SEMESTER III

PGCH3T08**: Spectroscopy-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Understand the symmetry properties of molecules*
2. *Interpret the structure of simple organic molecules using mass spectrometry*
3. *Correlate the presence of functional groups with IR frequencies*
4. *Apply the IR and Raman spectroscopy to simple molecules*

Unit - I: Symmetry properties of molecules and group theory:

Symmetry elements and symmetry operations. Properties of group. Point groups and Schoenflies symbols. Symmetry operations as a group. Matrix representations of groups. Multiplication table for C_{2v}, C_{3v} and C_{2h}. Reducible and irreducible representations. Similarity transformation. Classes of symmetry operations. Great Orthogonality Theorem. Derivation of character tables for H_2O and NH_3 using Great Orthogonality Theorem. Application of character tables in selection rules of IR, Raman and Electronic spectroscopy.

Unit - II:

A] **Mass spectrometry:** Theory, ion production (EI, CI, FD, FAB), ion analysis, ion abundance, isotopic contribution, Nitrogen-rule, types of fission processes, high resolution mass spectrometry, metastable peak, molecular ion peak, McLafferty rearrangement, mass spectral fragmentation of organic compounds alkanes, alkenes, alkynes, alcohols, amines, amides, acids, aldehydes, ketones, halides, Structure determination of organic molecules by mass spectrometry, problem based on mass spectral data

B] **Mössbauer spectroscopy**: Basic principle, experimental techniques, recoil emission and absorption, source, absorber, isomer shift, quadrupole interaction, magnetic hyperfine interaction, applications in determining electronic structure, molecular structure, crystal symmetry, magnetic structure, surface studies, biological applications.

Unit - III:

A] **Microwave spectroscopy**: Classification of molecules on the basis of M.I., rigid and non-rigid rotor, effect of isotopic substitution on transition frequencies, stark effect, microwave spectrometer, application in deriving: molecular structure, dipole moment, atomic mass and nuclear quadrupole moment.

B] **ESR spectroscopy**: Introduction, principle of ESR, ESR spectrometer, hyperfine coupling, zero field splitting, factors affecting g values, Kramer's degeneracy, application of ESR spectra to study free radicals like hydrogen, methyl radical, 1,4-semibenzoquinone, naphthalene, transition metal complexes, biological systems.

Unit IV:

A] **Infrared spectroscopy**: Diatomic molecules: Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero

point energy, isotope effect. The Anharmonic oscillator, the interactions of rotations and vibrations. P,Q,R branches, vibration of polyatomic molecules, selection rules, normal modes of vibration, group frequencies, overtone and combination frequencies. Structure determination of organic molecules by IR spectroscopy, problem based on IR spectral data

B] **Raman Spectroscopy**: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Selection rules, coherent anti-Stokes Raman spectroscopy, Structure determination from Raman and Infra-red spectroscopy.

Books suggested

1. Spectroscopic identification of organic compound-RM Silverstein, GC Bassler and TC Morril, John Wiley
2. Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiley
3. Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
4. Organic Spectroscopy-William Kemp, ELBS with McMillan
5. Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
6. Practical NMR Spectroscopy-ML Martin, JJ Delpench, and DJ Martyin
7. Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
8. Fundamentals of Molecular Spectroscopy-CN Banwell
9. Spectroscopy in Inorganic Chemistry-CNR Rao and JR Ferraro
10. Photoelectron Spectroscopy-Baber and Betteridge
11. Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
12. NMR –Basic Principle and Application-H Guntur
13. Interpretation of NMR spectra-Roy H Bible
14. Interpretation of IR spectra-NB Coulthop
15. Electron Spin Resonance Theory and Applications-W Gordy
16. Mass Spectrometry Organic Chemical Applications, JH Banyon

SEMESTER III

PGCH3T09: Advanced Organic Chemistry-I

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Identify a pericyclic reaction and categorize it as a cycloaddition, a group transfer reaction, a sigmatropic rearrangement, or an electrocyclic reaction,*
2. *Apply frontier molecular orbital (FMO) theory to rationalize selectivity and reactivity aspects of pericyclic reactions.*
3. *Understand the reaction mechanism of various common reagents employed in organic synthesis*
4. *Understand the reactivity of sulphur, silicon and phosphorous elements.*
5. *Apply pericyclic reactions for the synthesis of complex organic molecules*

Unit I: Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, classification of pericyclic reaction. FMO approach, Woodward-Hoffman correlation diagram method and Perturbation of Molecular Orbital (PMO) approach of pericyclic reaction under thermal and photochemical conditions Electrocyclic reactions, conrotatary and disrotatary motion for 4n and (4n+2) systems, Cycloaddition reaction with more emphasis on [2+2] and [4+2], Cycloaddition of ketenes, Secondary effects in [4+2] cycloaddition. Stereochemical effects and effect of substituents on rate of cycloaddition reaction, Diels-Alder reaction, 1,3-dipolar cycloaddition and chelotropic reaction. Sigmotropic rearrangement, suprafacial, and antarafacial shift involving carbon moieties, retention and inversion of configuration, [3,3] and [5,5] sigmotropic rearrangements, Claisen, Cope, Sommelet-Hauser rearrangements, Ene reaction, Nazarov cyclization, DeMayo reaction

Unit II: Oxidation

Oxidation of alkanes, aromatic hydrocarbons and alkenes, Dehydrogenation with S, Se, Fremy's salt, DDQ, chloranil, Oxidation with SeO_2, Epoxidation of olefins, application of epoxides, Sharpless asymmetric epoxidation, Dihydroxylation of olefins using $KMnO_4$, OsO_4, Woodward and Prevost dihydroxylation, Oxidative cleavage of olefins, Ozonolysis, Etard Reaction

Oxidation of alcohols: Chromium reagents, pyridinium chlorochromate (PCC), pyridinium dichromate (PDC), Collin and Jones reagent, Combination of DMSO with DCC, $(COCl)_2$, NCS, SO_3 and $(CH_3CO)_2O$ for oxidation of alcohols, Oxidation with MnO_2, Oppenauer oxidation, CAN, Tetrapropyl ammonium peruthenate, Fetizon's reagent, Chemistry and synthetic applications of $Pb(OAc)_4$, Dess-Martin periodane, IBX and related hypervalent iodine based oxidations

Conversion of ketones to α, β-unsaturated ketones and α-hydroxy ketones, Baeyer-Villiger oxidation, Dakin oxidation, Tamao-Fleming Oxidation, Oxidations with Dimethyl dioxirane (DMDO) and 2-sulfonyloxaziridines and chiral version

Unit III: Reduction

Catalytic heterogeneous and homogeneous hydrogenation, Hydrogenation of alkenes, alkynes and arenes, Selectivity of reduction, Mechanism and stereochemistry of reduction, Raney Ni-catalyst, Adam catalyst, Lindlar catalyst, Wilkinson catalyst

Reduction by dissolving metals, Reduction of carbonyl compounds, conjugated systems, aromatic compounds and alkynes. Birch reduction, Hydrogenolysis

Reduction by hydride transfer reagents, Meerwein-Pondorff-Verley reduction, Reduction with $LiAlH_4$ and $NaBH_4$, stereochemical aspects of hydride addition, Derivatives of $LiAlH_4$ and $NaBH_4$, Selectivity issues, Diisobutylaluminium hydride (DIBAL-H), Sodium cyanoborohydride, Reduction with boranes and derivatives Reduction of carbonyl group to methylene, Reduction with diimide and trialkylsilanes

Unit IV: Chemistry of P, S, Si, and Boron compounds

1) Phosphours and sulphur ylide: Preparation and their synthetic application along with stereochemistry

2) Umpolung concept: Dipole inversion, generation of acyl anion, use of 1,3-dithiane, ethylmethylthiomethylsulphoxide, *bis*-phenylthiomethane, metallated enol ethers, alkylidene dithiane, ketone thioacetals, 2-propenethiobismethyl thioallyl anion, thiaminehydrochloride based generation of acyl anion

3) Organoboranes- preparation and properties of organoborane reagents e.g. RBH_2, R_2BH, R_3B, 9-BBN, catechol borane. Thexylborane, cyclohexylborane, $ICPBH_2$, IPC_2BH, Hydrboration mechanism, stereo and regioselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes, Synthesis of *EE, EZ, ZZ* dienes and alkyenes. Mechanism of addition of IPC_2BH. Allylboranes-synthesis, mechanism and uses

4) Organosilicon compounds in organic synthesis, Me_3SiCl, Me_3SiH and Peterson reaction, Synthesis and reactions of alkenyl, alkynyl and aryl silanes

Books suggested

1. Organic Chemistry, J .Clayden, N .Greeves, S .Warren and P .Wothers, Oxford University Press
2. Some Modern Methods of Organic Synthesis-W .Carruthers
3. Principles of Organic Synthesis by R. O. C. Norman and James M. Coxon (Nelson Thornes Ltd)
4. Advance Organic Chemistry Part-B-F .A .Caray and R .J .Sundberg Plenum Press
5. Modern Organic Synthesis: An Introduction by G. S. Zweifel and M. H. Nantz (Wiley)
6. Organic Synthesis by Michael Smith , 4th Edition (Academic Press)
7. Pericyclic Reactions by I. Fleming, Oxford University Press, 1999
8. S. Sankararaman, Pericyclic Reactions – A textbook. Wiley-VCH, 2005.
9. Organic synthesis: The roles of boron and silicon by S. E. Thomas (Oxford Chemistry Primers)
10. The Chemistry of Organophosphorous-A .J .Kirbi and S.G .Warren
11. Organosilicon Compound-C .Eabon
12. Organic Synthesis via Bora- H. C. Brown
13. Organoborane Chemistry-T .P .Onak
14. Organic Chemistry of Boron-W Gerrard

Weblink to Equivalent MOOC on SWAYAM if relevant:

- Organic Photochemistry and Pericyclic Reactions: Dr. N.D. Pradeep Singh Department of Chemistry IIT Kharagpur, https://nptel.ac.in/courses/104105038
- Pericyclic Reactions and Organic Photochemistry: Prof. Sankararaman, IIT Madras https://nptel.ac.in/courses/104/106/104106077/
- Essentials of Oxidation, Reduction and C-C Bond Formation. Application in Organic Synthesis https://nptel.ac.in/courses/104/101/104101127/
- Reagents in organic synthesis: Prof. Subhas C. Pan, IIT Guwahati https://archive.nptel.ac.in/courses/104/103/104103111/
- Principles of Organic Synthesis: Prof. T. Punniyamurthy, IIT Guwahati, https://archive.nptel.ac.in/courses/104/103/104103110/

SEMESTER III

PGCH3T10**: Advanced Inorganic Chemistry**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Understand the crystal structures of simple inorganic molecules.*
2. *Understand the industrial applications of catalysis.*
3. *Apply the mechanism of metallo-enzyme actions in various life processes.*
4. *Apply simple methods of synthesis and characterization to nanomaterials.*

Unit I: Solid State Chemistry

Ionic Crystals and their structures, radius ratio rule, effect of polarization on crystals. Covalent structure type: Sphalerite and Wurtzite. Geometry of simple crystal AB type: NaCl, CsCl and NiAs. AB_2 type: Fluorite, antifluorites, Rutile structures. Li_2O, Na_2O, $CdCl_2$, CdI_2 structures.

Ternary Compounds ABO_3 type: Perovskite, Barium titanate, lead titanate, $CaTiO_3$, Tolerance factor, charge neutrality and deviation structures $FeTiO_3$.

Solids of AB_2O_4 type: Normal and inverse,2-3 and 4-2 spinel, packing of oxygen in tetrahedral and octahedral sites, sites occupancy number of sites surrounding each oxygen, application of charge neutrality principles, site preferences in spinel, distorted spinel. Hausmannite (Jahn-Teller distortions), Factors causing distortion in spinel.

