CENTURION UNIVERSITY OF TECHNOLOGY AND MANAGEMENT, ODISHA

SCHOOL OF BASIC SCIENCES

2 YEARS M.Sc. PROGRAMME
IN
APPLIED CHEMISTRY

2015-16

SEMESTER-I				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	MSCH4701	PHYSICAL CHEMISTRY-IV	3+1+0	4
2	MSCH4702	INORGANIC CHEMISTRY-IV	3+1+0	4
3	MSCH4703	ORGANIC CHEMISTRY-IV	3+1+0	4
4	MSCH4704	POLYMER CHEMISTRY	3+1+0	4
5	MSCL4701	CHEMISTRY LAB-VII	0+0+6	4
6	As per specified courses	**FREE ELECTIVE-I**	3+1+0	4
TOTAL CREDITS				24

SEMESTER-II				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	MSCH4801	PHYSICAL CHEMISTRY-V	3+1+0	4
2	MSCH4802	INORGANIC CHEMISTRY-V	3+1+0	4
3	MSCH4803	ORGANIC CHEMISTRY-V	3+1+0	4
4	MSCH4804	NUCLEAR CHEMISTRY	3+1+0	4
5	MSCL4801	CHEMISTRY LAB-VIII	0+0+6	4
6	As per specified courses	FREE ELECTIVE-II	3+1+0	4
TOTAL CREDITS				24

SEMESTER-III				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	MSCH5101	ADVANCED INORGANIC CHEMISTRY-IV	3+1+0	4
2	MSCH5102	ADVANCED ORGANIC CHEMISTRY-IV	3+1+0	4
3	MSCH5103	ADVANCED PHYSICAL CHEMISTRY-IV	3+1+0	4
4	MSCH5104	SOLID STATE CHEMISTRY	3+1+0	4
5	MSCL5101	CHEMISTRY LAB-VII	0+0+6	4
6	MSRM5101	INTRODUCTION TO RESEARCH	2+0+0	2
7	MSCS5101	SEMINAR	3-0-0	2
TOTAL CREDITS				24

SEMESTER-IV				
Sl no	**Subject Code**	**Subject**	**Contact Hours per week (L+T+P)**	**Credits**
1	MSCH5201	ORGANIC SPECTROSCOPY	3+1+0	4
2	MSCH5202	BIO-INORGANIC CHEMISTRY	3+1+0	4
3	MSCS5201	SEMINAR	3+1+0	4
4	MSCP5201	PROJECT	3+1+0	12
5	----------	----------	------	---
6	----------	----------	--------	-------
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TOTAL CREDITS				24

SEMESTER-I

PHYSICAL CHEMISTRY –IV (3-1-0)

Module –I: Chemical Dynamics [15 Lectures]

Methods of determining rate laws, Derivation of collision theory of reaction rates, steric factor, activated complex theory, steady state kinetics, kinetic and thermadynamic control of reactions. Treatment of unimolecular reactions.
Dynamics chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen -bromine and hydrogen - chlorine reactions) and oscillatory reactions (Belousov- Zhabotinski reaction), homogeneous catalysis, kinetics of enzyme reactions. general features of fast reactions, relaxation method. flash photolysis and the nuclear magnetic resonance method.

Module-II: Surface Chemistry [16 Lectures]
(A) Adsorption:
Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation). Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electrokinetic phenomenon), catalytic activity at surfaces.
(**B) Micelles:**
Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants counter ion binding to micelles, thermodynamics of micellization, phase separation and mass action models, solubilization, micro emulsion, reverse micelles.
C) Quantum chemistry- Discussion of solutions of the Schrodinger equation to some model systems viz. the harmonic oscillator, the rigid rotor, the hydrogen atom.
Approximate Methods:
The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

Module-III: Electrochemistry [14 Lectures]

Derivation of electrocapiliarity; Lippmann equations (surface excess), methods of determination, Structure of electrified. Interfaces, Over potentials, exchange current density, derivation of Butler-Volmer equation, TafelplolQauntum aspects of charge transfer at electrode - solution interfaces, quantization of charge transfer, tunneling. semiconductor, interfaces-theory of double layer at 14semiconductor-electrolyte solution interfaces, structuer of double layer interfaces. Effect of light at semiconductor solution interface.Electrocatalysis-influence of various parameters, Hydrogen electrode.Bioelectrochemistry, Theresholdmembrance phenomena, Nerst-Planck equation, Hodges-Huxley equations, core conductor models, electrocardiography. Polarography theory, IIkovic equation; half wave potential and its significance.

