CHHATRAPATI SHAHU JI MAHARAJ UNIVERSITY, KANPUR

STRUCTURE OF SYLLABUS FOR THE

PROGRAM: M.Sc. , SUBJECT: CHEMISTRY

Syllabus Developed by		
Name of BoS Convenor / BoS Member	**Designation**	**College/University**
DR. SUDHIR K SRIVASTAVA	Convenor	D.A.V. COLLEGE, CIVIL LINES, KANPUR

SEMESTER / YEAR	COURSE CODE	TYPE	COURSE TITLE	CREDITS	CIA	ESE	MAX. MARKS
IST YEAR / IST SEM	B020701T	CORE	INORGANIC CHEMISTRY-I	4	25	75	100
	B020702T	CORE	ORGANIC CHEMISTRY-I	4	25	75	100
	B020703T	CORE	PHYSICAL CHEMISTRY-I	4	25	75	100
	B020704T	CORE	SPECTROSCOPY	4	25	75	100
	B020705P	PRACTICAL	PRACTICAL	4	25	75	100
IST YEAR / IIND SEM	B020801T	CORE	INORGANIC CHEMISTRY-II	4	25	75	100
	B020802T	CORE	ORGANIC CHEMISTRY-II	4	25	75	100
	B020803T	CORE	PHYSICAL CHEMISTRY-II	4	25	75	100
	B020804T	ELECTIVE	ENVIRONMENTAL CHEMISTRY OR	4	25	75	100
	B020805T		SYMMETRY AND GROUP THEORY				
	B020806P	PRACTICAL	PRACTICAL	4	25	75	100
	B020807R	PROJECT	RESEARCH PROJECT	8	25	75	100
		MINOR ELECTIVE	FROM OTHER FACULTY (IN 1ST YEAR)	4/5/6	25	75	100
IIND YEAR / IIIRD SEM	B020901T	CORE	BIOINORGANIC, BIOORGANIC, BIOPHYSICAL CHEMISTRY	4	25	75	100
	B020902T	CORE	APPLICATION OF SPECTROSCOPY	4	25	75	100
	B020903T	ELECTIVES: ANY 2 TO BE CHOSEN	SOLID STATE CHEMISTRY	4	25	75	100
	B020904T		PHOTOCHEMISTRY	4	25	75	100
	B020905T		ORGANOTRANSITION METAL CHEMISTRY				
	B020906T		ANALYTICAL CHEMISTRY				
	B020907P	PRACTICAL	PRACTICAL	4	25	75	100
IIND YEAR / IVTH SEM	B021001T	ELECTIVES: ANY 4 TO BE CHOSEN	ORGANIC SYNTHESIS	4	25	75	100
	B021002T		HETEROCYCLIC CHEMISTRY	4	25	75	100
	B021003T		CHEMISTRY OF NATURAL PRODUCTS	4	25	75	100
	B021004T		MEDICINAL CHEMISTRY	4	25	75	100
	B021005T		POLYMERS				
	B021006T		NUCLEAR AND RADIO CHEMISTRY				
	B021007T		COMPUTATIONAL CHEMISTRY				
	B021008T		BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY				
	B021009T		INDUSTRIAL CHEMISTRY				
	B021010T		GREEN CHEMISTRY				
	B021011P	PRACTICAL	PRACTICAL	4	25	75	100
	B021012R	PROJECT	RESEARCH PROJECT	8	25	75	100

NOTE:

1. *A MINOR ELECTIVE FROM OTHER FACULTY SHALL BE CHOSEN IN 1ST YEAR (EITHER 1st / 2nd SEMESTER) AS PER AVAILABILITY.

2. In both years of PG program, there will be a Research Project or equivalently a research-oriented Dissertation as per guidelines issued earlier and will be of 4 credit (4 hr/week), in each semester. The student shall submit a report/dissertation for evaluation at the end of the year, which will be therefore of 8 credits and 100 marks

3. Research project can be done in form of Internship/Survey/Field work/Research project/ Industrial training, and a report/dissertation shall be submitted that shall be evaluated via seminar/presentation and viva voce.

4. The student straight away will be awarded 25 marks if he publishes a research paper on the topic of Research Project or Dissertation.

B020701T Inorganic Chemistry-I Semester-I

I Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagrams (Tri- and Penta atomic molecules), dπ-pπ bonds, Bent rule and energetics of hybridizations, some simple reactions of covalently bonded molecules.

II Metal-Ligand Equilibria in solution

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 it's thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

III Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factor affection, acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reaction, reaction without metal ligand, bond cleavage. Substitution reaction in square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reactions, electron transfer reactions, outer sphere type reaction, cross reaction and Marcus-HushTheory, inner sphere type reactions.

IV Metal –Ligand Bonding

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory.

Books Suggested:

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson , John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the elements, N.N. Greenwoods and A. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry Eds G.Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

B020702T Organic Chemistry-I Semester-I

I Nature of Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyper conjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and nonbenzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule,

Energy level of π- molecular orbitals, annulenes, antiaromaticity, ψ-aromaticity, homo aromaticity, PMO approach.

Bonds weaker than covalent-Crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes

II Stereochemistry

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 chiral carbon (biphenyl, allenes & spiranes) Chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorous.

III Reaction Mechanism: Structure and Reactivity

Types of mechanism, types of reaction, thermodynamic and kinetic requirements, kinetic And thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanism, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanion, free radicals, carbenes and nitrenes.

Effect of Structure on Reactivity

Resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

IV Aliphatic Nucleophilic Substitution

The SN_2, SN_1, mixed SN_1 and SN_2 and SET mechanisms. The neighbouring group mechanism, neighbour group participation by π and σ bonds, anchimeric assistance. Classical and non-classical carbocations, phenonium ions, carbonyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN_1 mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

V Aliphatic Electrophilic Substitution

Bimolecular mechanism- SE_2 and SE_1. The SE_1 mechanism, electrophilic substitution accompanied by double bond shift. Effect of substrate, leaving group and the solvent polarity on the reactivity.

Book Suggested:

1. Advanced Organic Chemistry- Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Corey and R.J. Sunderberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Skyes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd Prentice Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic Professional.
8. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.

B020703T Physical Chemistry-I Semester-I

I Quantum chemistry

A. Introduction to Exact Quantum Mechanical Results

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz,. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

B. Approximate Methods

The variation theorem, linear variation principle, Perturbation theory (first order and non degenerate). Application of variation method and perturbation theory to the Helium atoms.

C. Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunction for angular momentum, eigenvalue of angular momentum , operator using ladder operators, addition of angular momentum , spin, antisymmetry and Pauli exclusion principle.

D. Electronic Structure of Atoms

Electronic configuration, Russell- Saunders terms and coupling schemes, Slater Codon parameters, terms separation energies for the p^n and d^n configuration, magnetic effect, spin orbit coupling and Zeeman splitting, Introduction to method of self-consistent field the varial theorem.

E. Molecular Orbital Theory

Huckel theory of conjugated system ,bond order and charge density calculation application to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel theory.

II Thermodynamics

A. Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropy, Partial molar properties, partial molar free energy, partial molar volume

and partial molar heat content and their significance. Determination of these quantities.
Concept of Fugacity and determination of fugacity.

Non ideal systems, excess function for non ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient of electrolyte solutions, determination of activity and activity coefficient, ionic strength.

Application of phase rule to three component system, second order phase transition.

B. Statistical Thermodynamics

Concept of distributions, thermodynamic probability and most probable distribution. Ensemble averaging, postulate of ensemble averaging . Canonical, grand canonical and microcanonical ensembles, Corresponding distribution law (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. Application of partition functions.