Unit II: Organometallic Chemistry

Introduction of Organometallic Chemistry, counting of electrons, 16-18 rule, Ligand substitution reactions, Oxidative Addition: Concerted, S_N2 and radical mechanism, Reductive elimination, Migratory insertion and elimination reactions, Migration and insertion reactions Alpha-Migratory insertion and Alpha-Elimination Reactions, beta-migratory insertion, Beta-Elimination Reaction, Alpha-Abstraction and Beta-Abstraction, 4-Center Reactions [2+2] Reactions, External Attack by a Ligand and Reductive Coupling

Hydrogenation Reaction [mobohydride and dihydride catalyst] Stereoselective hydrogenation reaction, Wilkinson catalyst, Schrock-Osborn catalysts for hydrogenation, Carbonylation Reaction: Monsanto Acetic Acid Process, Hydroformylation, Hydrocarboxylation and Hydrocyanation, Ziegler-Natta polymerization

Palladium catalyzed cross-coupling reactions-Heck reaction, carbonylation, Wacker oxidation, Kumada, Stille, Sonogashira, Negishi and Suzuki coupling reactions and their importance, Applications of $Co_2(CO)_8$, $Ni(CO)_4$, $Fe(CO)_5$ and in organic synthesis. Transition metal carbenes, Fischer and Schrock carbenes, Olefin metathesis by I^{st} and II^{nd} generation catalyst, Schrock and Grubbs catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, application in the synthesis of homo and heterocyclic compounds, polymerization and synthesis of small organic molecules.

Unit -III

A) Metallo enzymes: The principle involved and role of various metals in i) Zn-enzyme: Carboxyl peptidase & Carbonic anhydrase. ii) Fe-enzyme: Catalase Peroxidase & Cytochrome P-450 iii) Cu-enzyme: Super Oxide dismutase iv) Molybdenum: Oxatransferase enzymes, Xanthine oxidase, Co-enzyme vitamin B_{12}, Structure of vitamin B_{12}. Co-C bond cleavage, Mutase activity of co- Enzyme B-12, Alkylation reactions of Methyl Cobalamin.

B) Electron transfer in biology: Structure and functions of metalloproteins in electron transfer proteins, cytochromes and Fe-S proteins, non-heme iron proteins; Rubredoxins, Synthetic models. Biological nitrogen fixation (*in-vitro* and *in-vivo*).

Unit-IV: Nanomaterials and Microscopic Techniques

A) Nanoparticles and nanostructure materials: Introduction, methods of synthesis: conventional and biogenic synthesis. Molecular Precursor routes to inorganic solids: Nanoporous Materials: Zeolites, metal oxides, composites & molecular sieves, composition-structure, preparation & applications.

B) Carbon-based nanomaterials: Introduction, synthesis methods: CNT, graphene-based materials, graphitic carbon nitride, quantum dot, carbon dot.

C) Techniques for nanomaterials authentication: X-Ray diffraction, Fourier Transform Infrared Spectroscopy, *U*V-Diffuse Reflectance Spectroscopy, X-ray Photoelectron Spectroscopy, Scanning Electron Microscopy, Transmission Electron Microscopy, Atomic Force Microscopy, Energy Dispersive X-Ray Analysis, Brunauer-Emmett-Teller analysis, Thermogravimetric Analysis.

Books suggested

1. Inorganic Chemistry, Third Edition, Shriver and Atkins, Oxford University Press.
2. Inorganic Chemistry, Fourth Edition, Catherine E. Housecroft and Alan G. Sharpe, Pearson, England.
3. Principles of Inorganic Chemistry, thirty third edition, B. R. Puri, L. R. Sharma, K. C. Kalia, Milestone Publisher & Disruptors, Delhi.
4. Organometallic Chemistry, Revised Second Edition, R. C. Mehrotra, A. Singh, New Age International Publication, New Delhi.
5. Basic Inorganic Chemistry, Third Edition, F. Albert Cotton, Geoffrey Wilkinson, John Wiley & Sons Inc.
6. Essentials of Bio-Inorganic Chemistry, Neerja Gupta, Monal Singh, Pragati Edition, Meerut.
7. Inorganic Chemistry, Gary L. Miessler and Donald A. Tarr, Pearson Education International, New York.

8. Inorganic Chemistry, Fourth Edition, James E. Huheey, Ellen A. Keitler, Richard L. Keitler, Pearson Education International, New York.
9. Emerging Nanomaterials and Their Impact on Society in the 21st century, N. B. Singh, Md. A.B. Hasan Susan, R.G. Chaudhary, Material Research Forum, Millerville, USA.
10. Concept and Models of Inorganic Chemistry, Third Edition, B. Douglas, D. McDaniel, J. Alexander, John Wiley & Sons Inc., New York.
11. Inorganic Chemistry, K. F. Purcell, J. C. Kotz, Cengage Learning, Delhi.
12. Nanoscale Materials in Chemistry, K. I. Kalbunde, John Wiley, New York.
13. Biogenic Sustainable Nanotechnology, R. P. Singh, A. R. Rai, A. Abdala, R. G. Chaudhary, Elsevier, Amsterdam, Netherland.
14. Introduction To Nanoscience and Nanotechnology, Chris Binns, John Wiley & Sons Inc., New York.
15. Carbon nanomaterials: synthesis, structure, properties and applications, R. Mathur, B. Singh, S. Pande, Taylor & Francis, Boca Raton.
16. Nanomaterials and Nanocomposites: Synthesis, Properties, Characterization Techniques, and Applications, R. K. Goyal, Taylor & Francis, Boca Raton.

SEMESTER III

PGCH3T11**: Elective (a) Inorganic Chemistry Special-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student would be able to*

1. *Understand structure and bonding in transition metal pi complexes*
2. *Elaborate advance materials including supramolecules and advanced nanomaterials.*
3. *Classify and characterize the coordination polymers*
4. *Understand mechanism of photophysical and photochemical processes*
5. *Explain various redox processes in complexes.*

Unit-I

Transition Metal Pi Complexes-Carbon multiple bonds. Nature of bonding, structural characteristics and synthesis, properties of transition metal pi- Complexes with unsaturated organic molecules, alkenes alkynes, allyl, diene, dienyl, arene and trienyl complexes. Application of transition metal, organometallic intermediates in organic synthesis relating to nucleophilic and electrophilic attack on ligands, role in organic synthesis.

Unit-II

A) Supramolecular chemistry: Definition, intermolecular bonds, concepts and perspectives, cationic recognition, anionic recognition, neural molecular recognition: self-assembly concept and its application in molecular and supramolecular chemistry, supra molecular chemistry, supramolecular devices and machines.

B) Inorganic pharmaceuticals: Lithium drugs, gold antiarithritic drugs, Bismuth drugs in the treatment of gastric ulcers, Cyclams as anti-HIV agents, Radio-diagnostic agents, contrast agents for MRI and X-ray imaging.

C) Nano structural materials: Nanofibres, MXenes (two-dimensional inorganic compounds), Molecular Precursor routes to Nanoporous Materials: Zeolites and molecular sieves, porous lamellar solids, composition-structure, preparation and applications.

Unit-III

A) **Coordination Polymers**: Coordination polymers and their classification. Synthesis and applications of coordination polymers. Use of polymeric ligands in synthesis of coordination polymers. Organosilicon polymers. Synthesis and their uses.

B) **Characterization of coordination polymers on the basis of**:

i) Spectra (UV, Visible, IR and NMR)

ii) Magnetic and thermal (TGA, DTA and DSC) studies

Unit-IV

A] Photophysical and photochemical properties of Gold(I) complexes: Introduction, Binuclear and trinuclear complexes, Mixed metal Systems, Photochemical reactivity, Solid state studies, Mononuclear Gold(I) complexes, Mononuclear three coordinate Gold(I) complexes

B) Redox reactions by Excited Metal Complexes: Energy transfer under conditions of weak interaction and strong interaction – exciplex formation, conditions of excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2- bipyridine and 1,10-Phenanthroline complexes.), illustration of reducing and oxidizing character of ruthenium(II); role of spin-orbit coupling, lie time of these processes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants in to high energy products, chemical energy in to light.

C) Excited States of Metal Complexes: Electronically excited states of metal complexes, charge transfer spectra, charge transfer excitations, methods for obtaining charge transfer spectra.

Books suggested

1. Anderson J.C.,LeverK.D.,Alexander J.M and Rawlings,R.D.,ELBS
2. GrayG.W.Ed.Thermotropic Liquid Crystals,John Wiley
3. Kelkar and Hatz Handbook of Liquid Crystals,ChemieVerlag.
4. Kalbunde K.I.,Nanoscale Materials in Chemistry,JohnWiley,NY.
5. Shull R.D.,McMichael R.D. and SwartzendrubL.J.,Studies of Magnetic Properties of Fine particles and their relevance to Mataerials Science, Elsevier Pub. Amsterdam
6. Optoelectronic Properties of Inorganic Compounds, D. Max Roundhill and John P. Fakler, Jr. Plenum Press, New York

SEMESTER III

PGCH3T11: Elective (b) Organic Chemistry Special-I

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Learn the important aspects of steroids and terpenoids.*
2. *Understand the biosynthesis of natural products.*
3. *Analyze the enzyme reactions involved in various life processes*
4. *Illustrate the structure elucidation of unknown naturally occurring organic compound*
5. *Apply the knowledge of organic reactions for the total synthesis of useful natural products*

Unit I

A) Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol, α-terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β-carotene, Vitamin A.

B) Genesis of biological isoprene unit, Biosynthesis (**ONLY**) of the following tepenoids: myrecene, linalool, geraniol, α-terpeneol, limonene, camphor, α-pinene, β-pinene, farnesol, β-bisabolene and squalene.

Unit- II

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, generalmethods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring,role of alkaloids in plants Structure, stereochemistry, and total synthesis of the following: Ephedrine, (+)-coniine, Nicotine, Atropine, Quinine, Reserpine and Morphine.

Biosynthesis (**ONLY**) of the followings: hygrine, tropinone, nicotine, pelletierine, conine.

Unit-III

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and total synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone and Aldosterone. Biosynthesis of steroids (lanosterol)

Unit IV

A) Plant Pigments: Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteolin, Quercetin, Myrcetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Cyanidin-7-arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and The Shikimate pathway: Biosynthesis of Cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavanoids.

B) Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE2 and PGF2 (E. J. Corey and Gilbert Stork synthesis only) and iodolactonization reaction.

Books suggested

1. Organic Chemistry Vol. II - I. L. Finar
2. Chemistry of Plant Natural Products: Sunil Kumar Talapatra and B. Talapatra (Springer)
3. Classical Methods in Structure Elucidation of Natural Products: *R. W. Hoffmann*, Wiley-VCH
4. A Fragrant Introduction to Terpenoid Chemistry: Charles S Sell (RSC)
5. Chemistry of Alkloids-S .W .Pelletier
6. Chemistry of Steroids-L .F .Fisher and M .Fisher
7. The Molecules of Nature-J .B .Hendricsion
8. Biogenesis of Natural Compound -Benfield
9. Natural Product Chemistry and Biological Significance -J .Mann, R .S Devison, J .B .Hobbs, D .V .Banthripde and J .B .Horborne
10. Introduction to Flavonoids-B .A .Bohm, Harwood
11. Chemistry of Naturally Occurring Quinines-R .H .Thomson
12. The Systematic Identification of Flavonoids -Marby, Markham, and Thomos

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Weblink to Equivalent MOOC on SWAYAM if relevant:

- Classics in total synthesis: Prof. Krishna P. Kaliappan, IIT Bombay (Useful for total synthesis of alkaloids, steroids and prostaglandins) https://archive.nptel.ac.in/courses/104/101/104101133/

SEMESTER III

PGCH3T11**: Elective (c) Physical Chemistry Special-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Understand, the concept of statistical function, and applications*
2. *Understand the applications of electrochemistry in various fields*
3. *Understand the theories of advanced chemical dynamics*
4. *Understand the various photophysical processes and their applications*

UNIT I: ELECTRICAL AND THERMAL PROPERTIES OF SOLIDS

A**)** Classical free electron theory, electrical conductivity, thermal conductivity, Wiedemann-Franz Law, Lorenz number, Electronic distribution in solids using Fermi Dirac Statistics, The Fermi Distribution function and effect of temperature, Quantum theory of free electrons, periodic potential, The Kronig-Penney Model, Brillouin Zones, Distinction between metals, insulators and intrinsic semiconductors based on above theory**.**

B**)** Thermal Properties**:** Specific heat of solids, Classical theory, Einstein**'**s theory of heat capacities, Debye theory of heat capacities or Debye T-cubed law.

