

FIRST SEMESTER

CHE 101- CORE THEORY: INORGANIC CHEMISTRY-I

UNIT-I: CO-ORDINATION COMPOUNDS

15 Hrs

Introduction to Crystal field Theory, CFSE and its calculation, Pairing energy, Splitting of 'd' orbitals in Trigonal bi pyramidal, square planar, square pyramid and pentagonal bipyramidal geometries, Jahn –Teller effect, Application of CFT, OSSE, site Selection in Spinels, Shortcomings of CFT, Evidence for covalency – Nephelauxetic effect. MOT of co-ordinate bonds – M.O. Diagrams for octahedral, tetrahedral and square planar complexes. Experimental evidences for π - bonding – Crystallography, Infrared spectroscopy and Photoelectron spectroscopy.

UNIT-II: CHEMISTRY OF NON-TRANSITION ELEMENTS

15 Hrs

General characteristics of the non- transition elements special features of individual elements ; Synthesis' properties and structure of their Halides and Oxides, Polymorphism of Carbon, Phosphorus and Sulphur, Synthesis, properties and structure of boranes, Carboranes, borazines, Silicates, Carbides, Sulphur-nitrogen compounds. Electron counting in boranes, Wades rules (Poly hedral skeletal electron pair theory), Isopoly and hetero poly acids.

UNIT-III: REACTION MECHANISMS IN COMPLEXES

15 Hrs

Reactivity of metal complexes. Inert and Labile complexes. Concept of Labile and Inert complexes in terms of Valence bond and Crystal Field theories. Taube's classification of complexes as labile and inert complexes. Dissociative (D) and Dissociative interchange Mechanism (Id) & Associative (A) and Associative interchange Mechanism (Ia). Substitution reactions in octahedral complexes- Acid Hydrolysis -factors affecting Acid Hydrolysis - Base Hydrolysis-conjugate Base Mechanisms - Anation Reactions -Substitution Reactions in Square Planar complexes- Trans effect – Mechanisms of Trans effect: polarization and π -bonding theories. Electron Transfer Reaction-Inner Sphere and outer Sphere Mechanisms- Marcus theory.

UNIT-IV: METAL π COMPLEXES-I

15 Hrs

Nature of π bonding, Classification of π ligands, π donor ligands and π -acceptor ligands.

Metal Carbonyls: Synthesis of metal carbonyls, Structures of metal carbonyls of the types $M(CO)_n$ ($M = Cr, Fe, Ni; n=4-6$), $M_2(CO)_n$ ($M=Co, Fe, Mn; n=8-10$), $M_3(CO)_n$ ($M=Fe, Ru$ and Os), $M_4(CO)_n$ ($M=Co, Rh, Ir$). IR Spectra of metal carbonyls (i) Detection of bridging and terminal CO ligand, (ii) Synergistic effect, EAN and 18-electron rule. Electron counting methods (i) Oxidation state method and (ii) Neutral Atom method.

Metal Nitrosyls: Synthesis of metal Nitrosyls, bonding, Electron donation by nitric oxide, Models for NO bonding (i) Covalent model and (ii) Ionic models, Structures of metal nitrosyls (1) $[Fe_4S_3(NO)]$ (2) $[Fe_2(NO)_2I_2]$ (3) $[(\phi_3P)_2Ir(CO)Cl(NO)]^+$ (4) $[(\phi_3P)_2Ru(NO)_2Cl]$, Detection of bridging NO ligand, Applications of metal nitrosyls.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John Wiley & sons. Inc., New York.
2. James E. Huheey, Inorganic chemistry- Principles of structure and reactivity, VI Edition 1993. Harper Collins College Publishers, New York.
3. J.D.Lee: Concise Inorganic Chemistry (Blackwell)
4. Gary Wolfsburg: Inorganic Chemistry (5th Ed. (Viva Books)
5. W.L.Jolly: Modern Inorganic Chemistry (McGraw-Hill)
6. B.N Figgis: Introduction to Ligand Fields (John-Wiley)
7. S.F.A.Kettle: Coordination compounds.
8. Coordination Chemistry. Bassalo & Jahnson.