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

C. Non equilibrium thermodynamics

Thermodynamics criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equation for different irreversible process (eg. heat flow, chemical reaction etc) transformations of the generalized fluxes and forces, non aquarium stationary states, phenomenological equations, microscopic reversibility and Onsager reciprocity relations, Electrokinetic phenomena, diffusion, electric conduction, Irreversible thermodynamics for biological systems, coupled reactions.

Book Suggested:

1. Physical chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum chemistry, Era N Levine, Prentice Hall.
4. Coulson's Valence, R. McWeeny, ELBS.
5. Chemical Kinetics, K.J. Laidler, McGraw- Hill.
6. Kinetics and mechanism of chemical transformations, J. Rajaraman and J. Kuriacose, McMillan.
7. Micelles, Theoretical and applied aspect, V. Moroi, Plenum.
8. Modern electrochemistry, Vol. 1 and Vol. 2, J.O.M. Bockris and A.K.N. Reddy, Plenum.
9. Introduction to polymer science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

B020704T Spectroscopy Semester-I

I Microwave spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field.

II Vibrational spectroscopy

A. Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energy of diatomic molecules, zero point energies, force constant and bond strengths, anharmonicity, Morse potential energy diagram, vibration- rotation spectroscopy, P,Q,R, Branches. Breakdown of Oppenheimer approximation; vibration of polyatomic molecules. Selection rules, normal mode 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 theory of Raman effect, pure rotational, vibrational and vibration- rotational, Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti-Stokes Raman spectroscopy (CARS).

III Electronic Spectroscopy

A. Atomic Spectroscopy

Energies to atomic orbitals, vectors, representation of momenta, and vector coupling, spectra of hydrogen atom and alkali metal atoms

B. Molecular Spectroscopy

Energy levels, molecular orbitals, vibranic transitions, vibrational transition and geometry of the excited states. Franck-Condon Principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative 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.

IV Magnetic resonance spectroscopy

A. Nuclear Magnetic Resonance spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factors influencing chemical shift, deshielding, spin-spin interaction, factor influencing coupling constant 'J', classification (ABX,AMX,

ABC,A_2 B_2 etc), spin decoupling, basic idea about instrument, NMR study of nuclei other than proton- ^{13}C, ^{19}F and ^{31}P, FT NMR, advantage of FT NMR, use of NMR in medical diagnostics.

B. Electron Spin Resonance spectroscopy

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the "g" value. Isotropic and anisotropic hyperfine coupling constant, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

C. Nuclear Quadruple Resonance Spectroscopy

Quadruple nuclei, quadruple moments, electric field gradient, coupling constant, splitting. Applications.

V Photoacoustic Spectroscopy

Basic principle of photoacoustic spectroscopy (PAS), PAS- gases and condensed system, chemical and surface applications.

Books Suggested:

1. Modern spectroscopy, J.M. Hollas, John Willey.
2. Applied Electronic Spectroscopy For Chemical Analysis. Ed.H, Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Method in Chemistry, R.S. Drago, Saunders College.
5. Introduction to Molecular Spectroscopy, G.M. Barrow, Mcgraw Hill.
6. Basic Principles of Spectroscopy, R. Chang. McGraw Hill.
7. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
8. Introduction of Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
9. Introduction of Magnetic Resonance, A. Carrington and A.D. Maclachlan, Harper and Row.

B020705P Practical Semester-I

The duration of Practical Examination will be of Eight Hours and will comprise two exercises.

The Distribution of marks will be as follows.

(a) Inorganic Exercise (one) 30
(At least six ions including minimum one rare element)
(b) Organic Exercise (one) 30
(c) Viva-voce 20
(d) Record/Assessment 20

Inorganic Chemistry

Qualitative Analysis

(a) Rare metal ions- Tl, Mo, W, Ti, Zr, Th, Zr, V, U (Two metal ions in cationic/anionic forms).

(b) Insoluble oxides, sulphates and halides.

Chromatography

Separation of cations and anions by

(a) Paper Chromatography

(b) Column Chromatography

Organic Chemistry

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using TLC and Column chromatography, chemical tests. IR spectra to be used for functional group identifications.

Books Suggested

1. Vogel's Text book of Quantitative Analysis, revised. J. Bassett, R. C. Denney. G.H. Jeffery and J. Mendham ELBS.
2. Synthesis and Characterization of Inorganic compounds, W.L. Jolly, Prentice Hall.
3. Experiments and Techniques in Organic Chemistry, D. Pasto. C. Johnson and M. Miller, Prentice Hall.
4. Macroscale and Microscale Organic experiments, K.L. Williamson. D.C. Heath.
5. Systematic qualitative Organic Analysis, H. Middleton, Adward Arnold.
6. Handbook of Organic Analysis Qualitative and Quantitative. H. Clark, Adward Arnold.
7. Vogel's text book of Practical Organic Chemistry, A.R. Tatchell, John Wiley.

B020801T Inorganic Chemistry-II Semester-II

I Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for Transition metal complexes (d^1-d^9 states), calculations 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.

II Metal π- Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyl for bonding and structural elucidation, important reactions of metal carbonyl; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

III Metal Clusters

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal – metal multiple bonds.

IV Isopropyl and Heterophyl Acids and Salts

Books Suggested:

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson , John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the elements, N.N. Greenwoods and A. Earnshow, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry Eds G.Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

B020802T Organic Chemistry-II Semester-II

I Aromatic Electrophilic Substitution

The arenium ion mechanism. Orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in the other ring system. Quantitative treatment of reactivity in substrate and electrophiles. Diazonium coupling. Vilsmeir reaction, Gattermann-Koch reaction.

II Aromatic Nucleophilic Substitution

The SNAr. SN_1, benzyne and SRN_1 mechanism. Reactivity effect of substrate, leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser and Smile rearrangements.

III Free radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism at aromatic substrate, neighour group assistance. Reactivity of aliphatic and aromatic substrate at a bridgehead. Reactivity in the attacking radicals. The effect of solvent on reactivity. Allylic halogention (NBS), oxidation of aldehyde to carboxylic acids, auto oxidation, coupling of alkyne and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hansdiecker reaction.

IV Addition to Carbon- Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, region 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.

V Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compound. Wittig reaction. Mechanism of condensation reactions involving enolates- Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reaction. Hydrolysis of esters and amides, ammonolysis of esters.

VI Elimination Reactions

The E_1, E_2 and E_1cB mechanisms and their spectrum. Orientation of the double bonds. Reactivity effects of substrate structures. Attacking base, the leaving group and the medium. Mechanism and orientation in the pyrolytic elimination.

VII Pericyclic Reaction

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allylic systems. Cycloadditions-antarafacial and suprafacial additions 4n and 4n+2 systems, 2+2 addition of ketene, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements-suprafacial and antarafacial shift of H, sigmatropic shift involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Book Suggested:

1. Advanced Organic Chemistry- Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Corey and R.J. Sunderberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Skyes, Longman.

4. Structure and Mechanism in Organic Chemistry, C.K Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd Prentice Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic Professional.
8. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.

B020803T Physical Chemistry-II Semester-II

I Chemical dynamics

Method of determining rate law, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and activated complex theory, and ionic reaction, kinetic salt effects, steady state kinetics, kinetics and thermodynamic control of reaction, treatment of uni molecular reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of Ethane) , photochemical (hydrogen -bromine and hydrogen-chlorine reactions) and oscillatory reaction (Belousov-Zhabotinsky Reactions), homogeneous catalysis, kinetics of enzyme reactions, general feature of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motion, probing the transition state, dynamics of barrier less chemical reactions in solution, dynamics of uni molecular reactions (Lindemann- Hinshelwood Kerala and Rice Ramsperger-Kassel-Marcus [RRKM]. Theory of unimolecular reactions).