UNIT II: ELECTROCHEMISTRY OF SOLUTION

A**)** OHP and IHP, potential profile across double layer region, potential difference across electrified interface; Structure of the double layer: Helmholtz-Perrin, Gouy Chapman model, Stern region, Graham Devanathan- Mottwatts, Tobin, Bockris, Devnathan Models**.**

B**)** Over potentials, exchange current density, derivation of Butler Volmer equation under near equilibrium and non-equilibrium conditions, Tafel plot

C**)** Electrical double lever, theories of double layer, electro-capillary phenomena, electro-capillary curve**.** Electro-osmosis, electrophoreses**.** Streaming and Sedimentation potentials**.** Zeta potentials and its determination by electrophoresis, influence of ions on Zeta potential**.**

UNIT III: CHEMICAL DYNAMICS - I

A**)** Dynamics of complex reactions**:** reversible, parallel, consecutive, concurrent and branching reactions, free radical and chain reactions, reaction between Hydrogen – Bromine and Hydrogen – Chlorine **(**thermal and photochemical**)**, decomposition of ethane, acetaldehyde, N_2O_5, Rice Herzfeld mechanism, Oscillatory autocatalytic and Belousov-Zhabotinsky reactions, Lotka-Volterra mechanism, the brusselator and the oregonator**.**

B**)** **Fast Reactions:** relaxation methods, flow methods, flash photolysis, magnetic resonance method, relaxation time and numerical**.**

UNIT IV: PHOTOCHEMISTRY

A**)** **Photophysical phenomenon:** Introduction, photo and photochemical excitation and de-excitation, fluorescence, delayed fluorescence, and phosphorescence, fluorescence quenching**:** concentration quenching, quenching by excimer and exciplex emission, fluorescence resonance energy transfer

between photoexcited donor and acceptor systems. Stern-Volmer relation, critical energy transfer distances, energy transfer efficiency, examples and analytical significance, bimolecular collisions, quenching and Stern-Volmer equation.

B) **Photochemical reactions:** photoreduction, photooxidation, photodimerization, photochemical substitution, photoisomerization, photosensitization, chemiluminescence, photochemistry of environment: Greenhouse effect.

Books suggested

1. G. M. Panchenkov and V. P. Labadev, " Chemical Kinetics and catalysis", MIR Publishing
2. E.A. Moelwyn- Hughes, "Chemical Kinetics and Kinetics of Solutions", Academic
3. K. J. Laidler, Chemical Kinetics, Third Edition (1987), Harper and Row, New York
4. J. Raja Ram and J. C. Kuriacose, Kinetics and Mechanism of Chemical Transformations MacMilllan Indian Ltd., New Delhi (1993)
5. J.G. Calvert and J.N. Pitts, Jr., Photochemistry, John Wiley and Sons, New York (1966).
6. K. K. Rohtagi-Mukherjee, Fundamentals of Photochemistry, New Age International, New Delhi(1986).
7. R. P. Wayne, Principles and Applications of Photochemistry, Oxford University Press, Oxford(1988).
8. N. J. Turro, Modern Molecular Photochemistry, Univ. Science Books, Sansalito (1991).
9. J. F. L. Lakowicz, Principles of Fluorescence Spectroscopy, 2nd Edition (1999), PlenumPublishers, NewYork.
10. F.W.Sears, " Introdction to Thermodynamics, Kinetic Theory of Gases and statistical mechanics". AddisonWesley
11. H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
12. M. C. Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub. Corp., New York,
13. N. J. Turro, V. Ramamurthy and J. C. Scaiano, Principles of Photochemistry – An Introduction, Viva Books, New Delhi, 2015.
14. G. A. Somorjai, Introduction to Surface Chemistry and Catalysis, Wiley, 2010.
15. M. C. Gupta, Statistical Thermodynamics, New Age International.
16. K. Huang, Statistical Mechanics, Wiley, New Delhi, 2003.
17. Andrew Maczek, Statistical Thermodynamics, Oxford University Press Inc., New York (1998).
18. B. K. Agarwal and M. Eisner, Statistical Mechanics, Wiley Eastern, New Delhi (1988).
19. D. A. McQuarrie, Statistical mechanics, Harper and Row Publishers, New York (1976).
20. J.O.M.Bokris and A.K.N.Reddy, "Modern Elcrtrochemistry". Wiley
21. S. Glasstone, "Introduction to Electrochemistry" Affilisated East West Press, New Delhi.
22. S. O. Pillai, Solid State Physics, New Age International, New Delhi, 2102.
23. D. R. Crow, " The Principle of electrochemistry", Chapman Hall
24. G. K. Agrawal, Basic Chemical Kinetics, Tata-Mc-Graw Hill Pvt., Ltd. 1990
25. K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.

26. Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.

NPTEL sources weblinks:

- Electrochemistry of solutions: https://archive.nptel.ac.in/courses/104/106/104106129/
- Chemical Dynamics https://nptel.ac.in/courses/104101128
- https://onlinecourses.nptel.ac.in/noc20_cy22/preview
- https://nsdl.niscpr.res.in/bitstream/123456789/251/1/Photochemistry%20revised.pdf

SEMESTER III

PGCH3T11**: Elective (d) Analytical Chemistry Special-I**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Explain the principles involved in radiation chemistry.*
2. *Compare various detectors used in radiochemistry and select among them for desired analysis.*
3. *Compare various voltammetric techniques for given type of analysis.*
4. *Understand the electrodes used in different voltammetric techniques and their comparison.*
5. *Design experiments for water quality assessment based on parameter under study.*

Unit-I: Radioanalytical Chemistry

Radioactivity, Law of radioactive decay, Half life and mean life, Elementary principles of GM and proportional counters, Gamma Ray Spectrometer, Ionization chamber, HPGe detector, NaI(Tl) detector**.** Preparation of some commonly used radioisotopes (^{22}Na, ^{60}Co, ^{131}I, ^{65}Zn, ^{32}P)**,** Use of radioactive isotopes in analytical and physico-chemical problems, Neutron Activation Analysis, Isotope Dilution Analysis, Radiometric titrations (Principle, Instrumentation, applications, merits and demerits), Radiochromatography, Carbon dating, Numericals based on above.

Unit-II: Stripping voltammetry

Stripping Voltammetry**:** Principle and technique in anodic and cathodic stripping voltammetry, applications to metal ion analysis, limitations**.**

Adsorptive stripping voltammetry: Principle, technique, applications to metal ions and organic analysis**.** Advantages over anodic stripping voltammetry**.** Catalytic effects in voltammetry**.**

Working electrodes: Mercury electrodes, carbon electrodes, film electrodes**.**

Electrochemical sensors (*Chemically modified electrodes****):*** Biosensors, catalytic sensors and gas sensors**.** Comparison of voltammetry with AAS and ICP-AES**.**

Unit-III: Electroanalytical methods

Electrogravimery: Theory of electrolysis. Electrode reactions. Decomposition potential. Overvoltage. Characteristics of deposits and completion of deposition. Instrumentation. Application in separation of metals.

Cyclic voltammetry**:** Principle and technique**.** Randles-Sevcik equation**.** Interpretation of voltammogram- reversible, irreversible and quasi-reversible systems**.** Applications of cyclic voltammetry in study of reaction mechanism and adsorption processes**.**

Unit IV: Water pollution and analysis

Sources of water pollution, composition of potable water, importance of water analysis, sampling and sample preservation, physico-chemical analysis of water. Mineral analysis (temperature, pH, conductivity, turbidity, solids, alkalinity, chloride, fluoride, sulphates, hardness), Demand analysis (DO, BOD, COD, TOC), nutrients (nitrogen-total, nitrate, nitrite, phosphate) and heavy metals (As, Cd,

Cr, Hg and Pb). A brief idea of coagulation and flocculation. Water treatment plants: Sand filters and other types of filters.

Books suggested

1. Essentials of Nuclear Chemistry: H. J. Arnikar (Willey Eastern Ltd)
2. Substoichiometry in Radioanalytical Chemistry: J. Ruzicka and J Stary (Pergamon Press)
3. Introduction to Radiation Chemistry: J. W. T. Spinks and R. J. Woods
4. Radiochemistry: A. N. Nesmeyanov (Mir Publications)
5. Instrumental Methods of Analysis: Willard, Meriit and Dean(Van Nostrand)
6. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
7. Vogel's Text Book of Quantitative Inorganic Analysis: Bassett, Denney, Jeffery and Mendham (ELBS)
8. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
9. Atomic Absorption Spectroscopy: Robinson (Marcol Dekker)
10. Instrumental Methods of Chemical Analysis: Braun (Tata McGraw-Hill)
11. Analysis of Water: Rodier
12. Laboratory manual of water analysis: Moghe and Ramteke (NEERI)
13. Electroanalytical chemistry: Joseph Wang
14. Electroanalytical stripping methods: Brainina and Neyman (Wiley-Interscience)
15. Trace analysis: S. Lahiri (Narosa Publishing House)
16. Electroanalytical Chemistry: Bard (Marcel-Dekker)
17. Chemistry in Engineering and Technology- Vol I and II: J.C. Kuriacose and J. Rajaram (Tata-McGraw Hill)

SEMESTER III

PGCH3T11**: Elective (e) Nuclear Chemistry**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course students will be able to

1. *Understand various modes and properties of radioactive disintegration.*
2. *Elaborate the working principles of various radiation detectors.*
3. *Elaborate the structure and properties of nucleus.*
4. *Identify most suitable methods of quantitative analysis using radioisotopes.*
5. *Develop quantitative and qualitative methods for chemical analysis.*
6. *Estimate absorbed and exposure doses using various dosimeters.*

Unit-I: Radioactive decay and detection **15h**

Natural radioactivity, successive radioactive decay and growth kinetics, radioactive equilibrium, ^{99}Mo-^{99m}Tc generator, half life, half life of mixed radioisotopes, decay schemes, its determination by experimental methods, statistical nature of nuclear radiation, treatment of nuclear data and calculation of standard deviation, probability. Various methods of detecting nuclear radiations, gas filled counters, ionization chamber, proportional and GM counters, scintillation detector and solid state detectors- Ge(Li), Si(Li) and HPGe.

Unit-II: Nuclear structure and reactions **15h**

Nuclear properties, mass size, spin and parity, nature of nuclear forces, liquid drop model, shell model, its evidence and advantages, comparison of the two models. Energetics of nuclear reaction, cross reaction, comparison with chemical reactions, various types of nuclear reactions, photonuclear, spallation and thermonuclear reactions.

Mass and charge distribution, release of energy and neutrons, spontaneous fission, nuclear reactors and their uses for power production, brief idea about thermal and fast breeder reactors, reprocessing of nuclear fuel, PUREX process, heavy water- manufacturing and use in reactors. accelerators, nuclear fusion.

Unit-III: Radioanalytical techniques **15h**

- ***Quantitative analysis:*** Neutron activation analysis (Principle, methodology, types and application), Isotope dilution analysis (Principle, methodology, types and applications), Radioimmunoassay (discovery, principle, set up of RIA, Principle of Immunoradiometric assay), Radiometric titrations (Principle, types)
- ***Chemical investigations:*** Reaction mechanism, structure determination, isotope exchange

- ***Physicochemical applications:*** Solubility of sparingly soluble salt, surface area
- ***Age determination:*** Tritium, Carbon-14 and Lead-206 dating.