CHE 102- CORE THEORY: - ORGANIC CHEMISTRY-I

UNIT-I: Stereochemistry

15 Hrs

Stereoisomerism-Stereoisomers Classification – Configuration and conformation.

Molecular Three dimensional representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions.

Molecular Symmetry & Chirality: Symmetry operations and symmetry elements (C_n & S_n). Criteria for Chirality. Dissymmetrization.

Optical isomerism: Molecular Symmetry and Chirality-Cahn-Ingold-Prelog rules R, S-nomenclature, stereoisomerism resulting from more than one chiral center, meso and pseudoasymmetric compounds - **Axial Chirality** - Stereochemistry of allenes spiranes - biphenyl derivatives and atropisomerism - **Planar chirality** - Ansa compounds and trans - Cycloalkenes - **Helicity.** Helically chiral compounds

Geometrical isomerism - E, Z - nomenclature - Physical and Chemical methods of determining the configuration of geometrical isomers-Stereoisomerism in 3, 4 and 5-membered cyclic compounds.

UNIT-II: Substitution Reactions

15 Hrs

i) Aliphatic Nucleophilic substitutions: The S_N2 , S_N1 , mixed S_N1 and S_N2 , SET mechanisms. Reactivity-effects of substrates, attacking nucleophiles, leaving groups and reaction medium. Common carbocation rearrangements – primary, secondary and tertiary. The neighbouring group participation (NGP) -anchimeric assistance, NGP by σ and π - bonds, phenonium ions, norbornyl and norbornenyl systems, Classical and nonclassical carbocations, NGP by halogens and heteroatoms (O,N,S) The S_N1 and S_N2' mechanisms. Nucleophilic substitution at an allylic, and vinylic carbons.

ii. Aromatic Nucleophilic Substitution: The S_NAr , S_N1 , benzyne and $S_{RN}1$ mechanisms. Reactivity - effect of substrate, structure, leaving group and attacking nucleophile. The von Richter, Sommelet - Hauser and Smiles rearrangements.

UNIT-III: Reactive intermediates

15 Hrs

Types of reactions, types of bond cleavage mechanisms, generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Thermodynamic and kinetic requirements, kinetic and thermodynamic control, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects.

UNIT-IV: Terpenoids

15 Hrs

Classification of terpenoids, occurrence, isolation, general methods of structure determination. Isoprene and special isoprene rule. Structure determination and synthesis of the following representative molecules: Farnesol, Zingiberine, Cadinene and Abietic acid.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J Sundberg, Plenum.
3. Structure and Mechanism in Organic Chemistry C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Principles of Organic Synthesis, R.O.C Norman and J. M. Coxon, Blackie Academic.
7. Stereochemistry, P.S.Kalsi, Wiley Eastern.
8. Text book of Organic Chemistry, M.C. Murry
9. Organic Chemistry, Vol I, I.L.Finar, ELBS Eds.

CHE : 103 A : COMPULSARY FOUNDATION : PHYSICAL CHEMISTRY- I

UNIT-I : Quantum Chemistry-I

15 Hrs

(A) Introduction to Exact Quantum Mechanical Results

Comparison of Classical and Quantum mechanics, Operator algebra, Eigen values and Eigen functions, Operators for momentum and energy, Degeneracy, Linear combination of Eigen functions of an operator, well behaved wave functions, Normalized and orthogonal functions, The schrodinger wave equation and the postulates of Quantum Mechanics, **Applications of Schrodinger wave equation:** Particle in one dimensional and three dimensional box, harmonic oscillator, rigid rotor, hydrogen atom and its applications. Hydrogen like wave function, hydrogen like orbitals and their representation, polar plots, contour plots and boundary diagram.

. **Approximate Methods:** The variation Theorem, Linear variation principle, perturbation Theory (first Order and non-degenerate), Application of variation Method and perturbation theory to the helium atom, The Born-Oppenheimer approximation.