II Surface chemistry

A. 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 film on liquids (Electrokinetic phenomena), catalytic activity at surfaces.

B. Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factor affecting the the CMC of surfactant, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

C. Macromolecules

Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization.

Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macro molecules, calculation of average dimensions of various chain structures.

III Electrochemistry

Electrochemistry of solution, 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, Graham- Devanathan-Mottwatts, Tobin, Bockris, Devanathan models.

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, electrolytic solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface.

Electrocatalysis- influence of various parameters. Hydrogen electrode.

Bioelectrochemistry, threshold membrane phenomenon, Nernst-Planck equation, Hodges-Huxley equations, core conductor models, Electrocardiography.

Polarography theory, Ilkovic equation; Half wave potential and its significance.
Introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

Book Suggested:

1. Physical chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum chemistry, Era N Levine, Prentice Hall.
4. Coulson's Valence, R. McWeeny, ELBS.
5. Chemical Kinetics, K.J. Laidler, McGraw- Hill.
6. Kinetics and mechanism of chemical transformations, J. Rajaraman and J. Kuriacose, McMillan.
7. Micelles, Theoretical and applied aspect, V. Moroi, Plenum.
8. Modern electrochemistry, Vol. 1 and Vol. 2, J.O.M. Bockris and A.K.N. Reddy, Plenum.
9. Introduction to polymer science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

B020804T Environmental Chemistry Semester-II

1. Environment

Introduction, the composition of the 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

The chemical composition of water bodies is lakes, streams, rivers, wetlands, etc. Hydrological cycle. Aquatic pollution-inorganic, organic, pesticides, agricultural, industrial and sewage, detergents, oil spills, and oil pollutants, water quality parameters-dissolved oxygen, biochemical oxygen demand, solids, metals, the 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), Residual chlorine and chlorine demand, purification and treatment of water.

3. Soils

Composition, micro, and macronutrients, Pollution-fertilizers, pesticides, plastics and metals, waste treatment.

4. Atmosphere

Chemical composition of atmosphere-particles, ions and radical and photochemical reactions in the atmosphere, smog formation, oxides of N,C,S,O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons, greenhouse 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. Radionuclide analysis, disposal of wastes and their management.

6. Environmental Toxicology

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes.

Books Suggested:

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.

2. Standard Methods of Chemical Analysis, F. J. Welcher vol. III, Van Nostrand Reinhold Co.
3. Environmental Chemistry, C. Baird, W. H. Freeman.
4. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
5. Environmental Chemistry, A.K. De, Wiley Eastern.

B020805T Symmetry and Group Theory Semester-II

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 groups of matrices (representation for the Cn, Cnv, Cnh, Dnh etc. groups to be worked explicitly).

Character of a representation. The great orthogonality theorem (without proof) and its importance.

Character tables and their use; spectroscopy.

B020806P Practical Semester-II

The Distribution of marks will be as follows.

(a) Inorganic Exercise (One preparation)	30
(b) Organic Exercise (One exercise from given list)	30
(c) Viva-voce	20
(d) Record/Assessment	20

Inorganic Chemistry

Preparation of following inorganic compounds-

(1) $VO(acac)_2$
(2) $TiO(C_9H_8NO)_2\ 2H_2O$
(3) cis-$K[Cr(C_2O_4)_2\ (H_2O)_2]$
(4) $Na[Cr(NH_3)_2\ (SCN)_4]$
(5) $Mn(acac)_3$
(6) $K_3[Fe(C_2O_4)_3]$
(7) Prussian Blue, Turnbull's Blue
(8) $[Co(NH_3)_6]\ [Co(NO_2)_6]$
(9) cis-$[Co(trien)\ (NO_2)_2]\ Cl.H_2O$
(10) $Hg[Co\ (SCN)_4]$
(11) $[Co(Py)_2\ Cl_2]$
(12) $[Ni(NH_3)_6]Cl_2$
(13) $Ni(dmg)_2$
(14) $[Cu(NH_3)_4]\ SO_4.\ H_2O$

Organic Chemistry

Organic Synthesis

Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by Column chromatography.
Oxidation: Adipic acid by chromic acid, oxidation of cyclohexanol.
Grignard reaction: Synthesis of triphenylmethanol from benzoic acid.
Aldol condensation: Dibenzal acetone from benzaldehyde.
Sandmeyer reaction: p-chlorotoluene from p-toluidine.
Acetoacetic ester condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.
Friedal Craft Reaction: Benzoyl propionic acid from succinic anhydride and benzene.
Aromatic electrophilic substitutions: Synthesis of p-nitroaniline and p-bromoaniline.
The Products may be characterized by Spectral Techniques.

Quantitative Analysis

Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation methods.

Estimation of amines/phenols using bromate bromide solution/ or acetylation method.

Determination of Iodine and Saponification values of an oil samples.

Determination of DO, COD and BOD of water sample.

Books Suggested

1. Vogel's Text book of Quantitative Analysis, revised. J. Bassett, R. C. Denney. G.H. Jeffery and J. Mendham ELBS.
2. Synthesis and Characterization of Inorganic compounds, W.L. Jolly, Prentice Hall.
3. Experiments and Techniques in Organic Chemistry, D. Pasto. C. Johnson and M. Miller, Prentice Hall.
4. Macroscale and Microscale Organic experiments, K.L. Williamson. D.C. Heath.
5. Systematic qualitative Organic Analysis, H. Middleton, Adward Arnold.
6. Handbook of Organic Analysis Qualitative and Quantitative. H. Clark, Adward Arnold.
7. Vogel's text book of Practical Organic Chemistry, A.R. Tatchell, John Wiley.

B020807R Research Project Semester-II

B020901T Bio-Inorganic, Bio-Organic and Biophysical Chemistry Semester-III

A. BIO-INORGANIC CHEMISTRY

1. Metal Ions in Biological Systems: Essential and trace metals.

2. Na^+/K^+ Pump: Role of metals ions in biological processes,

3. Bioenergetic and ATP Cycle: DNA polymerization, glucose storage, metal complexes in the transmission of energy, chlorophylls, photosystem I and photosystem II in water cleavage, model systems.

4. Transport and storage of Dioxygen: Heme protein and oxygen uptake, structure and function of hemoglobin, myoglobin, and hemerythrin, model synthetic complexes of iron, and copper

Books Suggested:

1. Progress in Inorganic Chemistry, vol. 18 and 38 Ed. J J. Lippard, Wiley.
2. Inorganic Biochemistry vol. I and II ed. G. L. Eichhorn, Elsevier.
3. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.

B. BIO-ORGANIC CHEMISTRY

1. 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. Fischer's lock and key and Koshland's induced fit hypothesis, concept, and active site identification by using inhibitors, affinity labeling, and enzyme modification by site-directed mutagenesis.

2. Mechanism of enzyme action: Transport state theory, orientation, and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease.

3. Co-Enzyme Chemistry: Cofactors as derived from Vitamins, coenzymes, prosthetic groups, apoenzymes, structure, and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxalphosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, vitamin B12, mechanism of reactions catalyzed by the above cofactors.

C. BIOPHYSICAL CHEMISTRY

1. Biological cell and its constituents: Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems, Helix coil transition.

2. Bioenergetics: Standard free energy change in biochemical reactions, exergonic, endergonic, hydrolysis of ATP, synthesis of ATP from ADP.

3. Thermodynamics of biopolymer solutions: Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction, and energy generation in the mechanochemical system.