Unit-IV: Radiation Chemistry **15h**

- ***Interaction of radiations with matter:*** Interaction of radiation (alpha, beta & neutrons) with matter, Interaction of electromagnetic radiation with matter by photoelectric, Compton scattering and pair production, Primary Radiation Effects (LET, Spur Model), Radiation Units (Roentgen, REM, Rad, Gray, Sievert), Measurement of dose Interconversions, calculation of absorbed dose, Radiation Dosimetry, Types of Dosimetry, Chemical dosimeters-Fricke dosimeter, ceric sulfate dosimeter, TLD badges
- ***Radiation induced reactions:*** Radiolysis intermediates (ions, free radicals, excited molecules), various free radical reactions, radiolysis of aqueous organic, inorganic systems, radiolysis of alcohols, halides, Industrial application of radiation

Books suggested

1. H. J. Arnikar - Essentials of Nuclear Chemistry (Willey Eastern Ltd)
2. G. Friendlander, J. W. Kennedy,E. S. Macias and J. M. Miller-Nuclear and Radiochemistry (Wiley Intersciences, New York)
3. G. R. Choppin and J. Rydberg- Nuclear Chemistry-Principles and Applications (Pergamon press, London)
4. B. G. Harvey-Introduction to Nuclear Physics and Chemistry(Prentice Hall of India)

A. N. Nesmeyanov - Radiochemistry- (Mir Publications)

5. M. N. Sastry-Introduction to Nuclear Science, Affiliated East-West Press, New Delhi
6. G. Hughes- Radiation Chemistry- Oxford University Press, London
7. V. Verschinskii and A. K. Pikeav-Introduction to Radiation Chemistry, Israel Publication, Jerusalem- Robinson (Marcol Dekker)
8. Farhat Aziz and M. A. J. Radgers-Radiation Chemistry-Principles and Applications, VCH Publishers FRC.
9. M. Hassinsky-Nuclear Chemistry and its application, Addison Wesley

SEMESTER III

Practical based on Elective Paper (Any one of the four special practicals)

PGCH3P06: Elective (a) Inorganic Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Prepare various complexes by wet chemical methods.*
2. *Carry out characterization of prepared complexes.*
3. *Interpret the electronic and magnetic properties of complexes.*
4. *Elucidate the spin states of various complexes using susceptibility studies.*
5. *Deduce the structures of crystalline solids.*
6. *Carry out photochemical reactions in complexes*

A) Complex preparations: Preparation and characterization of following complexes/organometallic compound including their structural elucidation by the available physical methods**. (**element analysis molecular weight determination, conductance and magnetic measurement and special studies**)**

1. Preparation of *cis* and *trans* potassium dioxalatodiaquochromate(III)
2. Preparation of hexa-aminecobalt(III) chloride
3. Preparation of *tris* (acetylacetonato) manganese(III)
4. Preparation of N-N *bis* (salicyldehyde) ethylene diaminonato nickel(II)
5. Preparation of trinitrotriaminocobalt(III)
6. Preparation of chloropentammine cobalt(III) chloride
7. To prepare copper(II) acetylacetonate complex
8. To prepare *cis* and *trans* bis (glycinato) Cu(II) monohydrate complex
9. To prepare dipyridineiodine(I) nitrate
10. Preparation of ammonium nickel(II) sulphate
11. *Any other complex depending on availability of chemicals.*

* Minimum 5 complexes should be prepared.

B. Nanomaterials and Synthesis Techniques

1. Preparation of Metal oxides and mixed oxides Nanomaterials by Conventional Methods (NiO, ZnO, TiO_2, CuO, Fe_2O_3, Fe_3O_4, Co_3O_4, $ZnFe_2O_4$, $ZnMn_2O_4$, $CuAl_2O_4$ and $NiFe_2O_4$)
2. Preparation of Metal oxides and mixed oxides Nanomaterials by Biogenic Methods (NiO, ZnO, TiO_2, CuO, Fe_3O_4, Fe_2O_3, Co_3O_4, $ZnFe_2O_4$, $ZnMn_2O_4$, $CuAl_2O_4$ and $NiFe_2O_4$)
3. Preparation of graphene oxide via *Hummer's* Method.
4. Preparation of graphitic carbon nitride using Urea, Thiourea, Melamine.

C) Separation techniques

1. Paper and thin layer chromatography
2. Ion exchange

3. Solvent extraction

D) Bioinorganic Chemistry

1. Extraction and absorption spectral study of chlorophyll from green leaves of student choice.
2. Separation of chlorophyll and their electronic spectral studies.
3. Preparation of plant extract using different parts of different biological sources.

Books suggested

1. Advanced Inorganic Analysis, S. K. Agarwal, K. Lal, Pragati Edition, Meerut.
2. Practical Inorganic Chemistry, G. Pass, H. Sutcliffe, Springer.
3. Practical Inorganic Chemistry - Marr & Rocket
4. Basic Concept of Analytical Chemistry - Khopkar S. M.
5. Vogel A: A Textbook of Quantitative Inorganic Analysis, Longman
6. Preparation And Properties of Solid-State Materials – Wilcox, Vol. IV & II, Dekker
7. The Structure and Properties of Materials – Vol IV, John Wulff, Wiley Eastern
8. Dutt P. K.: General And Inorganic Chemistry (Sarat Book House)
9. Fenton, David E.: Biocoordination Chemistry, Oxford
10. Jolly, W. L.: Inorganic Chemistry (4^{Th} Ed) Addison-Wesley
11. Bertini, et al: Bioinorganic Chemistry (Viva)
12. Katakis, D. And Gordon, G: Mechanism of Inorganic Reactions (J. Wiley)
13. Nanomaterials and Nanocomposites: Synthesis, Properties, Characterization Techniques, and Applications, R. K. Goyal, Taylor & Francis, Boca Raton.
14. Biogenic Sustainable Nanotechnology, R. P. Singh, A.R. Rai, A. Abdala, R. G. Chaudhary, Elsevier, Amsterdam, Netherland.

SEMESTER III

PGCH3P06: Elective (b) Organic Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Understand the types of reactions involved in organic synthesis.*
2. *Realize the various functional groups which are commonly present in simple organic molecules.*
3. *Develop skills to understand the reactions of different functional groups by the hands-on experience.*
4. *Characterize the synthesized compounds using IR spectroscopy*
5. *Draw the structures using Chem-Draw*

A) Organic preparations: Student is expected to carry out 4-7 two or three stage preparation from the following list. During preparation of organic compounds, the techniques such as crystallization, distillation, solvent extraction, TLC and column chromatography should be demonstrated.

1. Aniline → acetanilide →p-bromoacetanilide →p-bromoaniline
2. Aniline → Acetanilide →p-nitroacetanilide →p-nitroaniline
3. Benzaldehyde)thiamine hydrochloride→ (benzoin → benzil → benzilic acid
4. p-Nitrotoluene →p-nitrobenzoic acid→ PABA →p-iodobenzoic acid
5. p-Cresol → p-cresylacetate → 2-hydroxy-5-methyl acetophenone → 2-hydroxy chalcone
6. Benzophenone → Benzophenone oxime → Benzanilide → Benzoic acid +aniline
7. Aniline → aniline hydrogen sulphate → sulphanilic acid → Orange II
8. Aniline → N-arylglycine → indoxyl → indigo
9. Phthalimide → Anthranilic acid → Phenyl glycine-o-carboxylic acid → Indigo
10. Phalic anhydride → Phthalimide → Anthranilic acid → o-chlorobenzoic acid
11. Phalic anhydride → Phthalimide → Anthranilic acid →Diphenic acid
12. *Any other suitable three stage preparation as per the availability of chemicals*

B) Qualitative Analysis : Separation of the components of a mixture of three organic compounds)three solids, two solids and one liquid, two liquids and one solid, all three liquids and identification of any two components using chemical methods or physical techniques .Minimum 4-6 mixtures to be analyzed.

C) IR spectroscopy: The IR spectrum of minimum four synthesized compounds from the Section A should be interpreted.

D) Use of Computers- Chem Draw, Chem Sketch for drawing simple organic molecules, aliphatic and aromatic compounds should be demonstrated (2 hour activity).

Books suggested

1. Practical organic chemistry by FG Mann and BC Saunders
2. Text book of practical organic chemistry –by Vogel
3. The synthesis, identification of organic compounds –Ralph L. Shriner, Christine K.F. Hermann, Terence C. Morrill and David Y. Curtin

4. Compendious Practical Organic Chemistry: Preparations, Isolation, and Chromatography by Basavarajaiah S M, Nagesh G Y, Ramakrishna Reddy K
5. Advanced Practical organic chemistry by N.K. Vishnoi

SEMESTER III

PGCH3P06: Elective (c) Physical Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: *At the end of the course students will be able to*

1. *Inculcate the potential of establishing any new laboratory at UG or PG level.*
2. *Execute the theoretical principles in practical*
3. *Analyze and interpret the results of their performances*
4. *Inculcate the skills of preparing, maintaining and developing the chemicals and reagents*
5. *Understand the role of laboratory safety and preparedness*

Thermodynamics:

1. Determination of partial molar volume of solute and solvent **(**ethanol-water, methanol-water, KCl-water mixture**)**

Solutions:

2. Study the variation of solubility of potassium hydrogen tartarate with ionic strength using a salt having a common ion and hence determine the mean ionic activity coefficients**.**
3. Determination of temp**.** dependence of the solubility of a compound in two solvents having similar intermolecular interactions**(**benzoic acid in water and DMSO **–** water mixture**)** and calculation of the partial molar heat of solution**.**

Phase equilibrium:

1. To study the effect of addition of an electrolyte such as NaCl, KCl,Na_2SO_4,K_2SO_4 etc**.** on the solubility of an organic acid**(**benzoic acid or salicylic acid**).**
2. To determine the heat of crystallization of $CuSO_4$,$5H_2O$
3. To determine the heat of reaction involving precipitation of a salt $BaSO_4$
4. To determine transition temperature of $CaCl_2$ by thermometric method and to determine transition temperature of $CaCl_2$, sodium bromide by solubility method

Kinetics:

1. To determine the activation energy of hydrolysis of an ester by acid**.**
2. Kinetics of reaction between sodium thiosulphate and KI**.** Determination of rate constant; study of influence of ionic strength
3. Kinetics of decomposition of H_2O_2 catalysed by iodide ion**.** Also determination of activation energy of reaction**.**
4. Clock reaction**-** activation energy of bromide**-**bromate reaction**.**
5. Temp dependence of persulfate**-**iodide reaction by iodine clock method and calculation of thermodynamic and Arrhenius activation parameters**.** Study of ionic strength effect on persulfate**-**iodide reaction**.**
6. Kinetics of B**-**Z reaction; Kinetics of modified B**-**Z reaction
7. Investigate the Autocatalytic reaction between potassium permanganate and oxalic acid**.**
8. Determination of pKa value of a weak acid by chemical kinetic method **(**formate**-**iodine reaction**)**

Conductometry:

1. Estimate the concentration of H_2SO_4, CH_3COOH, $CuSO_4.5H_2O$ in a given solution by carrying out conductometric titration against NaOH solution.
2. Determine the eq. conductance of strong electrolyte (KCl, NaCl, HCl, KNO_3) at several concentration and hence verify Onsager's equation.
3. Carry out the following precipitation titration conductometrically. a. 50 ml.0.02N $AgNO_3$ with 1N HCl; b.50 ml.0.02N $AgNO_3$ with 1N KCl; c. 50 ml 0.004 N $MgSO_4$ with 0.1 N $Ba(OH)_2$; d. 50 ml 0.002 N $BaCl_2$ with 1 N Li_2SO_4; e. 50 ml.0.02 N $BaCl_2$ with 1N K_2SO_4
4. To determine degree of hydrolysis of aniline hydrochloride and hence to determine the hydrolysis constant of salt by conductometric method.
5. To determine pK of weak acids, succinic acid, acetic acid, Malonic acids, (dibasic acids).
6. Complexation between $Hg^{2+}$and I^- conductometrically.
7. To determine solubility product of lead chromate.
8. Kinetic study of saponification ethyl acetate by conductometry.

Potentiometry:

1. To prepare calomel electrode and to determine the potential of calomel electrode by potentiometry.
2. To determine stability constant of Fe^{3+} with potassium dichromate in presence of dilute sulphuric acid by redox titration.
3. To determine solubility product of Silver chloride by potentiometric method.
4. Determination of redox potential of the couples(Fe^{2+}/Fe^{3+},Co^{3+}/Co^{2+},Cr^{3+}/Cr^{2+},MnO_4^- /Mn2+(any two) and equilibrium constant.
5. Study of complex formation by potentiometry e.g.Ag^+-$S_2O_3^{-2}$, Fe^{3+}-SCN^-,Ag^+-NH_3(any two) and calculation of stability constant.
6. Transport number by potentiometry.
7. To determine degree of hydrolysis of aniline hydrochloride and hence to determine the hydrolysis constant of salt by potentiometry method.
8. To determine pK of weak acids, succinic acid, acetic acid, Malonic acids, (dibasic acids).
9. Complexation between $Hg^{2+}$and I^- conductometrically.