UNIT-II: Chemical Dynamics

15 Hrs

(A) **Theories of reaction rates:** Collision theory, steric factor. Theory of Absolute Reaction Rates-Reaction coordinate, activated complex and the transition state. Thermodynamic formulation of reaction rates.

(B) Unimolecular reactions: Lindemann, Lindemann-Hinshelwood, and RRKM theories. Termolecular reactions. Complex reactions-Rate expressions for opposing, parallel and consecutive reaction (all first order type)

(C) Chain reactions: Dynamic chain, hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane, photochemical reactions- $\text{H}_2\text{-Br}_2$, $\text{H}_2\text{-Cl}_2$ reactions, Autocatalysis, $\text{H}_2\text{-O}_2$ reaction explosion limits.

(D) Fast Reactions: Flow system – Temperature and pressure Jump Methods – Relaxation Techniques.

UNIT – III : Thermodynamics

15 Hrs

(A) Brief review of Thermodynamic concepts: Enthalpy, Concept of Entropy – Entropy as a state function – Entropy change in reversible process and irreversible process – Temperature – Entropy diagrams – Entropy change and phase change – Entropy of mixing – Entropy and disorder. Free energy and Gibbs – Helmholtz equation. Chemical Potential and Gibbs – Duhem equation.

(B) Statistical thermodynamics: Partial molar properties: their significance and determination of partial molar properties, fugacity and its determination. Concept of distribution, thermodynamic probability and most probable Distribution, Ensemble averaging, postulates of ensemble averaging, canonical, grand canonical and micro-canonical ensembles, partition functions, translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions, Entropy of monatomic gases (Sackur-Tetrad equation)

UNIT-IV : Electrochemistry I

15 Hrs

(A) Thermodynamic and Kinetic concept of Electrochemistry

Thermodynamic and Kinetic Derivation of Nernst Equation, Chemical and Concentration Cells with and without Transference, Liquid Junction Potential, Derivation of the Expression for Liquid Junction Potentials-its determination and elimination, Applications of EMF Measurements: (i) Solubility product, (ii) pH Determination, (iii) Potentiometric Titrations. ;

(B) Conductivity

Theory of Electrolytic Conductance, Derivation of Debye-Huckel Equation and its Verification, Debye-Huckel Effect, and Wien Effect, Kohlrausch law. Calculation of Solubility of Sparingly soluble Salt from Conductance Measurements.

Conductometric Titrations : Titration of Strong Acid Vs Strong Base (HCl vs NaOH) ; Titration of Weak Acid Vs Strong Base (AcOH vs NaOH); Titration of mixture of Strong and Weak Acids vs Strong Base ; Precipitation Titrations.

Books Suggested

1. physical chemistry, P. W. Atkins (ELBS)
2. Introduction to quantum chemistry, A. K. Chandra (Tata McGraw Hill)
3. Quantum Chemistry, Ira N. Levine (Prentice Hall)
4. Atomic Structure and Chemical bond, Manas Chandra.
5. Chemical Kinetics, K.J. Laidler (Mc Graw Hill)
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose (McMillan)
7. Thermodynamics for chemists, S. Glasstone
8. Chemical thermodynamics, I.M. Klotz
9. Statistical Thermodynamics, M. Dole
10. Modern Electrochemistry, Vol. I & II, J.O. M. Bockris and A.K.N.Reddy (plenum)
11. An Introduction to Electrochemistry (3rd ed.), S. Glasstone (Affiliated East-West)

CHE : 103 B : CHEMISTRY OF NANOMATERIALS AND FUNCTIONAL MATERIALS

UNIT-I: Fundamental Principles. Definitions and Classification of functional nanomaterials. Historical development. Size & Scale, Units, Scaling Laws, Atoms, Molecules, & Clusters, Supramolecules. Nanoscale Phenomena, Tunneling, Chemical Bonds (types and strength), Intermolecular Forces, Molecular and Crystalline Structures, Hierarchical Structures and Functionality, Surfaces and Interfaces, Bulk to Surface transition, Self-Assembly and surface reconstruction.