Books Recommended:

1. Physical Chemistry: P.W. Atkins, J.D. Paula, Oxford III University Press.
2. Introduction to Quantum Chemistry :A.K.Chandra, Tata McGraw Hill.
3. Quantum-Chemistry : Ira N. Levine, Prentice Hall.
4. Coulson's Valence: R Mc Weeny, ELBS.
5. Chemical Kinetics: K.J.Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation: J.Rajaraman and J.Kuriacose,
Mcmillan.
7. Micelles, Theoretical and Applied Aspects, V.Moroi, Plenum.
8. Modem Electrochemistry: Vol.-I and Vol. II, J.O.M. Bockris and A.K. N. Reddy, Plenum.

INORGANIC CHEMISTRY –IV (3-1-0)

Module-I

Theory of metal-ligand bonding [15 Lectures]

Octahedral and tetrahedral crystal field potential and its effect on d-wave function.The evaluation of l0Dq free ions in weak, medium and strong fields. Crystal-Field Theories:Limitation of crystal field theory, Elementary idea of Angular overlap model, molecular orbital theory for octahedral, tetrahedral and square planar complexes, σ and π bonding in molecular orbital theory,Lignad field theory. Analysis of Electronic Spectra of transition metal complexes at least for one system [d^n(Oh) or (Td)] .

Module -II
Electronic Spectra and Magnetic Properties of Transition Metal Complexes [16 Lectures]

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1, d9 states), Lignad field spectra of octahedral and tetrahedral complexes and calculations of Dq, B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemicalinformation,Term interaction and the energies of the levels,

Module-III

Symmetry and Group Theory in Chemistry [15 Lectures]

Symmetry elements and symmetry operation, definitions of group-subgroup, relation between orders of a finite group and its subgroup.Symmetry point group.Schonflies symbols, Matrix representations of groups (representation for the Cn, Cnv, Cnh, Dnh etc. groups to be worked out explicitly).Character of a representation.The great orthogonality theorem (without proof) and its importance. Character tables and their uses:application to selection rules.

Books Recommended:

1. Advanced Inorganic Chemistry: F.A, Cotton and G. Wilkinson, John Wiley.
2. Inorganic Chemistry: J.E. Huheey, E.A Keiter, RL. Keiter, Pearson Education.
3. Inorganic Electronic Spectroscopy: AB. P. Lever, Elsevier.
4. Magnetochemistry, RL. Carlin, Springer Verlag.
5. Comprehensive Coordination Chemistry eds.,-G. Wilkinson, RD. Gillars and J.A. McCleverty, Pergamon.
6. Chemical Application of Group Theory: FA Cotton, John Wiley.
7. Symmetry in Chemistry: Orchin and Jaffe.
8. Group theory: I .V. Raman, Tata McGraw Hill.
9. Group Theory & its Applications to Chemistry: KV. Raman, Tata McGraw Hill Publishing Company, New Delhi.

ORGANIC CHEMISTRY-IV(3-1-0)

Module-I [17 Lectures]

1) **Nature of Bonding in Organic Molecules :**

Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Alternant and non-alternant hydrocarbons.energy level of π-molecular orbitals, annulenes, antiaromaticity, ψ-aromaticity, homoaromaticity,PMO approach. Bonds weaker than covalent addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, Catenanes and Rotaxanes.

2) Stereochemistry

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotropic and diastereotropic atoms, groups and faces, stereospecifjc and, steroselective synthesis. Asymmetric synthesis.Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape.Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Module-II **[15 Lectures]**

1) Addition to Carbon-Carbon Multiple Bonds:
Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, region and chemoselectivity, orientation and reactivity, Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings.Hydroboration, Michael reaction.Sharpless asymmetric epoxidation.

2) **Elimination mechanism:** E 1 , E 2 , E 1 CB and E 2 CB mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Sayetzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidaton of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction,Shapiro reaction, Stereo chemistry of elimination reactions-alpha elimination.