Spectrophotometry:

1. To verify Beers law for solution of potassium permanganate and to find molar extinction coefficient.
2. To determine the indicator constant (pK_{In}) of methyl orange/red spectrophotometrically.
3. To determine the stability constant of reaction between Ferric ion solution and SCN^- ion solution by Job's method.
4. To determine the stability constant between Fe^{3+} and SCN^- ion solution by Ostwald and Frank method.

Polarography:

1. Determination of the half-wave potential of the cadmium ion in 1M potassium chloride solution.

2. Investigation of the influence of dissolved oxygen.
3. Determination of cadmium in solution.
4. Determination of lead and copper in steel.

Adsorption:

1. To verify Freundlich adsorption isotherm**.**
2. To verify Langmuir adsorption isotherm**.**
3. To verify Gibbs adsorption isotherm and to find surface excess concentration of solute**.**
4. Study of variation of surface tension of solution of n-propyl alcohol with concentration and hence determine the limiting cross section area of alcohol molecule

Transport Number:

1. To determine transport number by Hittorff's method
2. To determine the transport number by moving boundary method

Books suggested

1. Vogel A**:** A Textbook Of Quantitative Inorganic Analysis, Longman
2. Das and Behra, Practical Physical Chemistry
3. Carl W. Garland, Joseph W. Nibler and David P. Shoemaker, Experiments in Physical Chemistry, Mc-Graw Hill, 8th Edition, 2009.
4. Farrington Daniels, Joseph Howard Mathews, John Warren Williams, Paul Bender, Robert A**.** Alberty, Experimental Physical Chemistry, Mc-Graw Hill, Fifth Edition, 1956**.**
5. John W**.** Shriver and Michael George, Experimental Physical Chemistry, Lab Manual and Data Analysis, The University of Alabama in Huntsville, Fall 2006
6. Day And Underwood**:** Quantitative Analysis
7. Merits And Thomas**:** Advanced Analytical Chemistry
8. Ewing, G**.** W**.:** Instrumental Methods of Chemical Analysis, Mcgraw-Hill
9. Drago, R**.**S**:** Physical Methods in Inorganic Chemistry
10. Christian G**.**D**:** Analytical Chemistry
11. Khopkar S**.**M**.:** Basic Concept of Analytical Chemistry
12. Koltath And Ligane**:** Polorography
13. Braun**:** Instrumental Methods of Chemical Analysis
14. Willard, Merritt and Dean**:** Instrumental Methods of Chemical Analysis ,Van Nostrand
15. Strouts,Crifi; Llan And Wisin**:** Analytical Chemistry
16. Skoog S**.**A**.** And West D**.** W**.:** Fundamental of Analytical Chemistry
17. Dilts R**.**V**.:** Analytical Chemistry
18. Jahgirdar D**.**V **:** Experiments in Chemistry
19. Chondhekar T**.**K**:** Systematic Experiments in Physical Chemistry, Rajbhoj S**.**W**.**, Anjali Pubn**.**
20. Wlehov G**.** J**:** Standard Methods of Chemical analysis 6th Ed

SEMESTER III

PGCH3P06: Elective (d) Analytical Chemistry Special Practical

4 h per week *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Understand the fundamental principles forming basis for the instrumental methods of analysis.*
2. *Select most suitable technique for the desired analysis.*
3. *Identify experimental conditions necessary to carry out the analysis of different samples.*
4. *Compare results obtained through different techniques.*
5. *Formulate experiments based on optical and electroanalytical techniques.*
6. *Demonstrate working of each instrument used in analysis.*

pH-metry

1. Determination of percent Na_2CO_3 in soda ash by pH-metric titration.
2. Determination of isoelectric point of amino acid.
3. Determination of three dissociation constants of phosphoric acid.

Conductometry

1. Estimation of acids in mixtures.
2. Displacement titration of CH_3COONa with HCl.
3. Precipitation titration of $MgSO_4$ and $BaCl_2$.
4. Titration of mixture of CH_3COOH, H_2SO_4 and $CuSO_4$ with NaOH.
5. Determination of dissociation constants of weak acids.

Potentiometry

1. Estimation of Cl^-, Br^- and I^- in a mixture.
2. Determination of percent purity of phenol by potentiometric titration with NaOH.
3. Estimation of acids in mixtures.
4. Potentiometric titration of phosphoric acid with NaOH.

Electrogravimetry

1. Estimation of nickel and copper individually as well as in mixture.

Spectrophotometry

1. Simultaneous determination of chromium and manganese in given mixture.
2. Simultaneous determination of two dyes in a mixture.
3. Estimation of Mn in steel.
4. Estimation of Cu/Ni in alloys.
5. Estimation of iron in water sample using 1,10-phenanthroline.
6. Estimation of Fe(III) in given solution by photometric titration with EDTA (salicylic acid method).

Flame photometry

1. Estimation of Li, Na, K, Ca in vegetable/ soil / water samples.

Polarography

1. Determination of $E_{1/2}$ of Cd^{2+} and Zn^{2+} at DME.
2. Estimation of Cd^{2+} and Zn^{2+} in respective solutions by calibration curve and standard addition methods.

Cyclic voltammetry

1. Study of cyclic voltammograms of $K_3[Fe(CN)_6]$.

Turbidimetry and nephelometry

1. Estimation of sulphate in water sample by turbidimetry.
2. Estimation of phosphate by nephelometry.
3. Determination of molecular weight of polymer.

Polarimetry

1. Determination of specific and molar rotation of optically active compound.
2. Kinetics of inversion of cane sugar in the presence of HCl.
3. Determination of percentage of two optically active substances (d-glucose and d-tartaric acid) in mixture.

Applied analytical

1. Analysis of ores: Ca and Mg in Dolomite, Mn in Pyrolusite
2. Analysis of cement: Silica, alumina, ferric oxide, calcium and magnesium oxide, sodium and potassium oxide
3. Analysis of oils: Carbon residue, Acid value, Saponification value, Iodine value, Viscosity, Flash point, Cloud point, Aniline point
4. Analysis of drugs: Fe in capsule, ascorbic acid in vitamin-C tablet, Mg in milk of magnesia tablet/syrup
5. Bleaching powder: Available chlorine
6. Polymer analysis: Molecular weight, Saponification value, Iodine value
7. Food: Phosphoric acid in cola beverages by pH titration

Books suggested

1. Quantitative analysis**:** Day and Underwood **(**Prentice**-**Hall of India**)**
2. Vogel's Text Book of Quantitative Inorganic Analysis-Bassett, Denney, Jeffery and Mendham (ELBS)
3. Analytical Chemistry**:** Gary D**.** Christian **(**Wiley India**).**
4. Experiments and calculations in Engineering Chemistry- S. S. Dara (S. Chand and Co.)
5. Experiments in Chemistry-D. V. Jahagirdar (Himalaya)
6. Advanced Practical Chemistry-J. B. Yadav (Goel Publishing House)
7. Advanced Practical Chemistry-Jagdamba Singh (Pragati Prakashan)

Semester III

PGCH3P06: Elective (d) Nuclear Chemistry Practical

4 h per week Marks-50

1. Determination of working voltage of GM counter.
2. Study of nuclear counting statistics.
3. Attenuation of beta rays.
4. Determination of dead time of GM tube.
5. Study of geometry of GM counter.
6. Verification of inverse square law.
7. Determination and calibration of resolution of Cs-137by scintillation counter.
8. Determination and calibration of resolution of Co-60, Na-22 and Ba-133 by scintillation counter.
9. Determination of half life of Mn-56.
10. Determination of half life of I-128.
11. Determination of half life of Mn and I in a mixture.
12. Determination of neutron flux of Am-Be source by Indium foil.
13. Determination of absorbed dose of Co-60 using Fricke dosimeter.
14. Determination of $G(NO_2^-)$ of nitrate salt.
15. Determination of G(-Dye).
16. Determination of free iodine formed in radiolysis of ethyl iodide.

List of books:

1. H. J. Arnikar - Essentials of Nuclear Chemistry (Willey Eastern Ltd)
2. G. Friendlander, J. W. Kennedy,E. S. Macias and J. M. Miller-Nuclear and Radiochemistry (Wiley Intersciences, New York)
3. G. R. Choppin and J. Rydberg- Nuclear Chemistry-Principles and Applications (Pergamon press, London)
4. B. G. Harvey-Introduction to Nuclear Physics and Chemistry(Prentice Hall of India)
5. N. Nesmeyanov - Radiochemistry- (Mir Publications)
6. M. N. Sastry-Introduction to Nuclear Science, Affiliated East-West Press, New Delhi
7. G. Hughes- Radiation Chemistry- Oxford University Press, London
8. V. Verschinskii and A. K. Pikeav-Introduction to Radiation Chemistry, Israel Publication, Jerusalem- Robinson (Marcol Dekker)
9. Farhat Aziz and M. A. J. Radgers-Radiation Chemistry-Principles and Applications, VCH Publishers FRC.
10. M. Hassinsky-Nuclear Chemistry and its application, Addison Wesley

SEMESTER III

PGCH3P07: Research Project (RP)

8 h per week *100 Marks*

The objective of research project is to train the student in identifying the problem of research, develop the hypothesis, design the experiments/surveys to test the hypothesis, collect and analyse the data and draw conclusions from it. In addition, the aim is also to prepare the student to present the data in various forms such as project report, presentation in conferences and seminars and research paper. Research project is also aimed to prepare the student for doctoral research after the completion of the programme.

The student will have to carry out a research-based project work in the third and fourth semester. The project work may be carried out in the parent department or any other institute in collaboration with the parent institute. For this, the student will be attached to any of the national/regional/private research institute/organization for the duration of the third semester. If the student is working in the organisation other than the parent department, then it will be the responsibility of the student to attend the classes and other departmental activities in order to be eligible to appear for the examination. The student will be allotted the supervisor in the third semester; after which the student will finalize the topic of the project work in consultation with the supervisor.

The research project of the student will be evaluated on the basis of the project report submitted by him/her and the power point presentation made by him/her in the presence of internal and external examiner during the examination.

SEMESTER IV

PGCH 4T12: Spectroscopy-II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Interpret the structures of simple molecules using physical methods of analysis*
2. *Understand and interpret the NMR data*
3. *Analyze X ray diffraction data*
4. *Develop the skills of analytical ability*
5. *Execute out the combined application of spectral method*

Unit I:

A) Ultraviolet and visible spectroscopy: Natural line width, line broadening, transition probability, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels. General nature of band spectra. Beer- Lambert Law, limitations, Frank-Condon principle, various electronic transitions, effect of solvent and conjugation on electronic transitions, Fieser Wooodward rules for dienes, aldehydes and ketones. Structure differentiation of organic molecules by UV Spectroscopy

B) Photoelectron spectroscopy: Basic principles, photoelectric effect, ionization process, Koopman theorem, PES and XPES, PES of simple molecules, ESCA, chemical information from ESCA, Auger electron spectroscopy.

Unit II:

Nuclear Magnetic Resonance Spectroscopy: Magnetic properties of nuclei, resonance condition, NMR instrumentation, chemical shift, spin spin interaction, shielding mechanism, factors affecting chemical shift, PMR spectra for different types of organic molecules, effect of deuteration, complex spin spin interaction (1^{st} order spectra), stereochemistry, variations of coupling constant with dihedral angle, electronegativity, Karplus equation etc., classification of molecules as AX, AX_2, AMX, A_2B_2, Shift reagents. NMR studies of ^{13}C, chemical shift in aliphatic, olefinic, alkyne, aromatic, heteroatomic and carbonyl compounds, ^{19}F, ^{31}P. Structure determination of organic molecules by NMR spectroscopy

Unit III:

A) Application of NMR spectroscopy: FT-NMR, advantages of FT-NMR, two-dimensional NMR spectroscopy-COSY, HETCOR, NOSEY, DEPT, INEPT, APT, INADEQUATE techniques, Nuclear Overhauser effect, use of NMR in medical diagnosis

B) Problems based on structure determination of organic molecules by using NMR (^1H and ^{13}C nuclei) data, Structure elucidation using combined techniques including UV, IR, NMR and mass spectrometry (based on data and copies of the spectra)

Unit IV:

Diffraction techniques: X ray diffraction: Braggs condition, Miller indices, Laue method, Bragg method, Debye Scherrer method, identification of unit cells from systematic absences in diffraction pattern, structure of simple lattices and x-ray intensity, structure factor and its relation to intensity and electron density, absolute configuration of molecules.