UNIT-II: Properties and characterization of NanoMaterials. Size dependence of properties, Phenomena and Properties at Nanoscale, Brief introduction to calculational approaches, Mechanical / Frictional, Optical, Electrical Transport, Magnetic properties. Electron Microscopy, Scanning Probe Microscopies, Near field microscopy, Micro- and near field Raman spectroscopy, Surface-enhanced Raman spectroscopy, X-ray photoelectron spectroscopy

UNIT-III: Synthesis of Nanomaterials. Fabrication techniques: Self-Assembly, Self-Replication, Sol-Gels, Langmuir-Blodgett thin films, Nanolithography, Bio-inspired syntheses, Microfluidic processes, Chemical Vapor Deposition, Metals Colloidal gold, Silver and other metals clusters, Semiconductors, Cadmium Sulfide, silicon, Fullerenes / Carbon nanotubes, Nano-composites, Nanoporous Materials, Biological Materials. Applications of Nanomaterials. Nanoelectronics, Nanosensors, Environmental Biological, Energy storage and fuel cells

UNIT-IV: Overview of inorganic functional materials, their properties and applications. Introduction to solid state chemistry. Crystal structure and amorphous materials. Defects and non-stoichiometric solid solutions. Band theory and electronic conductivity. Synthesis and processing of inorganic materials. Properties of inorganic materials: superconductivity, magnetic, dielectric and optical properties

Books Suggested:

1. Nanomaterials- Synthesis, Properties and Applications, Edited by A.S. Edelstein and R.C. Cammarata, Institute of Physics Publishing, London, 1998.
2. Handbook of Nanostructured Materials and Nanotechnology, Edited by H.S. Nalwa Vols. 1-5, Academic Press (2000).
3. Science of Fullerenes and Nanotubes, by M.S. Dresselhaus, G. Dresselhaus and P.Eklund, Academic Press (1996).
4. Nanostructured Carbon for Advanced Applications, Edited by G. Benedek et al, Kluwer Academic Publishers (2001).

CHE : 104 A : ELECTIVE FOUNDATION: GENERAL CHEMISTRY-I

UNIT-I: TREATMENT OF ANALYTICAL DATA

15 Hrs

Precision and accuracy –mean and median values –Standard deviation – coefficient of variation, Types of errors: Determinate and indeterminate errors, confidence limits, significant figures, minimization of errors, statistical evaluation of data –T-test ,F- test , and X^2 –test. Correlation coefficient and coefficient of determination; Limit of detection (LOQ) ; Limit of determination(LOD) Sensitivity and selectivity of an analytical method.

UNIT-II: FLAME EMISSION AND ATOMIC ABSORPTION SPECTROSCOPY

15 Hrs

(a) **Flame Emission Spectroscopy:** Principles, chemical reactions in flames, Interferences, evaluation methods, flame photometer and experimental technique, procedure for determinations, limitations and disadvantages. Applications

(b)**Atomic Absorption Spectroscopy: Flame AAS:** Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences- Physical, Chemical, spectral and back ground correction, and methods of minimization

GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT-III:ECOSYSTEMS

15 Hrs

Concept of an ecosystem (Abiotic and biotic environment), structure and function of an ecosystem Producers, Consumers and decomposers. Energy flow in the ecosystem, (Nutrient cycle in the ecosystem) Ecological succession Food Chain, food webs and ecological pyramids. Introduction, types, characteristic features, structure and function of the following cosystems, Forest ecosystem, Grassl and ecosystem, Desert ecosystems aquatic ecosystems [ponds, streams, lakes, rivers, ocean estuaries].

UNIT-IV: ENVIRONMENTAL POLLUTION

15 Hrs

Definition a) Air pollution b) Water pollution c) Soil pollution d) Marine pollution e) Noise pollution f) Thermal pollution g) Nuclear pollution Solid waste management : Causes, effects and control measures of urban and industrial wastes. Environmental impact assessment.