Module-III **[14 Lectures]**

Organic Synthesis:
a) Synthetic design: Introduction, Retrosynthetic approach, Terminology in Retro synthetic analysis, One group disconnection, (alcohol, carbonyl compound, olefins and acids), Two group disconnections (beta-hydroxy compounds, alpha, beta-unsubstituted carbonyl compounds, 1,3-dicarbonyl compounds, 1,5 dicarbonyl compounds), Synthesis of some organic molecules by disconnection approach.
b) Formation of aliphatic Carbon-nitrogen bonds: Substitution and addition of nucleophilic nitrogen, reactions of electrophilic nitrogens, rearrangement of electron deficient nitrogen.
c) Organometallics in synthesis: Organo lithium, organo copper compounds, organoboranes,organometallic compounds of Zinc, Cadmium and mercury organo palladium compounds.

Books Recommended:

1. Advanced Organic Chemistry; Reactians Mechanism and Structure: Jerry March, John.Wiley.
2. Advanced Organic Chemistry: F A Carey and R J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry: Peter Sykes, Longman/Pearson Education.
4. Structure and Mechanism in Organic Chemistry: C K Ingold, Cornell University Press.
5. Organic Chemistry: R. T. Marrisan and R. N Boyd, Pentice- Hall/Pearson Education.
6. Modern Organic Reactions: H.O. House, Benjamin.
7. Principles of Organic Synthesis: R.O.C. Norman and J.M. Coxon, Blackie Academic &Professianal/ C.B.S. Publishers.
8. PericyclicReactions : S.M. Mukherji. Macmillan, India Ltd.
9. Reaction Mechanism in Organic Chemistry: S..M. Mukherjee and S.P. Singh, Macmillian. India. Ltd.
10. Organic Chemistry: J. Clyden, N. Grieves, S. Warren and P.Wather, Oxfard University Press.

11. Organic Reactions and Orbital Symmetry: T.L Gilchrist and R. C. Storr, Cambridge at the University Press.
12. Photo Chemistry and PericyclicReactions :Jagdamba Singh and Jaya Singh, New Age Internatianal.
13. Mechanism and Theory in Organic Chemistry: Thomas H. Lowry, Additian Wesley.
14. Stereochemistry by Eliel.
15. Stereochemistry by P.S.Kalsi
16. Stereochemistry by Nasipuri.

POLYMER CHEMISTRY (3-1-0)

Module I (14 Lectures)

Functionality, bi-functional and poly functional systems, classification and nomenclature of polymers, branching and crosslinking, glassy and crystalline states, thermodynamics of crystallization, kinetics of melting, crystal morphology, free volume, distribution of molecular size, stoichiometric imbalance.

Molecular weight, molecular weight distribution, polydispersity, degree of polymerization, molecular weight determination, viscosity of polymer solutions, molecular weight dependence of viscosity and size of polymer molecules.

Module II (12 Lectures)

Types of polymerization, polymerization techniques, copolymers and stereo-regular polymers, reactivity ratios, copolymer composition and microstructure, Price - Alfrey equation, Flory - Huggins theory, polymer fractionation, Mark – Houwink - Sakurada equation, diffusion coefficient and friction factor.

Module III (15 Lectures)

Elastic deformation, shear modulus and compliances, Maxwell model, Voigt model, dynamic viscoelasticity, molecular theory for viscoelasticity - Rouse model, Coefficient of viscosity, viscosity measurement, Power Law for pseudoplastic liquids, effect of shearing forces, segmental friction factor, Bueche theory.

Text Books

1. Gedde Ulf. W. Polymer Physics, Chapman & Hall London (1995)
2. Rodriguez, Ferdinand, Principles of Polymer Systems Mc. Craw – Hill, International BookCo. International Student Edn. 1985.
3. Cowie; JMG Polymers: Chemistry & Physics of Modern Materials, Nelson Thornes ltd.Chelterham, 2001
4. Hiemenz; Paul C. Polymer Chemistry- The Basic Concepts; Marcell&Deckker, Inc. New York (1984)
5. Polymer Science by V.R.Gowarikar, N.V.viswanathan and J.Sreedhar, New Age International.
6. Text book of Polymer science: F.M.Billmeyer, John wiley and sons.