Electron diffraction: scattering intensity vs scattering angle, Wierl equation, measurement techniques, elucidation of structure of simple gas phase molecules, low energy electron diffraction and structure of surfaces.

Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques, elucidation of structure of magnetically ordered unit cell.

Books suggested

1. Spectroscopic identification of organic compound-RM Silverstein,GC Bassler and TC Morril, John Wally
2. Introduction to NMR spectroscopy-R. J. Abraham, J. Fisher and P Loftus Wiely
3. Application of Spectroscopy to Organic Compound-J. R. Dyer, Printice Hall
4. Organic Spectroscopy-William Kemp, ELBS with McMillan
5. Spectroscopy of Organic Molecule-PS Kalsi, Wiley, Esterna, New Delhi
6. Practical NMR Spectroscopy-ML Martin, JJ Delpench, and DJ Martyin
7. Spectroscopic Methods in Organic Chemistry-DH Willson, I Fleming
8. Fundamentals of Molecular Spectroscopy-CN Banwell
9. Spectroscopy in Organic Chemistry-CNR Rao and JR Ferraro
10. Photoelectron Spectroscopy-Baber and Betteridge
11. Electron Spin Resonance Spectroscopy-J Wertz and JR Bolten
12. NMR –Basic Principle and Application-H Guntur
13. Interpretation of NMR spectra-Roy H Bible
14. Interpretation of IR spectra-NB Coulthop
15. Electron Spin Resonance Theory and Applications-W gordy
16. Mass Spectrometry Organic Chemical Applications, JH Banyon

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Weblink to Equivalent MOOC on SWAYAM if relevant:

- Application of Spectroscopic Methods in Molecular Structure Determination https://nptel.ac.in/courses/101/104/104106075/

SEMESTER IV

PGCH 4T13: Advanced Organic Chemistry II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Recognize the chemical reactions of carbonyl compounds and alkenes under photochemical conditions*
2. *Understand the stereochemistry of complex organic molecules*
3. *Apply the knowledge of enaolate chemistry in modern organic synthesis*
4. *Demonstrate the applications of stereochemistry of common organic reactions*
5. *Analyze the philosophy of synthesis of small molecules*

Unit I: Organic Photochemistry

Interaction of radiation with matter, types of excitation, rate of excited molecules, quenching, Quantum efficiency, quantum yield, transfer of excitation energy, singlet and triplet states, experimental methods in photochemistry of carbonyl compounds, and transition, Norrish type I and Norrish type II reactions Paterno–Buchi reaction, Photoreduction, Photochemistry of enones, Hydrogen abstraction rearrangement of unsaturated ketones and cyclohexadienones

Photochemistry of *p*-benzoquinones, photochemistry of aromatic compounds with reference to isomerization, addition and substitution Photochemical isomerization of *cis* and *trans* alkenes, Photochemical cyclization of reaction, Photo-Fries rearrangement, di-pi methane rearrangement, Photo theory reaction of anilides, photochemistry of vision, DeMayo reaction

Unit II:

Advanced Stereochemistry

A) Recapitulation of Stereochemical concepts- enantiomers, diastereomers, homo topic and heterotopic ligands, racemization and resolution methods, Chemo-, regio-, diastereo- and enantio-controlled approaches; Chirality transfer, Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, Felkin Anh rule, Houk model, Cram's chelate model. Asymmetric synthesis, use of chiral auxiliaries, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation

B) Stereochemistry of fused and bridged ring systems: Nomenclature, synthesis; stereochemical aspects of Perhydrophenanthrene, Perhydroanthracene, hydrindane, Steroids; Bridged system (bi, tri and polycyclo system) including heteroatoms, Bredt's Rule. Conformations of following compounds with justification of each: *cis* and *trans*-1,3- and l,4-di-t-butyl-cyclohexanes; Cis-4-di-t-butylcis-2,5-dihydroxycyclohexane; Twistane; bicyclo-[2.2.2]octane; Trans-anti-trans-Perhydro-anthracene and the lactone; cyclohexane-l,4-dione; 1,2,2,6,6-penta-methyl-4- hydroxy-4-phenylpiperidine; ψ-tropine; 2-hydroxy-2-phenyl quinolizidine; 4-*t*-butyl-4-methyl-l,3-dioxane; *cis*-and *trans*-2,5-di-t-butyl-l,3-dithianes; *cis*-2,5-di-t-butyl-l,3,2- dioxaphosphorinan-2-one

Unit III:

Alkylation of enolates and other carbon nucleophiles: Generation and properties of enolates and other stabilized carbaions, regioselectivity and stereoselectivity in enolate formation from ketones and esters, alkylation of enolates of ketones, aldehydes, esters, carboxylic acids, amides, and nitriles, Generation and alkylation of dianions, intramolecular alkylation of enolates, control of enantioselectivity in alkylation reactions, The nitrogen analogs of enols and enolates: Enamine and imine anions

Reactions of carbon nucleophiles with carbonyl compounds: Aldol addition and condensation reaction, mechanism, Control of regioselectivity and stereoselectivity of aldol reacions of aldehydes and ketones, Aldol addition reactions of enolates of esters and other carbonyl derivatives, Reaction of (*E*) or (*Z*)-enolates with chiral aldehydes, The Mukaiyama aldol reaction, Control of facial selectivity in aldol and Mukaiyama aldol reaction, Intramolecular aldol reaction and the Robinson annulation, Evans aldol reaction, Mannich reaction, Conjugate addition of enolates, organomettalic reagents and cyanide ion, Conjugate addition with tandem alkylations, Control of facial selectivity in conjugate addition reaction

Unit IV: Designing the synthesis based on retrosynthetic analysis

A) Disconnection Approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis

B) One Group C-C Disconnections: Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis

C) Two Group C-C Disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalisedcompounds, Michael addition and Robinson annelation, Methods of ring synthesis, Linear and convergent synthesis

Books suggested

1. N. J. Turro, "Modern Molecular Photochemistry" (MMP), University Press, Menlo Park, CA, 1978
2. A. Gilbert and J. Baggott, "Essentials of Molecular Photochemistry," CRC Press, London, UK, 1991
3. J. Mattay and A. Griesbeck, eds., "Photochemical Key Steps in Organic Synthesis", VCH, New York, 1994
4. J. D. Coyle, ed., "Photochemistry in Organic Synthesis", Royal society of Chemistry, London, 1986
5. Stereochemistry of Organic Compounds Principles and Applications by D. Nasipuri, 3rd Edition, New Age International (P) Ltd Publishers
6. Basic Stereochemistry of Organic Molecules, 2nd Edition, Book Syndicate Pvt. Ltd

7. Basic Organic Stereochemistry by Ernest L. Eliel, Samuel H. Wilen and Michael P. Doyle, 2001 edition, Wiley Interscience.
8. Advance Organic Chemistry Part-B-F .A .Caray and R .J .Sundberg Plenum Press (Useful for Unit III)
9. Organic Chemistry, J .Clayden, N .Greeves, S .Warren and P .Wothers, Oxford University Press
10. Some Modern Methods of Organic Synthesis-W .Carruthers
11. Principles of Organic Synthesis by R. O. C. Norman and James M. Coxon (Nelson Thornes Ltd)
12. Modern Organic Synthesis: An Introduction by G. S. Zweifel and M. H. Nantz (Wiley)
13. Organic Synthesis by Michael Smith , 4th Edition (Academic Press)
14. Organic Synthesis: The Disconnection Approach-S. Warren
15. Designing Organic Synthesis-S. Warren

Weblink to Equivalent MOOC on SWAYAM if relevant:

- Organic Photochemistry and Pericyclic Reactions: Dr. N.D. Pradeep Singh Department of Chemistry IIT Kharagpur, https://nptel.ac.in/courses/104105038
- Pericyclic Reactions and Organic Photochemistry: Prof. Sankararaman, IIT Madras https://nptel.ac.in/courses/104/106/104106077/
- A Study Guide in Organic RetrosynthesisL Problem Solving Approach: Prof. Samik Nanda, IIT Kharagpur https://nptel.ac.in/courses/104105087
- Stereochemistry: Prof. Amit Basak, IIT Kharagpur https://nptel.ac.in/courses/104105086
- Stereochemistry and Applications: Prof. A. R. Choudhury, IISER Mohali https://nptel.ac.in/courses/104106127
- Structure, Stereochemistry and Reactivity of Organic Compounds and Intermediates: A Problem-solving Approach: Prof. Amit Basak, IIT Kharagpur https://nptel.ac.in/courses/104105127

SEMESTER IV

PGCH 4T14**: Advanced Physical Chemistry**

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course, student will be able to*

1. *Understand the types and behavior of solids based on their structure.*
2. *Estimate various dependent parameters of under different influences.*
3. *Understand solid state reactions and synthesis process.*
4. *Understanding nano chemistry.*
5. *Identification of crystals and their analysis.*

UNIT I: SOLID STATE AND THEIR MAGNETIC PROPERTIES

A**)** Solid State Chemistry**:** Metals, Insulators and Semiconductors, Electronic structure of solids-band theory**.** Band structure of metals, Insulators and Semiconductors, Intrinsic and Extrinsic Semiconductors, p-n junction, energy band formation, forward bias and reversed bias p-n junction, their applications, Superconductors— types, Meissner effect, BCS theory, Low Temperature Superconductor **(**LTSC**)** and High Temperature Superconductor **(**HTSC**)**, Conventional and organic Superconductors, their applications**.**

B**)** Magnetic Properties**:** Behaviour of substances in magnetic field, effect of temperature, Curie and Curie-weiss law, calculation of magnetic moments, magnetic materials, their structure and properties, Applications, structure/ property relations, numerical**.**

UNIT II: ELECTRICAL PROPERTIES OF MOLECULES

Dipole moments of molecules, basic ideas of electrostatic interactions, polarizability, orientation polarization, Debye equations, limitation of the Debye theory, Clausius-Mossotti equation**.** electrostatic of dielectric medium, molecular basis of dielectric behavior, structural information from dipole moment measurements, use of individual bond dipole moments, application to disubstituted benzene derivatives, dipole moment and ionic character of a molecule, determination of dipole moment from dielectric measurements in pure liquids and in solutions**.** The energies due to dipole-dipole, dipole induced dipole and induced dipole-induced dipole interaction**.** Dispersion, dielectric loss and refractive index**.** Lennard-Jones potential**.**

UNIT III: THIN FILMS AND LIQUID CRYSTALS

(A) 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.

(B) Liquid crystals: Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases, smectic-nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular rearrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

UNIT-IV: CRYSTAL STRUCTURES

A) Introduction to crystals, Unit Cell and lattice parameters, Symmetry elements in crystals, Absence of fivefold axis, Space groups, The Bravais Lattices, Miller Indices, Bragg's Equation, seven crystal system, packing in crystals, Hexagonal Closest Packing (HCP) Cubic Closest Packing (CCP), Voids, packing fraction, Numerical.

B) **Lattice Defects:** Perfect and Imperfect crystals, point defects**,** Interstitial, Schottky defect, Frenkel defect, line defect and other entities, thermodynamics of Schottky and Frankel defects. Dissociation, theory of dislocation, plane defects- Lineage boundary, grain boundary, stacking fault, 3D defects, Defects and their concentrations, ionic conductivity in solids, Non stoichiometric compounds. Electronicproperties of Non-stoichiometric oxides.

Books suggested

1. S**.** O**.** Pillai, Solid State Physics, New Age International, New Delhi, 2102**.**
2. C**.**Kittel, **"** Introduction to solid state Physics**"**,Wiley
3. L**.**V**.**Azaroff, **"** Introduction to solids**"**, McGraw Hill

SEMESTER IV

PGCH4T15: Elective (a) Inorganic Chemistry Special II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student would be able to

1. *Understand the types and behavior cerasmic and composite materials.*
2. *Elaborate various types of ceramics and cementataceous composites.*
3. *Discuss corrosion types, reasons and solutions to corrosion problem.*
4. *Comprehend industrial materials and water treatment techniques.*
5. *Prepare a subject platform for energy sources and renewable fuel sources.*

Unit-I

a. Ceramic Materials: Classification of ceramics, dielectric properties and polarization properties of ceramics, piezo-, pyro- and ferro-electric effect of ceramics, sol-gel processing of ceramics. Examples and application of ceramics: oxides, carbides, borides, nitrides.

b. Composite Materials: Definition, glass transition temperature,fibersfor reinforced plastic composite materials (i.e. glass fibers, carbon fibres, and aramid fibers); concrets and asphalt materials. Application ofcomposite material.