Books Suggested:

1. Understanding enzymes, Trevor Palmer, Prentice Hall.
2. Enzyme Mechanisms Ed, M. I. Page and A. Williams, RSC.
3. Fundamental ofEnzymology, N. C. Price and L. Stevens, Oxford University Press.
4. Biochemistry, L. Stryer, W.H. Freeman.
5. Macromolecules: Structure and Function, F. Wold. Prentice Wall.
6. Biochemistry, Voet and Voet, John Wiley.

B020902T Applications of Spectroscopy Semester-III

Inorganic Chemistry

1. Vibrational spectroscopy: Symmetry and shapes of AB_2, AB_3, AB_4, AB_5, and AB_6, Mode of bonding of ambidentate ligands, ethylenediamine, and diketonato complexes, Application of resonance Raman spectroscopy, particularly for the study of active sites of metalloproteins.

2. 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,

3. 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 inequivalent MB atoms.

Organic Chemistry

1. Ultraviolet and Visible Spectroscopy: Various electronic transitions (185-800nm), Beer-Lambert law. The 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 effects in biphenyls.

2. Infrared Spectroscopy: Instrumentation and sample handling, 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 Fermi resonance, FTIR, IR of gaseous, solids, and polymeric materials.

3. 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), chemical exchange,

the effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first-order spectra), virtual coupling, stereochemistry, hindered rotation, Fourier transform technique, Nuclear Overhauser Effect (NOE), resonance of other nuclei-F, P.

4. ^{13}C NMR Spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic, and carbonyl carbon), coupling constants, Two-dimension NMR Spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

5. Mass Spectrometry: Introduction, ion production-EI, CI, FD, and FAB, factors affecting fragmentation, ion analysis, ion abundance, mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, meta stable peak, McLafferty rearrangement, Nitrogen rule, high- resolution mass spectrometry, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Infrared and Raman Spectra: Inorganic and Coordination Compounds, N. Nakamoto, Wiley
2. Physical Methods of Inorganic Chemistry, R. S. Drago, Saunders Company.
3. NMR, NQR, EPR, and Mossbauer Spectroscopy Inorganic Chemistry. R. V. Parish, Ellis Horwood.
4. Spectrometric Identification of Organic Compounds, Silverstein, Bassler and TMorrill, John Wiley.
5. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
6. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
7. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
8. Organic Spectroscopy, William Kemp, Mac publsihers, 3rd Edition, 2011.
9. C. N. Banwell and E. M. McCash; Fundamentals of Molecular Spectroscopy, 4th ed. Tata McGraw Hill, 1994.
10. D. L. Pavia, G.M. Lampman, G.S. Kriz and J. R. Vyvyan; Introduction to Spectroscopy, 5th ed. Cengage India, 2015.

B020903T Solid State Chemistry Semester-III

1. Solid State reactions

General principles, experimental procedures, co-precipitation as a precursor to solid-state reactions, kinetics of solid-state reactions.

2. Crystal Defects and Non-Stoichiometry

Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defect formation, color centers, non-Stoichiometry defects.

3. Electronic properties and band theory

Metals, insulators, and semiconductors, electronic structure of solid-band theory, the band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doping semiconductor, p-n-junction, superconductors, optical properties - optical reflectance, photoconduction-photoelectric effects, Magnetic properties-classification of materials, quantum theory of paramagnetic-cooperative phenomena-magnetic domains, hysteresis.

4. Organic solids

Electrically conducting solids, organic charge transfers complex, organic metals, new superconductors.

Books Suggested:

1. Solid State Chemistry and its Applications, A. R. West Plenum.
2. Principles of the Solid State, H.V. Keer, Wiley Eastern.
3. Solid State Chemistry, N.B. Hannay.

B020904T Photochemistry Semester-III

1. Photochemical Reactions

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

2. 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 reactions-photo dissociation, gas-phase photolysis**.**

3 . Photochemistry of alkenes

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

4. Photochemistry of carbonyl compounds

Intramolecular reactions of the carbonyl compounds-saturated, cyclic and acyclic, β, γ-saturated and α, β-unsaturated compounds, cyclohexadienones. Intermolecular cycloaddition reactions-dimerization, and oxetane formation.

5. Photochemistry of aromatic compounds

Isomerization, addition, and substitutions.

6. Miscellaneous photochemical reactions

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

Books Suggested:

1. Fundamental of Photochemistry, K. K. Rohtagi-Mukherji, Wiley-Eastern.
2. Molecular Photochemistry, N.J. Turro, W. A. Benjamin.
3. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
4. Photochemistry, R P. Kundall and A. Gilbert, Thomson Nelson.

B020905T Organotransition Metal Chemistry Semester-III

I Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

II Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

III Transition Metal π- complexes

Transition metalπ - complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

IV Transition Metal Compounds with bonds to Hydrogen

Transition metal compounds with bonds to hydrogen.

V Homogenous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions, activation of C-H bond.

VI Fluxional Organometallic Compounds

Fluxionality and dynamic equilibria in compounds such as η^2-olefin, η^3-allyl and dienyl complexes.

Books Suggested:

1. Principles and application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

B020906T Analytical Chemistry Semester-III

I Introduction

Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of Instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations- dissolution and decomposition. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks, Safety in the analytical laboratory.

II Errors and Evaluation

Definition of terms in mean and median. precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for, reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics in chemical analysis.

III Food Analysis

Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC Gas chromatography for organophosphates. Thin-layer chromatography for identification chlorinated pesticides in food products.

IV Analysis of Water Pollution

Origin of waste water, types, water pollutants and the effects. Sources of water pollution-domestic, industrial agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis parameter for analysis colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silicon phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.

V Analysis of Soil, Fuel, Body Fluids and Drugs

(a) **Analysis of soil:** moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.
(b) **Fuel analysis:** solid, liquid and gas, Ultimate and proximate analysis- heating values grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and gas-calorific value.
(c) **Clinical chemistry:** Composition of blood-collection and preservation of samples. Clinical analysis, serum electrolytes, blood glucose, blood urea, nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis-trace elements in the body.
(d) **Drug analysis:** Narcotics and dangerous drugs Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Books Suggested:

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West and F.J. Holler, W.B. Saunders
3. Analytical Chemistry- Principles, J.H. Kennedy, W.B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders
6. Principles of Instrumental Aanalysis. D.A. Skoog, W.B. Saunders.
7. Quantitative Analysis, R.A. Daty, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
10. Handbook of Instrumental Techniques For Analytical Chemistry, F. Settle, Prentice Hall.

B020907P Practical Semester-III

The Distribution of marks will be as follows.

(a) Inorganic Exercise (one)	30
(b) Physical Exercise (one)	30
(c) Viva-voce	20
(d) Record/Assessment	20

Inorganic Chemistry

Selection can be made from the following-

1. Sodium amide. Inorg. Synth., 1946,2 ,128.
2. Synthesis and thermal analysis of group (II) metal oxalate hydrate. J. Chem. Ed., 1988, 65,1024.
3. Atomic absorption analysis of Mg and Ca.
4. Trialkoxyboranes- Preparation, IR and NMR spectra.
5. $PhBCl_2$ Dichlorophenylborane- Synthesis in Vacuum line.
6. Preparation of Tin(IV) iodide, Tin(IV) chloride and Tin(II) iodide. Inorg. Synth., 1953, 4, 119.
7. Relative stability of Tin(IV) and Pb(IV). Preparation of ammonium hexochlorostannate $(NH_4)_2$ $SnCl_6$. ammonium hexachloroplumbate $(NH_4)_2PbCl_6$.
8. Hexa- bis (4-nitrophenoxy) cyclotriphosphazene.
9. Synthesis of trichlorodiphenylantimony(V) hydrate. Inorg. Synth., 1985, 23, 194.
10. Sodium tetrathionate $Na_2S_4O_6$.
11. Metal complexes of dimethyl sulfoxide (IR): $CuCl_2$. 2DMSO, $PdCl_2$. 2DMSO, $RuCl_2$. 4DMSO. J. Chem. Educ., 1982, 59, 57
12. Synthesis of metal acetylacetonate; magnetic moment, IR, NMR., Inorg. Synth. 1957, 5, 130; 1963, 1, 183.
13. Bromination of $Cr(acac)_3$. J. Chem. Edu., 1986,63,90.
14. Magnetic Moment of $Cu(acac)_2.H_2O$.
15. Cis- and Trans $[Co(en)_2Cl_2]^+$.
16. Separation of optical isomer of cis-$[Co(en)_2Cl_2]Cl$. J. Chem. Soc., 1960,4369.
17. Ion exchange separation of oxidation state, of vanadium. J. Chem. Educ. 1980, 57, 316; 1978, 55, 55.