Books Suggested

1. H.W.Willard, LL.Merritt and J.A.Dean: Instrumental Methods of Analysis
2. Vogel's Text book of Quantitative Inorganic Analysis.
3. Analytical Chemistry
4. Instrumental Methods of Analysis H.Kaur
5. Environmental Chemistry B.K. Sharma

CHE : 104 B : GREEN CHEMISTRY

UNIT-I

Fundamentals and significance of Green Chemistry: Discussion of the current state of chemistry and the environment and the definition of green chemistry. Assessment of the impact of chemistry in the environment and definition of risk hazard. An introduction to the tools of green chemistry and its fundamental principles.

Principles of Green Chemistry: Prevention of waste / by-products , Hazardous products- Designing of safer chemicals- Selection of appropriate solvents and starting materials- Use of protecting groups and catalysis- Designing of biodegradable products.

UNIT-II

Catalysis for Green Chemistry: Use of biocatalysts- Biochemical Oxidation, Biochemical Reduction, Enzyme Catalyzed Hydrolytic Process, Modified biocatalysis- transition metal catalysis- Reformatsky reaction, Wurtz reaction, Pinacol coupling, Simmons-Smith reaction, Mukaiyama reaction, Heck reaction, Ullmann's coupling.

UNIT-III

Solvent Free Reactions: Solvent free techniques- Reactions on solid mineral supports, Phase Transfer Catalysis- C-alkylation, N-alkylation, S-alkylation, Darzen's reaction, Wittig reaction. Ultrasound assisted green synthesis- Oxidation, Reduction, Hydroboration, Bouveault reaction, Strecker reaction, Microwave assisted green synthesis- Biginelli reaction, Aza-Michael reaction, Suzuki reaction, Stille reaction, Sonogashira reaction.

UNIT-IV

Ionic liquids: Definition- Types of Ionic Liquids-Synthesis of Ionic Liquids- Selection of ionic liquids- physical properties- Application in organic synthesis- alkylation, allylation, oxidation, reduction, polymerization, hydrogenation, hydroformylation, alkoxycarbonylation, carbon-carbon bond forming reactions, alkene metathesis.

Books suggested:

1. New Trends in Green Chemistry by V.K. Ahluwalia, M. Kidwai.
2. Green Chemistry: Environment Friendly Alternatives by Rashmi Sanghi, M M Srivastava
3. Green Solvents for Organic Synthesis by V.K. Ahluwalia, Rajender S. Varma
4. Green Analytical Chemistry by Mihkel Koel and Mihkel Kaljurand

FIRST SEMESTER PRACTICALS

CHE : 105 A : PRACTICAL - 1: INORGANIC CHEMISTRY

Semi Micro Qualitative Analysis:

Qualitative Analysis of a mixture containing four cations including two less common cations (viz., W, Mo, Se, Te, V, Ce, Th, Zr, Li and U).

CHE : 105 B : PRACTICAL – 1 : PHYSICAL CHEMISTRY

1. Calibration of volumetric apparatus and statistical analysis of the data.
2. Determination of critical solution temperature of phenol-water system and study the effect of electrolyte on CST.
3. Determination of Eutectic composition and temperature of binary system
4. Determination of distribution coefficient of benzoic acid between water and benzene.
5. Study the adsorption of acetic acid on charcoal and analysis of the data on the basis of Langmuir and Freundlich adsorption isotherms.
6. Determination of rate constant of acid hydrolysis of an ester and investigate the effect of catalyst concentration, reactant concentration and temperature.

CHE : 106 A : PRACTICAL – II : ORGANIC CHEMISTRY

Identification of single organic component by systematic qualitative analysis.

CHE : 106 B : PRACTICAL – II : GENERAL CHEMISTRY

Single step preparations

1. Preparation of aspirin
2. Preparation of p-nitroacetanilide
3. Preparation of p-bromoacetanilide

CHE : 107: (AUDIT COURSE) : HUMAN VALUES AND PROFESSIONAL ETHICS – I

Chapter I: Definition and Nature of Ethics – Its relation to Religion, Politics, Business, Law, Medicine and Environment. Need and Importance of Professional Ethics – Goals – Ethical Values in Various Professions.