Unit-II

A) Cementitious Materials: Difference between Blended and Non-Portland cements; Non-portland cements; high alumina cements, calcium sulfoaluminate cements, phosphate cements.Chemicals in cement hydration; hydration process, set retardersandaccelerators, plasticizers, slip-casting processing. Application of cementitousmaterials.

B) Bio-materials: Definition of biomaterials and biocompatibility;, Type of bio-materials: Metallic materials, Biopolymeric materials, Bioceramic materials (dense hydroxyapatite ceramics, bioactive glasses,and bioactive composites); Basic requirement of bone implants; Coating of hydroxyapatite on porous ceramics; Biomaterials in tissue attachments; Application of Biomaterials

Unit-III

A) Inorganic Chemicals as metallic Corrosion Inhibitors: Introduction, Principles of corrosion inhibitors, corrosion as an electrochemical process, Practical aspects of corrosion inhibition, Anion inhibitor properties in neutral electrolytes, some application of corrosion inhibitors (cooling water circulation-once through and open systems, engine radiation & cooling systems, central heating system, refrigeration plants and high chloride systems, water for steam raising, corrosion inhibitors for paintcoating).

B) Industrial gases: Introduction, Separation of gases from air,Hydrogen, Carbon dioxide, Carbon monoxide, Oxygen, Acetylene, Sulphur dioxide, Nitrous oxides.

C) Chemical explosives and propellants: Introduction, Potential energy of explosives , Properties of explosives, Manufacture of explosives , Explosives made by nitration, Dynamite , Commercial

high explosives containing no nitroglycerine , Initiating devices, Sporting and military explosives, Disruptive explosives for military use, Handling and storage of explosives.

Unit-IV

A) Applications of Biotechnology for the treatment of waste water: Introduction, Role of microorganism for the treatment of waste water, Application of biotechnology for a. high strength waste. b. Primary and secondary sludge c. Phenol & cyanide removal d. Solid phase extraction

B) Energy sources for future:

a. Solar Energy-Solar heating for homes and other buildings, electricity from solar thermal power collectors, electricity from photovoltaic cells.

b. Energy from biomass- Production of biomass, biofuels, biodiesel.

c. Geothermal energy,

d. water power

e. Tidal power.

f. Fuel Cells-Polymer electrolyte membrane fuel cells, Phosphoric acid fuel cell, Direct methanol fuel cell, Alkaline fuel cell, Regenerative(reversible) fuel cell, Clean cars for the future, Energy sources for the twenty first century.

Books suggested

1. Handbook of Industrial Chemistry,Vol.1, by K.H.Davis,F.S.Berner,Edited by S.C. Bhatia (CBS Publishers, Bangalore,2004)
2. Industrial inorganic chemistry, Karl Heinz Buchel, Hans-Heinrich Moretto, Peterwoditsch
3. Modern Electroplating, By M. Schlesinger and M. Paunovic (John Wiley and sons, Hoboken , New Jersey, 5th Edition2010)
4. Insight into Specialty Inorganic Chemicals-David Thompson (The Royal Society of Chemistry,1995)- Chapter 15.
5. New Trends in Green Chemistry (2nd Edition)-V.K.Ahluwalia and M.Kidwai (AnamayaPublishers, 2007)
6. Environmental Chemistry by A. K. Bagio.
7. Principles of Environmental Chemistry by James Girard Bartlett Publishers.
8. Waste Water Engineering by Calf& Eddy.
9. Waste Water treatment for pollution control by Arceivala.
10. Principles of water quality Control by T. H. Y Tebbut.
11. Manual on Sewage &Sewage treatment, Ministry of Works, New Delhi.

SEMESTER IV

PGCH4T15: Elective (b) Organic Chemistry Special-II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: *At the end of the course students would be able to*

1. *Understand the reactivity of organometallic compounds*
2. *Demonstrate the applications of organometallic reagents in C-C bond formation*
3. *Understands the reactivity of heterocyclic compounds in various reaction conditions*
4. *Understand the electrophilic, nucleophilic reactions and synthesis of various heterocycles*
5. *Justify the need of protecting groups in organic synthesis*

Unit I:

Organometallic compounds of Group I and II Metals: Synthesis and applications of organolithium and organomagnesium reagents, nucleophilic addition to aldehyde, ketones, ester, epoxide, CO_2, CS_2, isocyanates, ketenes, imines, amides, lactones, Stereochemistry of Grignard addition to carbonyl compounds, *o*-metallation of arenes using organolithium compounds, Organocopper reagents: Preparation and applications in C-C bond forming reaction, mixed oragnocuprates, Gilman's reagent. Organo Hg and Cd reagents in organic synthesis, Reformatsky reaction, Barbier reaction

Unit II: Heterocycles-I

a) Ring Synthesis: Introduction, Cyclization reactions: Reaction types, displacement at saturated carbon, intramolecular nucleophilic addition to carbonyl groups, intramolecular addition of nucleophiles to other double bonds, cyclizations on to triple bonds, radical cyclizations, cabene and nitrene cyclization, electrocyclic reactions, reactions and structural effects of heterocyclic rings, ,3 - dipolar cycloadditions producing five - membered heterocycles, Hetero Diels-Alder reaction, [2+2] cycloaddition, ene reactions, Palladium catalysis in the synthesis of Benzo - Fused heterocycles

b) Three and four membered heterocylces: Aziridines, Oxiranes, Thirienes, Azetidines, Oxetanes and Thietanes

C) Azoles: Structural and chemical properties; Synthesis of pyrazole, isothiazole and isoxazole; Synthesis of imidazoles, thiazoles and oxazoles; Nucleophilic and electrophilic substitutions; Ring cleavages, Carbonyldiimidazole as coupling agent

Unit III: Heterocycles-II

A) Benzofused heterocycles: Synthesis of indole, benzofuran and benzo-thiophene, quinoline and isoquinoline Nucleophilic, electrophilic and radical substitutions; Addition reactions; Indole rings in biology, Synthesis and reactions of coumarin

B) Diazines: Structural and chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines; Nucleophilic and electrophilic substitutions.

C) Synthesis of following bioactive compounds: Vitamin B6, Ondansetron, Serotonin, Indometacin, Cyanamid, fentiazac, trimethoprim, papaverine

Unit IV:

A) Protection and de-protection of functional group in organic synthesis: Hydroxyl group- alkyl ether, benzyl ether,acyl, PMB, Trityl, TMS, TBDMS, THP, MOM, MEM, MIP ether; Diol- Acetone, Cyclohexanone; Amines- Benzyl, Acyl, CBZ, BOC, FMOC, Carboxyl group-Ester, DCCI, DIPCDI; Ketone and aldehydes- Glycol, Thioglycol, Ketal, Acetal; Othroesters as protecting groups, Protection deprotection approach - In Solid phase synthesis of polypeptide

B) Total synthesis selected molecules: FR-900848, cubane, biotin, longifolene and taxol, Endiandric Acid A, B, C and D

Books suggested

1. Organometallics: A concise Introduction, Ch. Elshebroicn and A. Salzer, VCH, chapters, 12-16
2. Organotransition Metal Chemistry: Applications to Organic Synthesis, S.G. Davies, Permagaon 1982.
3. Organometallics in Organic Synthesis – Swan & Black
4. Organometallic Chemistry - E.J. Elias and Gupta
5. Aromatic Heterocyclic Chemistry (Oxford Chemistry Primers) by David T. Davies
6. Heterocyclic Chemistry (3rd Edition) by Thomas. L. Gilchrist (Useful for Unit II)
7. Heterocyclic Chemistry by John A. Joule and K. Mills
8. The Chemistry of Heterocycles: Structure, Reactions, Syntheses, and Applications by Theophil Eicher and Siegfried HauptmannPrincipal of Modern Heterocyclic Chemistry-L .A .Paquelte
9. Heterocyclic Chemistry-Morton
10. An Introduction to Chemistry of Heterocyclic Compound-J .B .Acheson
11. Heterocyclic Chemistry by Dr Thomas. L. Gilchrist 3rd edition (Prentice Hall) for Unit II
12. Protective Groups in Organic Synthesis-T. W. Greene
13. Organic Chemistry, J .Clayden, N .Greeves, S .Warren and P .Wothers, Oxford University Press
14. Modern Organic Synthesis: An Introduction by G. S. Zweifel and M. H. Nantz (Wiley)

Weblink to Equivalent MOOC on SWAYAM if relevant:

- Organometallic Chemistry: Prof. D. Maiti, IIT Bombay
  https://nptel.ac.in/courses/104/101/104101079/
- Metal Mediated Synthesis: Prof. D. Maiti, IIT Bombay
  https://nptel.ac.in/courses/101/104/104101092/
- Transition Metal Organometallics in Catalysis and Biology: Prof. P. Ghosh, IIT Bombay
  https://archive.nptel.ac.in/courses/104/101/104101123/
- Classics in total synthesis: Prof. Krishna P. Kaliappan, IIT Bombay
  https://archive.nptel.ac.in/courses/104/101/104101133/
- Heterocyclic Chemistry: Prof. D. R. Mal, IIT Kharagpur
  https://archive.nptel.ac.in/courses/104/105/104105034/

SEMESTER IV

PGCH4T15: Elective (c) Physical Chemistry Special-II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course students will be able to

1. *Execute the chemical dynamical calculations and research applications*
2. *Understand the applications of electrochemistry in industrial as well as research applications*
3. *Analyze the applications of radiation chemistry*
4. *Gain the knowledge of battery technology and their operations so as to work in the concerned research field*
5. *Understand, analyze and execute the concepts of quantum mechanics in various fields*

UNIT-I CHEMICAL DYNAMICS - II

A) Overview of Arrhenius rate law, Non-conventional equilibrium between reactants and activated complexes. Potential energy surfaces and reaction coordinate. Derivation of transition state theory-based equation for rate constant of bimolecular reaction. Prediction of rate constant using partition function and comparison with that given by collision theory. Arrhenius equation and activated complex theory. Transmission coefficient, quantum mechanical tunneling,

B) Reactions in solution: Cage effect, diffusion-controlled reactions, volume of activation its determination and correspondence with entropy of activation, Ionic reactions: Primary (Ionic strength) and Secondary salt effect and their nature.

UNIT II CORROSION AND CORROSION ANALYSIS

A) Scope and economics of corrosion, causes (Change in Gibbs free energy), Electrochemical Series and Galvanic series, dry (atmospheric) and wet (electrochemical) corrosion, other types of corrosion-Pit, Soil, chemical and electrochemical, inter-granular, waterline, microbial corrosion, measurement of corrosion by different methods, factors affecting corrosion, passivity, galvanic series, protection against corrosion, design and material selection.

B) Thermodynamics of corrosion, corrosion measurements (Weight loss, OCP measurements, polarization methods), passivity and its breakdown, corrosion prevention (electrochemical inhibitor and coating methods).

UNIT – III: RADIATION CHEMISTRY AND BATTERY TECHNOLOGY

A) Interaction of radiation with matter, radiation track spurs and γ-rays. Linear energy transfer, Bathe's equation for linear energy transfer, Bresstrahlung effect, Passage of neutron through matter, Interaction of γ -radiation with matter, photoelectric effect and Compton effect, pair production phenomena, units of measuring radiation absorption, Chemical Dosimeters, Fricke Dosimeter and Ceric Sulphate Dosimeter, Conversion of measured dose values, Radiolysis of water, Radiolysis of some aqueous solutions. Effect of radiation on biological substances, genetic effects, Radiation effects on organic compounds and Polymers.

B) Battery Technology: basic concept, classification of batteries, primary, secondary and reserve batteries, Construction, working and application of Acid Storage batteries, Lithium -MnO_2 batteries, Nickel- Metal hydride batteries, Fuel Cells, Construction and working of $H_2O_2$and

methanol-O_2 Cell.

UNIT IV: THE LIQUID STATE AND SOLUTIONS

A] Introduction, The van der Waals Approximation, Cell theory, Hole Theory, Radial Distribution Function Methods, Radial Distribution Functions and the Thermodynamic Functions, Other Theories, Applications of these theories.