18. Determination of Cr(III) complexes. $[Cr(H_2O)_6]NO_3.3H_2O$, $[Cr(H_2O)_4Cl_2]Cl.2H_2O$, $[Cr(en)_3]Cl_3$, $Cr(acac)_3$. Inorg. Synth., 1972, 13,184.
19. Preparation of N,N bis(salicyldehyde)ethylenediamine, salen H_2, Co(salen) J. Chem. Educ., 1977, 54,443; 1973; 50,670. Determination of O_2 absorption by Co(salen) Acct. Chem. Res., 1975, 8, 384. Reaction of oxygen adduct with $CHCl_3$ (deoxygenation).
20. Preparation of Fe(II) chloride (use it as Friedel-Crafts chlorination source). J.Org. Chem., 1978, 43, 2423; J. Chem. Edu., 1984, 61,645; 1986, 63, 361.
21. Reaction of Cr(III) with a multidentate ligand; a kinetics experiment (visible spectra Cr-EDTA complex.) J.A.C.S., 1953. 75, 5670.
22. Preparation of [Co(phenanthroline-5,6- quinone]. J. Chem. Soc., A., 1970, 447, J. Chem. Edu, 1977, 54,710.
23. Preparation and use of Ferrocene. J. Chem. Edu, 1966,43,73; 1976, 53,730.
24. Preparation of copper glycine complex-cis and trans bis glycinato Copper(II). J. Chem. Soc. Dalton , 1979, 1901, J. Chem. Edu, 1982, 59,1052.
25. Preparation of phosphine Ph_3P and its transition metal complexes.
26. Any other experiment such as Conversion of p-xylene to terephthalic acid catalyzed by $CoBr_2$ (homogeneous catalysis).

Spectrophotometric Determinations
(a) Manganese /Chromium/Vanadium in steel sample.
(b) Nickel/ Molybdenum/Tungsten/Vanadium/Uranium by extractive spectrophotometric method.
(c) Fluoride/nitrite /phosphate
(d) Iron-phenanthroline complex: Job's Method of continuous variations.
(e) Zirconium-Alizarin Red-S complex: Mole-ratio method.
(f) copper-Ethylene diamine complex: Slope ratio Method.

Flame Photometric Determinations
(a) Sodium and potassium when present together
(b) Lithium/calcium/barium/strontium
(c) Cadmium and magnesium in tap water.

Chromatographic Separations
(a) Cadmium and zinc
(b) Zinc and magnesium
(c) Thin-layer chromatography-separation of nickel, manganese, cobalt and zinc.
Determination of Rf values.
(d) Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.

Physical Chemistry

Adsorption

To study the surface tension concentration relationship for solutions (Gibbs equation).

Phase Equilibria

(i) Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone system).
(ii) Determination of glass transition temperature of given salt (e.g. $CaCl_2$) conductometrically.

(iii) To construct the phase diagram for three component system (e.g. Chloroform-acetic acid -water).

Chemical Kinetics

(i) Determination of the effect of (a) change of temperature (b) change of concentration of reactants and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
(ii) Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
(iv) Flowing clock reactions (Ref: Experiments in Physical Chemistry by Showmaker).
(v) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

Solutions

(i) Determination of molecular weight of non volatile and non electrolyte / electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
(ii) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behavior that occurs with a strong electrolyte.

Electrochemistry

Conductometry

(i) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
(ii) Determination of solubility and solubility product of sparingly soluble salts (e.g. $PbSO_4$, $BaSO_4$) conductometrically.
(iii) Determination of the strength of strong and weak acids in a given mixture conductometrically.
(iv) To study the effect of solvent on the conductance of $AgNO_3$/acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
(v) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

Potentiometry/pH metry

(i) Determination of strength of halides in a mixture potentiometrically.
(ii) Determination of the valency of mercurous ions potentiometrically.
(iii) Determination of the strength of strong and weak acids in a given mixture using a Potentiometer/pH meter.
(iv) Determination of temperature dependence of EMF of a cell.
(v) Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
(vi) Acid-base titration in a non-aqueous media using a pH meter.

(vii) Determination of activity and activity coefficient of electrolytes.

(viii) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.

(ix) Determination of the dissociation constant of monobasic/dibasic acid by Albert, Serjeant method.

(x) Determination of thermodynamic constants. ΔG, ΔS and ΔH for the reaction by e.m.f. method.

$Zn + H_2SO_4 \rightarrow ZnSO_4 + 2H$

Polarimetry

(i) Determination of rate constant for hydrolysis / inversion of sugar using a polarimeter.

(ii) Enzyme kinetics-inversion of sucrose.

Books Suggested

1. Vogel's Text book of Quantitative Analysis, revised. J. Bassett, R. C. Denney. G.H. Jeffery and J. Mendham ELBS.
2. Synthesis and Characterization of Inorganic compounds, W.L. Jolly, Prentice Hall.
3. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
4. Findley's Practical Physical Chemistry, B.P. Levitt, Longman.
5. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

B021001T Organic Synthesis Semester-IV

I Organometallic Reagents

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

Group I and II metal organic compounds

Li, Mg, and Zn compounds.

Transition metals

Cu, Pd, Ni and Fe compounds.

Other Elements

S, Si and B compounds.

II 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.

Oxidations with ruthenium tetraoxide, iodobenzenediacetate and thallium (III) nitrate.

III 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 oxine groups.

Hydrogenolysis.

IV Rearrangements

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

A detailed study of the following rearrangements-

Pinacol-pinacolone. Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Beckmann, Hofman, Curtius, Schmidt, Baeyer-Villiger.

Books Suggested:

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers. Cambridge University Press.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B. F. A. Carey and R.J. Sundberg, Plenum Press.
6. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

B021002T Heterocyclic Chemistry Semester-IV

I Nomenclature of Heterocycles

Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles.

II Aromatic Heterocycles

General chemical behaviour of aromatic heterocycle, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in 1H NMR-spectra. empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations).

Heteroaromatic reactivity tautomerism in aromatic heterocycles.

III Non-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, pyramidal inversion and 1,3,-diaxial interaction.

Stereo-electronic effects anomeric and related effects. Attractive interactions- hydrogen bonding and intermolecular nucleophilic- electrophilic interactions.

IV Heterocyclic Synthesis

Principle of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions

V Small Ring Heterocycles

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

VI Six-membered Heterocycles with One Heteroatom

Synthesis and reactions of pyrylium salts and pyrones and their comparision with pyridinium&thiopyrylium salt and pyridones.

Synthesis and reactions of quinolizinium benzopyrylium salts, coumarins and chromones.