Chapter II: Nature of Values – Good and Bad, Ends and Means, Actual and Potential Values, Objective and Subjective Values, Analysis of Basic Moral Concepts – Right, Ought, Duty, Obligation, Justice, Responsibility and Freedom, Good Behavior and Respect for Elders, Character and Conduct.

Chapter III: Individual and Society: Ahimsa (Non-Violence), Satya (Truth), Brahmacharya (Celibacy), Asteya (Non Possession) and Aparigraha (Non-stealing). Purusharthas (Cardinal virtues) - Dharma (Righteousness), Artha (Wealth), Kama (Fulfillment Bodily Desires), Moksha (Liberation), Crime and Theories of Punishment – (a) Reformatory, Retributive and Deterrent, (b) Views on Manu and Yajñavalkya

Chapter IV: Bhagavad Gita – (a) Niskama Karma, (b) Buddhism – The Four Noble Truths – Arya ashtanga marga, (c) Jainism - Mahavratas and Anuvratas. Values Embedded in Various Religions, Religious Tolerance, Gandhian Ethics.

Books for study:

1. John S Mackenzie: A Manual of ethics
2. “The Ethics of Management” by Larue Tone Hosmer, Richard D. Irwin Inc.
3. Management Ethics – Integrity at work by Joseph A. Petrick and John F. Quinn, Response Books, New Delhi.
4. “Ethics in Management” by S.A. Shelekar, Himalaya Publishing House.
5. Harold H. Titus: Ethics for Today
6. Maitra, S.K: Hindu Ethics
7. William Lilly: Introduction to Ethics
8. Sinha: A Manual of Ethics
9. Manu: Manava Dharma Sastra or the Institute of Manu: Comprising the Indian System of Duties: Religious and Civil (ed) G.C. Haughton.
10. Sasruta Samhita: Tr. KavirajKunjanlal, KunjanlalBrishagratha, Chowkamba Sanskrit Series, Vol I,II and III, Varanasi, Vol I PP, 16-20, 21-32 and 74-77 only.
11. Charaka Samhita: Tr. Dr. Ram Karan Sarma and Vaidya Bhagavan Dash, Chowkambha Sanskrit Series Office. Varanasi I, II, III Vol I PP 183-191.
12. Ethics, Theory and Contemporary Issues. Barbara Mackinnon, Wadsworth/Thomson Learning, 2001.
13. Analyzing Moral Issues, Judith A. Boss, Mayfield Publishing Company, 1999.
14. An Introduction to Applied Ethics (Ed.) John H. Piet and Ayodya Prasad, Cosmo Publications.
15. Text Book for Intermediate First Year Ethics and Human Values, Board of Intermediate Education – Telugu Academy, Hyderabad.
16. I.C. Sharma Ethical Philosophy of India. Nagin& Co Julundhar.

M.Sc., CHEMISTRY
SECOND SEMESTER

(NEP – 2020 CBCS syllabus of the students admitted from 2021-22)

CHE : 201 : CORE THEORY: INORGANIC CHEMISTRY-II

UNIT – I: TRANSITION METAL II – COMPLEXES -II

15 Hrs

Transition metal π – complexes with unsaturated organic molecules – alkenes, alkynes, diene, dienyl and Cyclopentadienyl complexes and arene complexes-general methods of preparation, properties, nature of bonding and structural features – Important reactions relating to Nucleophilic and Electrophilic attack on ligands and to organic synthesis.