CHEMISTRY LABORATORY-VII (0-0-6)

INORGANIC CHEMISTRY PRACTICAL

1. Qualitative analysis of mixtures containing not more than six radicals , (organic acid radicals
should be excluded, less common metal ions Mo, W, Ti, V, Zr, U (two metal ions in cationic / anionic forms), insoluble-oxides, sulphates and halides may be included]
2. Separation of cations and anions by (a) paper chromatography and column chromatography (b) ion exchange technique.

Books Recommended:

1. Vogel'-s Qualitative Inorganic Analysis (revised) : G. Svehla, Longman.
2. Inorganic Experiments: J. DerckWoollins, VCH.
3. Microscale Inorganic Chemistry: Z. Szafran, RM. Pike and M.M: Singh, Wiley.
4. Practical Inorganic Chemistry: G. Marr, B.W. Rockett Van Nostrand.

SEMESTER-II

PHYSICAL CHEMISTRY-V 3-1-0)

Module-I

Electronic Structure of Atoms: [04 Lectures]
Electronic configuration. Russell-Saunders terms and coupling schemes, magnetic effects: spin-orbit coupling and Zeeman splitting.

Molecular Orbital Theory: [05 Lectures]
Huckel theory of conjugated systems, bond order and charge density calculation.Applications to ethylene, butadiene, cyclopropenyl radical, and cyclobutadiene.

Classical Thermodynamics [10 Lectures]
Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies.Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance.Determination of these quantities.Concept of fugacity and determination of fugacity.

Module-II

Non-ideal systems: [04 Lectures]
Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients, ionic strength.

StatsticalThermodynamics : [10 Lectures]
Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function. Applications of partition functions. Heat capacity behaviour of solids – chemical equilibria and equilibrium constant in terms of partition functions,

Module-III

Vibrational Spectroscopy: Infrared Spectroscopy: [12 Lectures]
Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P. Q. R. branches. Breakdown of Oppenheimer approximation, vibrations of polyatomic molecules, Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities; far IR region, metal-ligand vibrations, normal co-

ordinate analysis.

Raman Spectroscopy: [10 Lectures]
Classical and quantum theories of Raman effect Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, Mutual exclusion principle. Resonance Raman Spectroscopy (RRS), Coherent Antistokes Raman Spectroscopy(CARS).

Books Recommended
1. Atkin's Physical Chemistry: P.W. Atkins,J.D. Paula, Oxford University Press
2. Introductory to Quantum Chemistry:4th Ed., AK Chandra, TataMcGraw Hill.
3. Quantum Chemistry: Ira N. Levine, Prentice Hall.
4. Coulson's Valence: R Mc Weeny, ELBS.
5. Physical Chemistry Vol-II: .RL. Kapoor, Mcmillan Publication.
6. Statistical Thermodynamics: M.C Gupta, New Age Pvt Publication.
7. Fundamentals of Molecular Spectroscopy : C.N. Banwell, McGraw-Hill.
8. Basic Principles of Spectroscopy: R. Chang, McGraw Hill.
9. Theory and Applications of U.V. Spectroscopy: H.H. Jaffe and M. Orchin, IBH-Qxford.
10. Quantum Chemistry : R K Prasad.

INORGANIC CHEMISTRY-V(3-1-0)

Module-I

Metal π -Complex. [12 Lectures]
Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding preparation,bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine and ligands.

Metal Clusters: [08 Lectures]
Higher boranes, carboranes, metalloboranes and, metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Module –II

Metal -Ligand Equilibria in Solution [15 Lectures]
Type of complex equilibria in solution and types of complex equilibrium constant , factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

Reaction Mechanism of Transition Metal Complexes [15 Lectures]

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, Acid hydrolysis, factors affecting acid hydrolysis and base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate base mechanism, reaction without metal ligand bond cleavage. Substitution reactions in square planar complexes. The trans effect, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions, Marcus-Hush theory, Inner sphere type reactions.

Books Recommended:

1. Advanced Inorganic Chemistry: A Comprehensive Text: FA Cotton and G. Wilkinson, John Wiley.
2. Inorganic Chemistry: Principles of Structure and Reactivity: J.E. Huheey, E.A. Keiter and
R.L. Keiter, Addition Wisley Publishing Company.
3. Comprehensive Coordination Chemistry eds.: G. Wilkinson, R.D. Gillars and JA McCleverty, Pergamon.
4. Inorganic reactions by Basalo and Pearson.