VII Six-Membered Heterocycles with Two or More Heteroatoms

Synthesis and reactions of diazines, triazines, tetrazines and thiazines.

VIII Seven-and Large Membered Heterocycles

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

Books Suggested:

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-Inter Science.
6. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C. W. Rees, eds. Pergamon Press.

B021003T Chemistry of Natural Products Semester-IV

I Terpenoids and Carotenoids

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol, α- Terpeneol, Menthol, Zingiberene, Abiatic acid and β-Carotene.

II Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants.

Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine, Atropine, Quinine and Morphine.

III Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation structure determination and synthesis of Cholesterol, Bile acids, Androsterone., Testosterone, Estrone, Progestrone, Aldosterone.
Biosynthesis of steroids.

IV Plant Pigments

Occurrence, nomenclature and general methods of structure determination, isolation and synthesis ofApigenin, Luteolin, Quercetin, Myrcetin Quercetin-3-glucoside, Vitexin, Cyanidin-7-arabinoside, Hirsutidin.

Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway

V Porphyrins

Structure and synthesis of Hemoglobin and Chlorophyll.

VI Prostaglandins

Occurrence, nomenclature, classification, biogenesis and physiological effects.Synthesis of PGE_2, and PGF_2.

Pyrethroids and Rotenones

Synthesis and reactions of Pyrethroids and Retenones. (For structure elucidation, emphasis is to be placed on the use of spectral parameters wherever possible).

Books Suggested:

1. Natural Products: Chemistry and Biological Significance J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope an J.B. Harborne, Longman Essex
2. Organic Chemistry, Vol 2, I L. Finar. ELBS.
3. Stereoselective Synthesis: A Practical Approach M.Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed, S. Coffe Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from 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-Rahman and M.I. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers

B021004T Medicinal Chemistry Semester-IV

I Drug Design

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting 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, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis, LD-50, ED-50 (Mathematical derivations of equations excluded).

II Pharmacokinetics

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in the rapeutics. Mention of uses of pharmacokinetics in drug development process.

III Pharmacodynamics

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition sulphonamides membrane active drugs, drug metabolism, xenobiotics biotransformation, significance of drug metabolism in medicinal chemistry.

IV Antineoplastic Agents

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors.

V Cardiovascular Drugs

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators.

Synthesis of amyl nitrate, sorbitrate.

VI Local Anti infective Drugs

Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, acid ciprofloxacin, norfloxacin, dapsone, ethionamide, ethambutal and chloroquin.

VII. Psychoactive Drugs – The chemotherapy of Mind

Introduction neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone, neurochemistry of mental diseases, antipsychotic drugs – the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs.

Synthesis of diazepam, oxazepam and chlorazepam.

VIII. Antibiotics

Cell wall biosynthesis, inhibitors – Lactam rings, antibiotics inhibiting, protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin.

Books Suggested:

1. Introduction to Medicinal Chemistry, A. Gringuage, Wiley-VCH
2. Wilson And Gisvold Es Text Rook of Organic Medicinal and Pharmaceutical Chemistry. Ed. Robert F.Dorge.
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 Ch-14), 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. Leilnicer. John Wiley.

B021005T Polymers Semester-IV

I. 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 reactions. Polymerization in homogeneous and heterogeneous systems.

II. Polymer Characterization

Polydispersion - Average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods Analysis and testing of polymers-chemical analysis of polymers, spectroscopic methods, X-ray diffraction study, Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue. impact. Tear resistance. Hardness abrasion resistance.

III. Structure and Properties

Morphology and order in cryststalline polymers-configurations of polymer chains. Crystal structures of polymers, morphology of cryststalline 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 and Tg effects of molecular weight diluents, chemical structure, chain topology, branching and cross linking, property requirements and polymer utilization.

IV. Polymer Processing

Plastics, elastomers and fibres. Compounding Processing Techniques; Calendering, die casting, rotational casting. film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

V. 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.

Books Suggested:

1. Textbook of Polymer Science, F. W. Billmeyer. Jr.Wiley.
2. Polymer Science. V. R. Gowarikar, N.V. Viswanathan and J. Sreedhar, Wiley - Eastern.
3. Functional Monomers and Polymers , K. Takemoto, Y. Inaki and R.M. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of polymers, J.M.G. Cowie, Blackie Academic and Professional.

B021006T Nuclear and Radio Chemistry Semester-IV

I. Introduction

Some Historical Landmarks in Nuclear and Radiochemistry. Nuclear Structure and Stability (Nucleus shape, Isotopes. Isobars, lsotones, Nuclear lsomensm and Isomeric Transitions. Nuclear forces, Nuclear Mass & Binding Energy. Frequency distribution of stable Isotopes & Nuclear stability N/Z ratio), Nuclear Reactions, Notation Q-value of Nuclear reactions, Coulomb Barrier, Reaction Cross-section, Types of reactions. Scattering reactions (- Induced reactions, Neutrons induced, Proton induced, Deutmn, Photon, Heavy ion induced reactions), Natural Radioactivity, Artificial Radioactivity, Nuclear fission and Nuclear fusion; Radioactivity and Types of Nuclear decay - Types and Kinetics of Radioactive Decay.

II. Radiation detection and Measurements

Interaction of Radioactive with matter, Electromagnetic Interaction (Photoelectric Effect, Compton Scattering and Pair Production), Photo-tube and Photo-multiplier tube, General Principles of Radioactivity Detection and Fundamental particles in Detectors and Nuclear Spectroscopy, Semiconductor Detector.

III. Nuclear Models

Nordhem rules and Magic numbers, Liquid- Drop Model, Fermi-Gas Model, Nuclear -Shell Model, The Optical Model and The collective Model. The Quantum Mechanical Nuclear Potentials- The square well potential, The Harmonic Oscillator potential, The Exponential potential, The Guassian potential and the Yukawa potential.

IV. Nuclear Reactor & Device

Fisson Chain Reaction- Radiations Decaying into channel width (Fission Cross Section, Control rods operated Neutron Flux and Nuclear chain reactions and MPDQ-92- Computer Program), Fission and Fertile isotopes. Nuclear Fuel, Fuel Cladding, Moderator, Coolant, Control Rods, Sensing elements, Conversion & Radioactivity; Nuclear Reactors- Boiler Water Reactor, Pressurised Water Reactor, Pressurised Heavy Water Reactor, Light- Water Gas Cooled Reactor, Advanced Gas Cooled Reactor, High Temperature Reactor, INDIAN REACTORS (Apsara, Cirus, Dhurva), Indian Kota Heavy Water Plant and Madras Atomic Power Station; Various Thermochemical Reactors, Laser Fusion Reactors, Lekka -8 (Japanese) Fusion, India's.Tokmann Aditya Toridal Reactor, Accelerates- Vande Graff Accelerator, Linear Accelerator. Cyclotron Reactor, Suchrocyclotron Accelerator; Nuclear Materials- **URANIUM -** Uranium Enrichment & Uranium as Fuel. Uranium Metal Ingot, Uranium di-oxide pellet. Freshly prepared Ammonium Diuraruite, Freshly prepared Magnesium diuranate, **PLUTONIUM -** Plutonium Based Fuels, Plutonium Metals, Plutonium Oxide Powder. Safety Aspects of Plutonium, **THORIUM -** Thorium Components, Thorium Breeders and Thorium Fuel Cycle, **HEAVY WATER -** Deuterium Enrichment Process and Radiolysis of Water, **ZIRCONIUM & ALLOYS, BERYLLIUM -** Use of Beryllium in Nuclear System and its application in other industries.

