Leaver, J. M. Alexander and R. D. Rawlings, ELBS
5. Thermotropic liquid Crystals, Ed. G. W. Gray, John Wiley.
6. Handbook of liquid crystals, Kelker and Hatz, Chemie Verlag.

CH5 201 Research or Industrial Project / Viva (L-T-P-C: 0-0-20-10)

CH5 202 Student Seminar (Based on Recent Research Articles) (L-T-P-C: 0-0-2-2)

CH5 203 Pharmaceutical Analysis (L-T-P-C: 2-0-0-2)

Unit 1: Pharmaceutical Analysis I

Sources of impurities in pharmaceuticals (chemicals, raw materials, methods of manufacture, reagents, solvents, atmospheric and microbial contaminants) and storage effects. Limit tests, solubility tests, disintegration tests, stability studies, impurity profile of drugs, Process analytical technology, quality audits etc. Validation of manufacturing and analytical equipment, process validation in production of pharmaceuticals, development of new analytical / bioanalytical method and its validation.

Unit 2: Pharmaceutical Analysis II

Assay of main classes of pharmaceuticals-with reference to Introduction-Type-Properties-Method of Analysis

Electrochemical Methods: Potentiometry and conductometry. Flame photometry, Atomic absorption spectrophotometry, nuclear magnetic resonance spectroscopy and mass spectrometry

Spectroscopic Methods: Ultraviolet, visible, Infrared and Raman spectroscopy

Chromatographic Methods: Ion exchange, column, paper, thin layer, gas and high performance liquid chromatography.

Assay of polymorphs in pharmaceutical Industry- introduction to polymorphs, methods of identification and analysis of polymorphs using Near-IR, Raman, XRPD, solid state NMR, DSC,TGA. Methods of analysis of common excipients /additives in formulations. Determination of active constituents in presence of these excipients.

Suggested Books:

1. Pharmaceutical Analysis, T. Highchi and E. Brochmann, Hanssen Interscience.
2. The quantitative analysis of drugs, D.C. Garrent, Chapman and Hall.
3. Pharmaceutical Analysis, A.H. Backett and J.B. Stenlake, Chapman and Hall.
4. Methods of drug analysis, S .F .Granbowrshll, Lee and Fehiger .
5. Analysis of drug and chemicals, N. Evers, W. Smith and C. Grikin.
6. Isolation and identification of drugs, E. G.J Clerks, Pharmaceutical Press.
7. Pharmaceutical analysis, A textbook for pharmacy students and pharmaceutical chemists, David G.Watson, Churhill Livingstone, 2000.
8. The practical evaluation of phyto pharmaceuticals, Brain K.R and Turner T.T Wright-Scientechnica, Bristil.

CH5 204 Chemistry of Nanomaterials (L-T-P-C: 2-0-0-2)

Unit 1: **Synthesis of Nano Materials**

Introduction: Definition and terminologies, nano particle morphologies, size dependent properties like optical, electrical and magnetic properties.

Synthesis of nano materials Physical methods: Mechanical methods, methods based on evaporation, laser ablation, sputtering, CVD, MBE.

Chemical methods: Quantum dots and 1D nano materials (chemical precipitation method, synthesis in confined media like reverse micelles, zeolites etc), synthesis from molecular precursors and molecular clusters, sol-gel method. 2D nano materials (L-B thin films, Self Assembled Monolayers, soft lithography).

3D nano materials and biological methods: Synthesis using microorganisms, use of natural templates like DNA. Biomimetic synthesis of nano particles. Synthesis of graphemes and nano composites

Unit 2: **Techniques for Characterizing Nano materials and Applications of Nano materials (15 h)**

Ellipsometry, and dual polarization interferometry (DPI) as methods used to obtain nano-gram masses, nano-scale thicknesses, and the optical properties of ultra-thin assemblies.

Infrared spectroscopy of nano-assemblies. Attenuated-total reflection (ATR) and grazing incidence angle techniques. Reflection-absorption IR spectroscopy (RAIRS). Surface enhanced Raman spectroscopy (SERS).

Imaging techniques: AFM, STM, SEM, EDX, imaging ellipsometry.

Optical microscopy. Fluorescence/phase contrast microscopy, confocal microscopy, total internal reflection microscopy (TIRM), Brewster angle microscopy (BAM), Nano-optics and local spectroscopy. Scanning near-field optical microscopy and photon scanning tunneling microscopy, scanning Plasmon near-field optical spectroscopy (SPNM), near-field optical spectroscopy, fluorescence spectroscopy, near field nonlinear optics.