ORGANIC CHEMISTRY-V(3-1-0)

Module-I

Reaction Mechanism: Structure and Reactivity: [15 Lectures]

Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin - Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects.

Photochemistry: [10 Lectures]

First order Photo chemical processes, Photo reactions : Dissociation , Reduction, Isomerisation, cycloaddition, Paterno-Buchi reaction, Norrish type-I & II reactions, Di-Pi methane reaction, Photochemistry of Arenes.

Module-II

Methodologies in organic synthesis [07 Lectures]

Ideas of synthones and retrones.Functional group transformations and interconversions of simple functional groups.

Six membered Heterocycles with one heteroatom [05 Lectures]
Synthesis and reactions of pyrilium salts and pyrones and their comparison pyridinium and thiopyrylium salts and pyridones. Synthesis and reactions of coumarins, chromones.

Six membered Heterocycles with two and more Heterocycles [08 Lectures]
Synthesis and reactions of diazines&triazines. Seven membered Heterocycles , Synthesis and reactions of azepines, oxepines&thiepines. unctionalities.

Module-III

PericyclicReactions: [19 Lectures]
Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1, 3, 5 – hexatriene and allyl system. Classification of pericyclicreactions.WoodWard – Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions, conrotator and disrotatory motions; 4n, 4n+2 and allylsystems.Cycloadditions, antarafacial and suprafacial additions; 4n and 4n+2 systems, 2+2 addition of ketenes.1, 3 - dipolar cycloadditon and cheletropic reactions.

Sigmatropic rearrangements -suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3 - and 5, 5 – sigmatropic rearrangements: Claisen, Cope and aza-Cope rearrangements,Ene reaction.

RECOMMONDED BOOKS
1.Modern synthetic reactions-(Benjamin) H. O. House.
2.Reagents in organic synthesis-(John Wiley) Fieser and Fieser
3.Principles of organic synthesis-(Methuen) R. O. C. Norman
4.Hydroboration- S. C. Brown.
5.Advances in Organometallic Chemistry- (A.P.)F. C. A. Stone and R. West.
6.Organic Chemistry (Longman)Vol. I & Vol. II- Finar
7.Oxidation by-(Marcel Dekker) Augustin
8.Advanced Organic chemistry 2nd Ed. R R. Carey and R. J. Sundburg.
9.Tetrahydron reports in organic chemistry- Vol.1, No. 8.
10. Organic Synthesis-(Prentice Hall)R. E. Ireland.
11. Homogeneous Hydrogenation-(J. K.) B. R. James.
12. Comprehensive Organic Chemistry- (Pargamon) Barton and Ollis.
13. Organic reactions- various volumes- R. Adams.
14. Some modern methods of Organic synthesis-(Cambridge) W. Carruthares.

NUCLEAR CHEMISTRY(3-1-0)

Module-I

Systematic Study of alpha, beta and gamma decays [15 Lectures]
Alpha decay, energy curve, spectra of alpha particles, Giger-Nuttal law, theory of alpha decay, penetration of potential barrier, potential barrier, potential well, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect.

Nuclear Structure and Stability [08 Lectures]
Binding energy, empirical mass equation, The nuclear models, the shell model, nuclear spin, parity &magnetic moments of odd mass numbers nuclei.

Module-II

Nuclear reaction [08 Lectures]

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

Nuclear fission [07 Lectures]

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and A symmetric fission, decay chains and delayed neutrons.