B] Introduction to solutions, Lattice Models, Ideal solutions, non-ideal or regular Solutions (Bragg-Williams Approximation), Incomplete Miscibility, Dilute Solutions, Polymer Solutions.

Books suggested

1. G.M.Panchenkov and V.P.Labadev, " Chemical Kinetics and catalysis", MIR Publishing
2. E.A. Moelwyn- Hughes, " Chemical Kinetics and Kinetics of Solutions", Academic
3. K.J.Laidler, Chemical Kinetics, Third Edition (1987), Harper and Row, New York
4. J.Raja Ram and J.C.Kuriacose, Kinetics and Mechanism of Chemical Transformations McMilllan IndianLtd., New Delhi (1993)
5. C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, **Vol 1**., Elsevier Publications, New York, 1969.
6. Gholam-Abbas Nazri, Gianfranco Pistoia, Lithum Batteries-Science and Technology, Springer, 2003.
7. C. H. Bamford and C. F. H. Tipper, Comprehensive Chemical Kinetics, **Vol 2**., Elsevier Publications, New York, 1969.
8. S. Glasstone, K. J. Laidler and H. Eyring, The Theory of Rate Processes, Mc-Graw Hill, New York, 1941.
9. Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
10. D. Mcquarie and J. Simon, Physical Chemistry – A Molecular Approach, University Press, 2000
11. G. M. Barrow, Physical Chemistry, Tata Mc-Graw Hill, V edition 2003.
12. H. K. Moudgil, Text Book of Physical Chemistry, Pretice Hall of India, New Delhi, 2010.
13. S. O. Pillai, Solid State Physics, New Age International, New Delhi, 2102.
14. C.Kittel, **"** Introduction to solid state Physics**"**,Wiley
15. L.V.Azaroff, **"** Introduction to solids**"**, McGraw Hill
16. Santosh Kumar Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer 2006.
17. N. B. Hanny, Treaties in Solid State Chemistry, 4th Edn,
18. N. B. Hanny, "Solid State Chemistry"
19. M. C. Day and J Selbin, Theoretical Inorganic Chemistry, Reinhold Pub. Corp., New York,
20. C.N.Rao. Nuclear Chemistry
21. B. G. Harvey, Introduction to Nuclear Physics and Chemistry, Prentice Hall, Inc. (1969).
22. H.J. Arnikar, Essentials of Nuclear Chemistry, 4th Edition (1995), Wiely-Eastern Ltd., New Delhi.
23. W. Loveland, D. Morrissey and G. Seaborg, Modern Nuclear Chemistry, Wiley-Interscience, 2006.

24. P. P. Milella, Fatigue and Corrosion in Metals, Springer, 2013.
25. Corrosion- Understanding the Basics, asminternational.org, 2000.
26. H. H. Uhlig, Corrosion and Corrsion Control – 3rd edn, John Wiley and sons, New York.
27. J. W. T. Spinks and R. J. Woods, An Introduction to Radiation Chemistry, John Wiley and sons., New Yoek, 1975.
28. K. L. Kapoor, Text Book of Physical Chemistry, Vol – I to Vol-VI, 2011.

SEMESTER IV

PGCH4T15: Elective (d) Analytical Chemistry Special-II

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student will be able to

1. *Understand the fundamental principles forming basis for the instrumental methods of analysis.*
2. *Select most suitable technique for the desired analysis.*
3. *Identify experimental conditions necessary to carry out the analysis of different samples.*
4. *Formulate experiments based on optical and electroanalytical techniques.*
5. *Demonstrate working of each instrument used in analysis.*

Unit-I: Optical methods of analysis-IV

Inductively coupled plasma-atomic emission spectroscopy: Principle, atomization and excitation. Plasma source and sample introduction. Instrumentation. Comparison of ICP-AES with AAS. Applications.

X-ray fluorescence spectroscopy: Principle. Instrumentation: wavelength and energy dispersive devices. Sources and detectors. Comparison between wavelength and energy dispersive techniques. Sample preparation for XRF. Matrix effects in XRF. Applications in qualitative and quantitative analysis.

Electron microscopy: Principle, instrumentation and applications of scanning electron microscopy (SEM) and transmission electron microscopy (TEM)

Unit-II: Electrochemical methods of analysis-IV

Ion selective electrodes: Theory of membrane potential. Types of ion-selective electrodes. Construction of solid state electrodes, liquid membrane electrodes, glass membrane electrodes and enzyme electrodes, Selectivity coefficients, Glass electrodes with special reference to H^+, Na^+ and K^+ ions. Applications of ISE in analysis of environmentally important anions like F^-, Cl^-, Br^-, I^-, NO_3^- and CN^-. Advantages of ISE.

***Coulometry*:** Principle. Coulometry at constant potential and constant current. Instrumentation. Applications and advantages of coulometric titrations.

***Electrochemical microscopy*:** Introduction to scanning probe microscopy (SPM), scanning tunneling microscopy (STM), atomic force microscopy (AFM) and scanning electrochemical microscopy (SECM).

Unit-III: Thermal methods of analysis

Introduction to different thermal methods, Thermogravimetry (TG and DTG), Static thermogravimetry, quasistatic thermogravimetry and dynamic thermogravimetry, Instrumentation-Balances, X-Y recorder, Stanton-Redcroft TG-750, Thermogram, Factors affecting thermogram, Applications of thermogravimetry, Differential Thermal Analysis (DTA)- Theories, DTA curves, Factors affecting DTA curve, Applications of DTA, simultaneous determination in thermal analysis, Differential Scanning Calorimetry (DSC)- Introduction, Instrumentation, DSC curves, factors affecting DSC curves, applications, Thermogravimetric titration-Theory, Instrumentation and applications.

Unit-IV: Air pollution and analysis

Air pollution and analysis-classification of air pollutants, sources of air pollution and methods of control, sampling of aerosols and gaseous pollutants and their effects, SO_2, NO_2, CO, CO_2, particulates-SPM, RSPM, High Volume Sampler, Fabric Filters, Cyclones (direct and Reverse), ESP, ozone layer, Green house effect, Heat Islands, Acid Rain.

Books suggested

1. Essentials of Nuclear Chemistry: H. J. Arnikar (Willey Eastern Ltd)
2. Substoichiometry in Radioanalytical Chemistry: J. Ruzicka and J Stary (Pergamon Press)
3. Instrumental Methods of Analysis: Willard, Meriit and Dean(Van Nostrand)
4. Instrumental Methods of Analysis: G. Chatwal and S. Anand (Himalaya Publishing House)
5. Vogel's Text Book of Quantitative inorganic Analysis: Bassett, Denney, Jeffery,Mendham (ELBS)
6. Advanced Analytical Chemistry: Meites and Thomas (McGraw-Hill)
7. Atomic Absorption Spectroscopy: Robinson (Marcel Dekker)
8. Instrumental Methods of chemical Analysis: Braun (Tata McGraw-Hill)
9. Radiochemistry: A. N. Nesmeyanov (Mir Publications)
10. Analysis of Water: Rodier
11. Ion selective electrodes: Koryta (Cambridge University Press)
12. Industrial Chemistry: Arora and Singh (Anmol Publications)
13. Diffraction Methods: John Wormald (Clarendon Press)
14. Electroanalytical Chemistry: Bard (Dekker)
15. Analytical Chemistry by Open Learning (Wiley)
16. An Introduction to Electron Diffraction: Beeston (North Holand Publishing Co.)
17. Material Science and Engineering: V. Raghavan (Printice-Hall of India)
18. Practical Physical Chemistry: J. B. Yadav (Goel Publishing House)
19. Indian Pharmacoepia, Vol-I, II and III.

Web link for related NPTEL courses

Analytical Chemistry: https://nptel.ac.in/courses/104105084

SEMESTER IV

PGCH4T15: Elective (e) Physical Organic Chemistry

60 h (4 h per week): 15 h per unit *100 Marks*

Course Outcomes: At the end of the course, student will be able to

- *describe molecular structure by the use of the valence bonding theory and molecular orbital theory*
- *use kinetics as a tool for understanding reaction mechanisms - use kinetic data for interpretation of reaction mechanisms*
- *determine if a reaction is acid or base catalyzed (specific or general catalysis) from kinetic data, and feel comfortable in making estimates on reaction mechanisms by use of the Hammett equation as a tool in studies of organic reactions*
- *interpret data for the inclusion of isotops and how this can be used in mechanistically studies of organic reactions*
- *suggest additional experiments to "prove" or "disprove" a proposed reaction mechanism - use Woodward and Hoffman's "selection rules" for pericyclic reactions*

Unit I:

A) Concepts in Molecular Orbital (MO) and Valence Bond (VB) Theory: Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi empirical methods and ab inito and density functional methods. Scope and limitations of several computational programmes.

Quantitative MO theory – Huckel molecular orbital (HMO) method as applied to ethane, allyl and butadiene. Qualitative MO theory – ionization potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital interaction diagrams. MO of simple organic systems such as ethee, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity.

Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve-crossing model-nature of activation barriers in chemical reactions.

B) **Principles of Reactivity:** Mechanistic significance of entropy, and Gibb's free energy. Arhenius equation. Transition state theory. Uses of activation parameters, Hannond's postulate. Bell-Evans-Polanyl principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

Unit II:

A) Kinetic Isotope Effect: Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

B) **Structural Effects on Reactivity:** Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of σ–values. Reaction constant p. Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model, σ_I and $\boldsymbol{\sigma_R}$–scales.

C) **Solvation and Solvent Effects: Q**ualitative understanding of solvent-solute effects on reactivity. Thermodynamics measure of solvation. Effects of solvation on reaction rates and equilibria. Various empirical indexes of solvation based on physical properties, solvent-sensitive reaction rates, spectroscopic solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model.

Unit III:

A) Acids, Bases, Electrophiles, Nucleophiles and Catalysis: Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilic scales Nucleofugacity. The –effect. Amvbibalent nucleophiles. Acid-base catalysis- specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding-micellar catalysis.

B) **Steric and Conformational Properties:** Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtion-Hammett principle.

C) **Nucleophilic and Electrophilic Reactivity:** Structural and electronic effects on S_N1 on S_N2 reactivity. Solvent effects. Kinetic isotope effects. Intramolecular assistance. Electron transfer nature of S_N2 reaction. Nucleophilicity and S_N2 reactivity abased on curve- crossing model. Relationship between polar and electron transfer reactions. S_E2-Ar reaction. Structural effects on rates and selectivity. Curve-crossing approach to electrophilic reactivity.

Unit IV:

A) Radical and Pericyclic Reactivity: Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors effecting barrier heights in additions, regioselectivity in radical reactions, Reactivity, specificity and periselectivity in pericyclic reactions.

B) Supramolecular Chemistry: Properties of covalent bonds – bond length, inter-bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy. Intermolecular forces, hydrophobic effects. Electrostatic, induction, disperision and resonance energy. Magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects. Hydrogen bond.

Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principle. Cryptands, cyclophanes, calixeranes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

Books suggested

1. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. L. Salem and W.L. Jorgensen, Academic Press.
3. Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Jarper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular. Modeling, W.B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman.\
6. Supramolecular Chemistry, Concepts and Perspectives, J.M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

SEMESTER IV

PGCH4P08: Major Research Project

12 h per week *200 Marks*

The objective of research project is to train the student in identifying the problem of research, develop the hypothesis, design the experiments/surveys to test the hypothesis, collect and analyse the data and draw conclusions from it. In addition, the aim is also to prepare the student to present the data in various forms such as project report, presentation in conferences and seminars and research paper. Research project is also aimed to prepare the student for doctoral research after the completion of the programme.

The student will have to carry out a research-based project work in the third and fourth semester. The project work may be carried out in the parent department or any other institute in collaboration with the parent institute. For this, the student will be attached to any of the national/regional/private research institute/organization for the duration of the fourth semester. If the student is working in the organisation other than the parent department, then it will be the responsibility of the student to attend the classes and other departmental activities in order to be eligible to appear for the examination. The student will be allotted the supervisor in the third semester; after which the student will finalize the topic of the project work in consultation with the supervisor.

The research project of the student will be evaluated on the basis of the project report submitted by him/her and the power point presentation made by him/her in the presence of internal and external examiner during the examination.