Size determination: DLS, XRD, TEM.

Applications of nano materials: Optical and bio sensors, Energy cell, Catalysis, Drug delivery systems, Waste remediation Risk assessment and management of nano particles

Suggested Books:

1. Chemistry of nano materials, Volume I & II, Ed. C N R Rao, A. Muller, A K Cheetham Wiley, VCH.(2004).
2. Introduction to Nanotechnology C P Poole Jr., F J Owens, Wiley (2006)
3. Nanotechnology, M. Ratner and D. Ratner, Pearson.

CH5 205 Advanced Heterocyclic Chemistry (L-T-P-C: 2-0-0-2)

Unit 1: Introduction

Nomenclature of Heterocycles Replacement and systematic nomenclature (Hantzsch-Widmansystem) formon cyclic, fused and bridged heterocycles. General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bondlengths, ringcurrent and chemical shifts in ^{1}HNMR-spectra, empirical resonance energy, delocalization energy and Dewarresonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramid alinversion and 1,3-diaxial interaction. Stereo-electroniceffects-anomericandrelatedeffects.Attractiveinteractions-hydrogen bonding and intermolecular nucleophilic-electrophilic interactions

Unit 2: Heterocyclic Synthesis

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes.

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes

General classification, chemistry of some important meso-ionicheterocyclesoftype-A and Band their applications.

Synthesis and reactions of pyryl;um salts and pyrones and their comparison with pyridinium &thiopyrylium salts and pyridones.

Synthesis andreactions of quinolizinium and benzopyrylium salts, coumarins and chromones

Synthesis and reactions of azepines, oxepines, thiepines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

Unit 3: Heterocyclic Systems Containing P, As, Sb

Heterocyclic rings containing phosphorus: introduction, nomenclature, synthesis and characteristics of 5- and 6-membered ring systems-phosphorinanes, phosphorines, phospholanes and phospholes.

Heterocyclic rings containing As and Sb: Introduction, synthesis and characteristics of s- and 6-membered ring systems.

Heterocyclic rings containing 8: introduction, synthesis, reactivity and spectral characteristics of 3-,5-and 6-membered ring systems.

Suggested Books:

1. Heterocyclic Chemistry Vol.1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L Gilchrist, Longman Scientific Technical.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.

CH5 206 Environmental and Green Chemistry (L-T-P-C: 2-0-0-2)

Unit 1: Environmental Chemistry

Environmental Chemistry of water Properties of Water, Major aquatic chemical processes

Water Pollution: Types, sources and consequences of water pollution.sewage and waste water treatment and recycling Environmental Impact Assessment. Environmental auditing. Carbon credits Soil Pollution: Physical and chemical properties of soil ,soil micro-organisms and their functions, Different kinds of synthetic fertilizer (N, P and K) and pesticides-their interactions with different components of soil. Their toxicityand pollution. Industrial effluents of different kinds, their interactions with soil components, problems of toxic heavy metals and pollution. Deterioration of soil due to mining activities .Soil Pollution Control

Unit 2: Green Chemistry

Green Chemistry: Definition, tools and principles of green chemistry, evaluation of starting materials and reaction types. Solvent free systems, supercritical fluids, ionic liquids as catalysts and solvents

Emerging Green Technologies: Photochemical reactions (advantages and challenges), examples, chemistry using microwaves, sonochemistry, electrochemical syntheses.

Waste Minimization techniques: Concept of Recycling, recovery and reuse, Bioremediation of wastes and soils, phytoremediation of soils and sediments

Suggested Books:

1. Environmental Pollution analysis, S.M. Khopkar, Wiley Eastern Ltd., Environmental Chemistry, S.K. Banerji, Prentice Hall of India Pvt. Ltd., New Delhi
2. Environmental Chemistry, Stanley Manahan, Lewis Publishers CRC Press, USA. 6th Edition
3. Identification and Analysis of Organic Pollutants in water L.H. Keith, Arber Science Publications.
4. Standard methods for examination of water and waste water analysis, American Public
5. Health Association, New York. Chemical treatment and water purification, F .J. Belan, Mir Publishing House, Moscow.
6. Standard Methods for Examination of Water and waste water analysis American Public Health Association, N.Y. Water and water pollution (Hand Book) Ed., Seonard'L. Ciacere, Vol. (I to IV), Marcel Dekker Inc. N.Y. (1972).