Module-III

Reactor Theory [10 Lectures]
Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a thermal reactor, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

Reference Books.
1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley
2. B.G. Harvey, Nuclear Chemistry
3. Hassinsky: Translated by D.G. Tuck, Nuclear Chemistry and its application: Addison Wiley
4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry
5. Maeclefort: Nuclear Chemistry: D.VanNostrand

6. An N.Nesmeyannoy: Radiochemistry: Mir
7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V.Nost& EWAP
8. N.Jay: Nuclear Power Today Tomorrow: ELBS
9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
10. Essentials of Nuclear Chemistry, W.J. Arnikar, John Wiley
11. Nuclear and Radiation Chemistry: B.K. Sharma, Krishna Publication
12. A Introduction to Nuclear Physics: R. Babber. And Puri

CHEMISTRY LAB-VIII (0-0-6)

Three stage preparations starting with 5g or less & TLC.
1. Estimation of sulphur, nitrogen and functional groups, pharmaceutical analysis.
2. Polyfunctional analysis of organic compounds
3. Organic preparations
i. Preparation of benzanilide by Beckmann rearrangement
ii.. Preparation of anthranilic acid
iii.. Preparation of phthalimide
iv. Preparation of N- bromosuccinamide
v. Preparatin of p- Amino benzoic acid
vi. Preparation of p- chloro nitrobenzene by Sandmeyer reaction
vii. Preparation of p- Idonitrobenzene by Sandmeyer reaction
viii. Pinacol- Pinacolone rearrangement

3. Separation of two colour compounds by column chromatography method.

REFERENCES BOOKS:

1. A Textbook of Practical Organic Chemistry – A. I. Vogel.
2. Practical Organic Chemistry – Mann & Saunders.
3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
4. Organic Synthesis Collective Volumes.
5. Organic Reactions (Wiley).

Semester-III

Advanced Physical Chemistry-IV (3-1-0)

Module I **(18 Lectures)**

Electronic spectra of molecule:

Introduction, Absorption of light; The Beer–Lambert Law. and its deviation, relation between molar extinction coefficient and absorption cross section, Electronic spectra of diatomic molecules: The Born-Oppenheim Approximation, vibrational coarse structure, intensity of Vibrational-electronic spectra: the Franck–Condon principle, notation of energy levels and electronic transitions, Electronic spectra of polyatomic molecules: auxochromo and chromophore, Selection rules, applications.

Nuclear Magnetic Resonance Spectroscopy:

Introduction, Theory of Nuclear magnetic resonance, chemical shift, factors affecting chemical shift, spin-spin splitting, Advanced NMR techniques, Application of NMR

Module II **(16 Lectures)**

Photophysical Chemistry I:

Fluorescence:

Introduction, principles and instrumentation; choice of light sources, monochromators, choice of optical filters and various detector systems used, Jablonski Diagram, Characteristics of Fluorescence Emission, Fluorescence Lifetimes and Quantum Yields, Stoke's shift, fluorescence excitation spectrum, Fluorescence Anisotropy. Effects of solvents on the fluorescence spectrum: (general effects and specific effects, derivation of the equation, Temperature Effects)

Module III **(10 Lectures)**

Photophysical Chemistry II:

Fluorescence quenching and Resonance Energy Transfer: Different mechanism of fluorescence quenching & applications, Different mechanisms of energy transfer (Forster and Dexter mechanism), selection rules for energy transfer, non-vertical energy transfer, Forster Resonance Energy Transfer (FRET), typical examples and choice of dyes and applications.

Data analysis: **(6 Lectures)**

Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

Reference Books:

- Chemical application and group Theory; F.A. Cotton, 3rd edition (1999).
- Fundamentals of Photochemistry; K. K. Rohatagi-Mukherjee.
- Molecular Fluorescence: Principles and Applications; Bernard Valeur.

- Principles of Fluorescence Spectroscopy; Springer; 3rd edition (2006), J. R. Lakowicz.
- Basic Principle of Analytical Chemistry ; S.M. Khopkar.

Chemistry Laboratory-VII(0-0-6)

1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law.
2. Verification of Onsager's limiting law.
3. Conduct metric titration of a mixture of HCl+CH_3COOH with NaOH
4. Determination of solubility product of $BaSO_4$.
5. Potentiometric titration of strong acid with strong base.
6. Determination of temperature coefficient and energy of activation of hydrolysis of ethyl acetate.
7. To determine the rate constant of base hydrolysis of ester titrometrically.
8. pH meter: Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid.
9. To study the simultaneous equilibria in benzoic acid – benzene- water system.
10. Conductometry: Hydrolysis of NH_4Cl or CH_3COONa or aniline. Hydrochloride, Determination of dissociation constant of acetic acid, Hydrolysis of ethyl acetate by NaOH.