UNIT – II: ELECTRONIC SPECTRA OF COMPLEXES

15 Hrs

Russel-Saunders coupling – Spectroscopic term symbols- Derivation of term symbols of p^2 and d^2 configuration, Hole Formulation, Energy ordering of terms (Hund's Rules), Splitting of energy levels and spectroscopic states in Octahedral field, Selection rules – Break – down of selection rules

Orgel diagrams, Definition and utility–Orgel Diagrams for d^1 to d^9 configurations in Octahedral and tetrahedral fields. Interpretation of electronic spectra of high spin octahedral and tetrahedral complexes of Ti(III), V(III), Cr(III), Mn(III), Mn(II), Fe(II), Fe(III), Co(III), Co(II), Ni(II) and Cu(II) complexes, Calculation of Dq and B^1 parameters for Cr(III) and Ni(II) complexes.

Tanabe – Sugano diagrams, Differences between Orgel diagrams and Tanabe – Sugano diagrams, Tanabe – Sugano diagrams of d^2 to d^6 and d^8 configurations. Charge transfer spectra- LMCT and MLCT.

UNIT – III: MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES

15 Hrs

Diamagnetism and paramagnetism-orbital and spin contributions, spin-orbit coupling, Hund's third rule and Energies of J levels – Curie law and Curie – Weiss law- Ferromagnetism and antiferromagnetism – Temperature independent magnetism Magnetic susceptibility and its determination by Gouy's and Faraday methods.

Calculation of magnetic moment from magnetic susceptibility, spin-only formula, Orbital contribution to magnetic moment (Oh and Td Complexes) –Paramagnetism and crystalline fields – Ti (III), V (III), VO^{2+} , Cr (III), Mn (II), Fe (III), Co(II), Ni (II) and Cu (II). Magnetic Exchange in copper acetate and other dimmers – spin cross over in complexes.

UNIT –IV: CATALYSIS

15 Hrs

Homogeneous catalysis, Metal ion catalyzed reactions – Redox potentials and processes –

Mechanism of redox processes involving ligands – Factors affecting redox potentials - other types of metal catalyzed reactions – Reactions involving Ag (I) , Cu (II) and Os (VIII) – Reactions of Oxyanions – Factors affecting rate (General discussion only) – Induced reactions – Free radical reactions – Thermal decomposition of peroxy disulphate – Fe(III) – S_2O_8 reactions – chain reactions – H-Br reactions, H_2O_2 – S_2O_8 reactions.

Books Suggested

1. Inorganic Chemistry principles of Structure and Reactivity 6th Edition. James E. Huheey.
2. Organometallic Chemistry: R.C.Mehrotra and Singh.
3. R. S. Drago: Structural methods in Inorganic Chemistry.
4. H. H. Willard, L. L. Merritt, Jr., J. A. Dean and F. A. Settle, Jr.: Instrumental Methods of Analysis (CBS Publishers).
5. R. L. Carlin: Magnetic Chemistry. R. L. Datta and A. Syamal: Elements of Magnetic Chemistry.

CHE : 202 : CORE THEORY: ORGANIC CHEMISTRY-II

UNIT-I: Reaction mechanism-I

15 Hrs

Electrophilic addition to carbon carbon double bond: Stereoselective addition to carbon carbon double bond; anti addition- Bromination and epoxidation followed by ring opening. Syn addition of OsO_4 and $KMnO_4$. Elimination reactions Elimination reactions E_2 , E_1 , E_{1CB} mechanisms. Orientation and stereoselectivity in E_2 eliminations. Pyrolytic syn elimination and α -elimination, elimination Vs substitution. Factors influencing the elimination reactions Determination of reaction mechanism: Determination of reaction mechanism: Energy profiles of addition and elimination reactions, transition states, product isolation and structure of intermediates, use of isotopes, chemical trapping, crossover experiments. Use of IR and NMR in the investigation of reaction mechanism.

UNIT-II: Molecular Rearrangements:**15 Hrs**

Rearrangements to electron deficient Carbon atom:

Pinacol-Pinacolone, Wagner-Meerwein, Dienone-Phenol and Demjoneve Rearrangements

Rearrangements to electron deficient Nitrogen atom:

Hofmann, Curtius, Schmidt and Beckmann Rearrangements.