V. Applications of Isotopes

Production of Isotopes. Radiopharmaceuticlas and Radio-nuclide Therapy- NAME of the Pharmaceuticals and their application and Radioimmunoassay; Radiation, Sterilization of Medical Products. Food Preservation and Gamma Radiography, Age Determination (Carbon Dating, Diagnostic Radiopharmaceutical - Bone Density Measurements, Bone Imaging, Cardiovascular Studies. Central Nervous System, Environmental Radioactivity and Safety-Natural Radionuclides, Fall out from Nuclear Weapons Testing.

VI. Radioactive and Nuclear Techniques

Radioactive Analytical Techniques, Radiometric Titrations. Prompt Gamma Neutron Activation Analysis. Charged Particle Activation Analysis, Particle Induced X-ray emission analysis (PIGS).

Book Suggested:

1. Nuclear and Radioactivity- Friedlander G; Kennedy J.M Mamas E.S., Miller J.M., Wiley Inter Science N.Y. (1981).
2. Introduction to Nuclear Physics and Chemistry- Harvey B.G., Prentice Hall Engle-wood Cliffs (N.J.) 1963, EKE Edn (1965).
3. Source Book of Atomic Enemy, Glasstone S. Affiliated Ease-West Press, New Delhi 1969.
4. Environmental Chemistry P.S. Sindhu, New Age International. New Delhi.

5. Nuclear Reactions R. Singh & S. N. Mukherjee, New Age International. New Delhi.
6. Nuclear and Radiochemistry (Text book Arnikar, New Age International. New Delhi.

B021007T Computational Chemistry Semester-IV

Fortran/C Programming and Numerical Methods

Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc.

a. Solutions of Equations

Bisection. regular falsi, Newton-Raphson and related methods for solving polynomial and transcendental equations. Convergence, Errors and ill-conditioning.

b. Linear Simultaneous Equations

Gaussian elimination, Gauss - Seidel method, Gauss-Jordan method. Pivoting strategy. Errors and ill conditioning.

c. Eigen values and Matrix Diagonalization

Jacobi and Householder methods, analysis of errors.

d. Interpolation

Newton forward and backward difference, central difference formulae. Lagrange and Herrnite interpolation. Polynomial wiggle problem.

e. Numerical Differentiation

Solution of simple differential equations by Taylor series and Runge-Kutta methods.

f. Numerical Integration

Newton-Cotes formulae, Romberg integration. errors in integration formulae.

The students should develop computer programes for some of the above numerical methods.

i. Running of Advanced Scientific Package

The students are expected to get hands on experience of running a few selected advanced level scientific software packages after a brief introduction to the basic theory and methodology. ab initio quantum chemical packages such as GAUSSIAN/GAMES with carefully designed exercises for illustrating various features of the packages. Semi empirical/Dynamics/Simulation packages such as MOPAC. CHARM. AMBER. QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design etc.

II Introduction to Networking and Search using Internet

Book Suggested:

1. Computational Chemistry, A. C. Norris, John Wiley.
2. Computer Programming in FORTRAN 77, R. Rajaraman, Prentice Hall.

3. Numerical Analysis. C.E. Frogberg, Macmillan.
4. Numerical Analysis, A Practical Approach, M. J. Maron, John Wiley.
5. Numerical Methods for Scientists and Engineers. H.M. Antia, Tata McGraw Hill.

B021008T Bioinorganic and Supramolecular Chemistry Semester-IV

I Metal Storage Transport and Biomineralization

Ferritin, transferrin and siderophores

II Calcium in Biology

Calcium in living cells, transport and regulation, molecular aspects of Intramolecular processes, extracellular binding proteins.

III Metalloenzymes

Zinc enzymes carboxypeptidase and carbonic anhydrase. Iron enzymes-catalase. peroxidase and cytochrome P-450. Copper enzymes- superoxide dismutase. Molybdenum oxatransferase enzymes- xanthine oxidase. Coenzyme vitamin B_{12} .

IV Metal- Nucleic Acid Interactions

Metal ions and metal complex interactions, Metal complexes-nucleic acids.

V Metals in Medicine

Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

VI Supramolecular chemistry

Concepts and language.

(A) Molecular recognition : Molecular receptors for different types of molecules, design and synthesis of coreceptor molecules and multiple recognition.

(B) Supramolecular reactivity and catalysis.

(C) Transport processes and carrier design.

(D) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

(E) Host guest chemistry, cation, anion, neutral guest binding. Physicochemical method of investigation of supramolecular associates.

Some example of self-assembly in supramolecular chemistry.

Books Suggested:

1. Principle of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books
3. Inorganic Biochemistry Vol. I and II ed. G.L Eichhorn, Elsevier.

4. Progress in Inorganic Chemistry, Vols. 18 and 38 Ed. J.J. Lippard, Wiley.
5. Supramolecular Chemistry, J.M. Lehn, VCH.
6. Supramolecular Chemistry, Jonathan W. Steed, J.L.Atwood.
7. Supramolecular Chemistry, Jear-Merie Lehn.

B021009T Industrial Chemistry Semester-IV

Unit 1: Cement, Ceramic and Glass

Composition of cement, mixing of cement clinker with Gypsum, Setting of cement. Composition, Physical and Chemical properties of Glass, Varieties of glass, Introduction to ceramics.

Unit 2: Composites

Introduction, constituents of composites, Types, of composites, Microscopic and Macroscopic Composites, Dispersion, Strength, Particle and Fiber- reinforced Composites.

Unit 3: Fertilizers

N - Ammonia, Ammonium nitrate and Urea; P - Phosphoric acid, Single and Triple superphosphate, DAP; K- Potassium Nitrate and Muriate of potash.

Unit 4: Petrochemicals and Lubricants

Introduction, Occurrence, Composition of Petroleum, Natural gas, cracking, refining, octane rating, cetane number, flash and fire point determination.
Lubricating oils and additives, Naphtha crackers and Profile of their products, Synthetic and Blended oils.

Unit 5: Paints

General characteristic, their function, Manufacture and Classification, Enamels, Emulsion paints, Water based paints. Formulation of paints: Function of vehicles, solvent, thinner, pigment, dyes, filler, resins, drier, insecticides, additives in paint formulation.

Books Suggested:

1. Oliver Kahn, Molecular Magnetism, VCH Publishers, UK,1993.
2. W. D. Callisters, Materials Science and Engineering: An Introduction, Wiley, 2006.
3. N. W. Aschcroft and N. D. Mermin Solid State Physics, Holt, Rinehart and Winston, New York, 1976.
4. J. C. Anderson, K. D. Leaver, J. M. Alexander and R. D. Rowlings Materials Science. ELBS, 2003.
5. Kelker and Hatz , Hand Book of Liquid Crystals, 2nd Ed. Wiley, 2014.
6. V.C. Malshe and Meenal Sikchi, Basics of Paint Technology, Part I & II, 2008,
7. G.P.A. Turner, Introduction to Paint Chemistry, Chapman& Hall, 1967.

B021010T Green Chemistry Semester-IV

Unit 1: Introduction Principle and Concepts of green Chemistry

Need for green chemistry, Inception and evolution of green chemistry, Twelve principles of Green Chemistry with their explanation and examples, Designing a green synthesis using these principles, Green chemistry in day to day life.

Unit 2: Non Traditional Greener Alternative Approaches

Different approaches to green synthesis: Use of green reagents in organic synthesis-Dimethyl carbonate, Polymer supported reagents- Peracids and Chromic acids, Green Catalysis , role of catalysis in sustainable development , homogeneous and heterogeneous catalyst, Introduction , advantages and applications of Biocatalyst.