Reference Books:

- Experimental Physical Chemistry: RC Das and B Behera
- Practical physical chemistry: B Viswanathan and P.S .Raghavan
- Practical chemistry: Vogel

Solid State Chemistry (3-1-0)

Module I **(12 Lectures)**

Crystal Structure

(a) Crystal lattice, Crystal planes, Miller indices, Bragg's law, Determination of crystal structure (NaCI, KCI, ZnS, and CsCl), Structure of elements and compounds.

(b) Bonding in Solids: Vander waal's force, force of covalency, bonding in ionic solids, Born-Harber cycle, theoretical evaluation of lattice energy, imperfections in solids, Schottky and Frenkel defects.

Module II **(15 Lectures)**

Electronic structure of solids-band theory:

Band structure of Solid: Metals and their properties; semiconductors: Intrinsic and extrinsic semiconductors, Fermi Levels; Hall effect, Semiconductors devices: p-n junctions and other devices; insulators-dielectric, ferroelectric, pyroelectric and piezoelectric properties; ionic conductors.

Module III **(15 Lectures)**

Mechanical Properties of Solids: Stress, strain, deformation, tensile properties, ductility, and other mechanical properties of metals

Magnetic properties: Dia, para, Ferro, ferri, and antiferro magnetic types; soft and hard magnetic materials; magneto resistance.

Reference Books:

- Solid State Chemistry by D. K. Chakrabarty.
- Solid State Chemistry and its Applications by R. West, John Wiley & Sons, 1984.
- Solid State Chemistry - An Introduction by L. Smart and E. Moore, Chapman & Hall, 1992.
- Principles of the Solid State by H. V. Keer, Wiley Eastern Limited, 1993.
- Solid State Chemistry by K. Chakrabarty, New Age Publishers, 1996.
- Principles of Materials Science and engineering, Navneet Gupta, 2nd Ed, Dhanpat Rai & Co.

Advanced Inorganic Chemistry-IV (3-1-0)

Module I

Instrumental Method of Analysis: (8 Lectures)

Atomic absorption and Flame emission spectral method and their application in quantitative analysis. Molecular absorption and emission spectroscopy in quantitative analysis. Light scattering technique including nephlometry and Raman spectroscopy.

Electron Spin Resonance Spectroscopy: (5 Lectures)

Theory, instrumentation, g-values, hyperfine splitting, ESR spectra of systems with more than one unpaired electrons, double resonance, ENDOR and ELDOR techniques.

Mossbauer Spectroscopy: (8 Lectures)

Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects,Quadrupole splitting, Magnetic hyperfine interaction.

Module II

Homogeneous and Heterogeneous Catalysis: (10 Lectures)

Stiochiometric reactions for Organometallic catalysts: Dissociation & Substitution, Oxidative addition & carbonylation, Oxygen transfer from Peroxo and Oxo Species, Reductive & Hydride elimination, Insertion,Displacement and Isomerization reaction. Hydrogenation, Hydroformylation, Wacker (Smidt) Process, Olefin Metathesis, Fischer-Tropsch synthesis, Zeigler-Natta polymerization, Water gas reaction.

Module III

Mechanism Of Substitution Reactions: (15 Lectures)

The nature of substitution reactions, Kinetic Application of Crystal Field Theory.Acid hydrolysis of octahedral Co (III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group. Base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, Test of conjugate base mechanism. Anation reaction.

Electron Transfer Reactions:

Introduction, electron tunneling hypothesis, Marcus-Hush theory, atom transfer reactions, one and two electron transfer, inner sphere and outer sphere reaction, electron transfer through extended bridges and the hydrated electron.

Reference Books:

- Spectroscopy Vol. I & II : Walker & Straw.
- Fundamentals of Molecular Spectroscopy: C.N. Banwell.
- Molecular Spectroscopy: P.S. Sindhu.
- Fundamentals of Molecular Spectroscopy: G.M. Barrow.
- Mechanisms of Inorganic Reactions : F. Basolo and R.G. Pearson.
- Inorganic Chemistry : Cotton and Wilkinson (4th Ed).

Advanced Organic Chemistry-IV (Biomolecules) (3-1-0)

Module I **(15 Lectures)**

Amino Acids, Peptides and Proteins:

Classification and functions of amino acids and proteins, Chemical reactions of amino acids, alkali titration of amino acids, Synthesis of peptides, α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Primary, secondary, tertiary and quaternary structures of proteins. Tertiary structure of protein- folding and domain structure. Quaternary structure.

Module II **(10 Lectures)**

Lipids:

Classification and Function of lipids, Structural lipids in membranes, lipids with specific biological activities, Resolution and Analysis of lipids, Biological membrane and transport.

Module III **(15 Lectures)**

Purine and pyrimidine of nucleic acids, base pairing via H–bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. Overview of Replication, Transcription and Translation processes, Sequencing ofnucleic acids, Genetic code, Recombinant DNA.

Reference Books:

1. Principles of Biochemistry, A. L. Lehinger, Worth Publications.

2. Biochemistry, Voet and Voet, John Wiley.

Semester IV

Bio-Inorganic Chemistry (3-1-0)

Module I (**18 Lectures)**

Organometallic Chemistry:

18-Electron Rule, Ligands in Organomettallics,Synthesis, bonding and reactions of Alkyl, Aryl, Alkylidenes, Alkylidynes, Allyl, Dienyl,Arene & Trienyl complexes, Cyclic p systems (3 to 8 membered rings) and Fullerene complexes. Spectral analysis of Organometallic Complexes.

Module II **(18 Lectures)**

Metalloporphyrins And Iron-sulphur Protein

Iron porphyrins (Heme proteins): Hemoglobin (Hb), Myoglobine (Mb) their behavior asoxygen carrier and oxygen uptake protein, O_2 affinity cooperativity and Bohr's effect, Heme protein as electron carrier with particular reference to reference to cytochrome-c and cytochrome-450, and cytochrome oxydase. Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle). Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

Module III **(18 Lectures)**

Metalloenzymes

Preliminary idea about enzyme, co-enzyme and metalloenzyme, Enzyme-substrate binding problem, The Michaelis-Menten's equation, carboxypeptidase, carbonic anhydrase and their biological significance, oxydases, nitrogenases and its role in nitrogen fixation, Interchangeability of zinc and cobalt enzyme Supramolecular Chemistry**:** Host guest chemistry, chiral recognition and catalysis, molecular recognition, biomimetic chemistry, crown ethers, cryptates. Cyclodextrine, cyclodextrinbased enzyme models, calixarenes, Ionophores.

Reference Books:

- Basic Inorganic Chemistry (3rd ed) : Cotton ,Wilkinson & Gaus.
- Inorganic chemistry (4th Ed) : Huheey, Keiter & Keiter.
- Bioinorganic and Suparmolecular Chemistry: Bhagi, G.R.Chatwal.
- Bio-Inorganic chemistry : E.Ochiai.

Bio-Inorganic chemistry : R.W. Hay.

Organic Spectroscopy (3-1-0)

Module I **(12 Lectures)**

Ultraviolet Spectroscopy:

Woodward- Fisher rules for conjugated dienes and carbonyl compounds; Calculation of λ max. Ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

IR Spectroscopy:

Characteristic vibrational frequencies of alkanes; alkenes; alkynes; aromatic compounds; alcohols; ethers; phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters; amides, acids, Anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones; FT-IR of gaseous; solids and polymeric materials.

Module II **(12 Lectures)**

Nuclear Magnetic Resonance Spectroscopy:

The nature of spinning particles, interaction between spin and a magnetic field. Population of energy levels, The larmor precession . relaxation times . the meaning of resonance and the resonance condition. NMR experiment, significance of shielding constants and chemical shift . the origin and effect spin - spin coupling , factors affecting chemical shift, chemical analysis by NMR. Exchange phenomena, 13C NMR spectroscopy, double resonance and nuclear-overhauser effect.

Module III **(10 Lectures)**

Mass Spectrometry:

Introduction, ion production, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, nitrogen rule. High-resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Structural problems based on combined spectroscopic techniques.

Reference Books

- W. Kemp, Organic spectroscopy ELBS.
- D.W. Williams and Flemming, Spectroscopic methods of organic compound.
- Silverstein and Basallar, Spectroscopic identification of organic compounds.
- P.S. Kalsi Spectroscope of organic compounds (New age publisher).
- Jafee and Orchin, Theory and application of U.V.