Unit 3: Application of Non-conventional Energy Sources

Introduction of microwave induce synthesis: Microwave activation, equipment, time and energy benefits, limitations, Organic transformations under microwaves- Fries rearrangement , Diels -Alder reaction, Decarboxylation, saponification of ester.
Introduction of ultrasound assisted green synthesis: Instrumentation, Physical aspects, application in organic transformations.

Unit 4 Environmentally Benign Solutions to organic solvents:

Ionic liquids as green Solvents: Introduction, properties and types of ionic liquids, Synthetic applications- Diels -Alder reaction.
Aqueous phase reactions: Synthesis applications- 1,3- Dipolar Cycloadditions, Carbon-Carbon bond-forming processes and bromination reactions. Role of supercritical Carbon dioxide in green chemistry, Ethyl lactate as a renewable green solvent: Properties and applications.

Unit 5: Synthesis of Nanomaterials:

Greener synthesis of Nanomaterials –Magnetic Nanoparticles, MW assisted nano catalysis in water, Synthesis of Nanoparticles using Bacteria , Yeast, Algae and Fungus.

Books Suggested:

1. P.A.G. Blackie, *Organic synthesis in water*, Springer (1998).
2. P.T. Anastas, *Green Chemistry: Theory and Practice*, Oxford University Press (2002).
3. M. Lancaster, *Green Chemistry: An Introductory Text*, Royal Society of Chemistry (2016).

B021011P Practical Semester-IV

The Distribution of marks will be as follows.

(a) Organic Exercise (one)	30
(b) Physical Exercise (one)	30
(c) Viva-voce	20
(d) Record/Assessment	20

Organic Chemistry

Qualitative Analysis

Separation, purification and identification of the components of a mixture of three organic compounds (three solids or two liquids and one solid, two solids and one liquid), using TLC for checking the purity of the separated compounds, chemical analysis, IR, PMR and mass spectral data.

Multi-step Synthesis of Organic Compounds

The exercises should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

Photochemical reactions

Benzophenone ⟶ Benzpinacol ⟶ Benzpinacolone
Beckmann rearrangement: Benzanilide from benzene
Benzene ⟶ Benzophenone ⟶ Benzophenone oxime ⟶ Benzanilide
Benzilic acid rearrangement: Benzilic acid from benzoin
Benzoin ⟶ Benzil ⟶ Benzilic acid
Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline Fisher- Indole synthesis:
Preparation of 2-phenylindole from phenylhydrazine.
Enzymatic synthesis
Enzymatic reduction: Reduction of ethyl acetoacetate using Baker's yeast to yield enantiomeric excess of S(+) ethyl-3-hydroxybutanoate and determine its optical purity.
Biosynthesis of ethanol from sucrose.
Synthesis using microwaves
Alkylation of diethyl malonate with benzyl chloride.
Synthesis using phase transfer catalyst
Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide

Extraction of Organic Compounds from Natural Sources

1. Isolation of caffeine from, tea leaves.
2: Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported).
4. Isolation of nicotine dipicrate from tabacco.
5. Isolation of cinchonine from cinchona bark.
6. Isolation of piperine from black pepper.
7. Isolation of lycopene from tomatoes.
8. Isolation of β-carotene from carrots.
9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
10. Isolation of eugenol from cloves.
11. Isolation of (+) limonine from citrus rinds.

Paper Chromatography

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper, chromatography and determination of Rf values.

Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS).

Spectrophotometric (UV/VIS) Estimations

1. Amino acids
2. Proteins
3. Carbohydrates
4. Cholesterol
5. Ascorbic acid
6. Aspirin
7. Caffeine

Physical Chemistry

Number of hours for each experiment: 3-4 hours

A list of experiments under different headings are given below. Typical experiments are to be selected from each type.

Thermodynamics

(i) Determination of partial molar volume of solute (e.g., KC1) and solvent in a binary mixture.
(ii) Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO- water mixture) and calculate the partial molar heat of solution.

Spectroscopy

(i) Determination of pKa of an indicator (e.g., methyl red) in (a) aqueous and (b) micellar media.
(ii) Determination of stoichiometry and stability constant of inorganic (e.g. ferric-salicyclic acid) and organic (e.g. amine-iodine) complexes.
(iii) Characterization of the complexes by electronic and IR spectral data.

Polarography

(i) Estimation of Pb^{2+} and Cd^{2+}/Zn^{+} and Ni^{2+} ions in a mixture of Pb^{2+} and Cd^{2+}/Zn^{+} and Ni^{2+} by polarography.
(ii) Determination of dissolved oxygen in aqueous solution of organic solvents.

Electronics

This lab course will have theory as well as practicals and the lectures shall be delivered during lab hours.

Basic Electronics

Notations used in an electric circuit, study of electronic components and colour codes, conversion of chemical quantities into electrical quantities. Transducer illustration with electrodes, thermocouples and thermistors.

Passive components: Resistors, capacitors and inductors with some emphasis on solid state properties of materials. Net works of resistors. Thevenin's theorem, superposition theorem, loop analysis, R C circuits, L R circuits, LCR circuits. Illustration of the use of the circuits in NQR spectroscopy, Mossbauer spectroscopy, cyclic voltametry and in power supplies as filter circuits.

Active Components

Introduction to ordinary diodes and Zener diodes with some emphasis on p-n juction as a solid state property. Use of diodes as rectifiers, clipping and clamping circuits Power supplies.

Transistors: An extension of p-n juction to p-n-p and n-p-n transistors. Characteristics of transistors, hybrid parameters; transistor circuits as amplifiers, high impedance (preamplifier) circuits. Darlinction pairs differential amplifiers.

Operational Amplifiers

Ideal characteristics; inverter, summer integrator, differentiator, voltage follower, illustrative use of operational amplifiers.
Introduction to Fourier transform in instrumentation .

List of Experiments in Electronics

- Measurements of resistance with multimeter.
- To measure the resistance of the given ammeter
- Voltage measurement with CRO
- Familiarising with CRO
- Use of a Wheatstone Bridge for accurate measurement of resistance
- Capacitor as a charged storage device
- To study the behaviour of parallel charged capacitors in series charged capacitors placed in parallel
- The use of LCR Bridge
- Response characteristics of RC network
- Response characteristics of LR network
- Response characteristics of LCR network
- Verification of Kirchoff's laws
- To study the Lissajou's figures
- Measurement of e.m.f. with thermocouple
- To plot the characteristic curve of a diode.
- Half-wave and full-wave rectifier
- Clipping and clamping circuits
- Capacitors filter for full-wave rectifier
- Voltage doubler, Zener stabilized bipolar power supply
- Transistor characteristics
- Differential amplifier
- Transistor amplifier
- Introduction of an operational amplifier as a voltage follower
- Op-Amp as non-inverting and inverting amplifier
- Simple integration differentiation with Op-Amp. 741
- Op- Amp. as comparator
- Designing and fabrication of a printed circuit board
- Setting up of a thermostat: Constant temperature bath
- Four-probe method for resistivity measurement

Books Suggested:

1. The Systematic Identification of Organic Compounds, R.S. Shriner and D.Y. Curtin.
2. Semimicro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entrikin and E.M. Hodnett
3. Experimental Organic Chemistry, M.P. Doyle and W.S. Mungall.
4. Small Scale Organic Preparations, P.J. Hill.
5. Organometallic Synthesis, J.J. Fisch and R.B. King Academic
6. Experimental Physical Chemistry, D.P. Shoemaker C.W. Garland and J.W. Niber, McGraw Hill Interscience.
7. Findlay's Practical Physical Chemistry, Revised B.P. Levitt, Longman.
8. Experiments in Physical Chemistry, J.C. Ghosh, Bharat Bhavan.

B021012R Research Project Semester-IV