Rearrangements to electron deficient Oxygen atom: Baeyer-Villiger and Dakins Rearrangements

Rearrangements to electron rich Carbon atom: Favorski and Neber Rearrangements

Aromatic and Sigmatropic Rearrangements: Fries and Claisen Rearrangements

UNIT III: Three and four membered heterocycles:**15 Hrs**

Systematic nomenclature (Hantzsch-Widmann system) and Replacement nomenclature for monocyclic heterocycles (Three and four membered rings). Synthesis and chemical reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes, and thietanes.

UNIT-IV: Alkaloids**15 Hrs**

Occurrence, isolation, general methods of structure elucidation and physiological action, degradation, classification based on nitrogen heterocyclic ring, structure elucidation and synthesis of the following: Atropine, Papaverine and Quinine.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J Sundberg, Plenum.
3. Structure and Mechanism in Organic Chemistry C.K.Inglod, Cornell University Press.
4. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
5. Modern Organic Reactions, H.O. House, Benjamin.
6. Principles of Organic Synthesis, R.O.C Norman and J. M. Coxon, Blackie Academic.
7. Stereochemistry, P.S.Kalsi, Wiley Eastern.
8. Text book of Organic Chemistry, M.C. Murry
9. Text book of Organic Chemistry, Fessendon and Fessendon.
10. Text book of Organic Chemistry, T.W. Solomon,
11. Organic Chemistry, Vol II, I.L.Finar, ELBS Eds.
12. Heterocyclic chemistry T.L Gilchrist, Longman Scientific Technical
13. An Introduction to the Heterocyclic compounds, R M Acheson, John Wiley.

CHE : 203 A : COMPULSARY FOUNDATION : PHYSICAL CHEMISTRY-II**UNIT-I: Quantum Chemistry-II****15 Hrs**

(A) **Angular momentum:** Importance of Angular momentum, Rotations and angular momentum, Eigen functions and Eigen values of angular momentum, Ladder operator, addition of angular momenta, spin, antisymmetry and pauli Exclusion principle. Anti symmetry of the molecule, Slater determinant. ;

(B) **Molecular Orbital Theory**

Atomic Orbitals, Simple Molecular Orbitals, Hybrid Atomic Orbitals, Shapes and energies of Molecular Orbital, Systems of Organic Molecules (Ex: Methane, Ethylene, Acetylene). Huckel theory of conjugated systems, π -bond order and charge density calculations, application of Huckel theory to ethylene, butadiene and benzene.

UNIT-II: Surface Chemistry**15 Hrs**

Surface tension, capillary action, pressure difference across curved surface, (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET adsorption isotherm, derivation of BET equation, limitations of BET equation, estimation of surface area from BET equation, Surface films on liquids. Concept of electric double layer model- Helmholtz perrin, Gouy- Chapman and stern models (no derivation)

Micells: Surface active agents, classification of surface active agents micellisation, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, thermodynamics of micellisation, emulsions, reverse micelles.

UNIT-III: SYMMETRY AND GROUP THEORY**15 Hrs**

Definition of a group, rules that are set for a group, sub-group, order of a group, Relation between order of a finite group and its sub-group, conjugacy relations and class of a group, symmetry elements and symmetry operation. Symmetry point group (MLS, MHS and MSS), Schoenflies symbols - Representation of groups by matrices, character of a representation, Determination of character of a group, group multiplication tables, reducible - irreducible representations The great orthogonality theorem (without proof) - character tables (H_2O, NH_3) and their use in spectroscopy, Mulliken character tables.

Irreversible Electrode phenomenon:

Reversibility and irreversibility, Dissolution and deposition potentials, Decomposition voltage, overvoltage, diffusion overvoltage, charge transfer overvoltage, concentration overvoltage-hydrogen and oxygen overvoltages, Tafel plots, Exchange current density and Transfer coefficient, Butler-Volmer equation for one electron transfer processes.

Polarography:

Theory, classification, principle, Instrumentation of Polarography, DME, HMDE diffusion current, Ilkovic equation, DC-Polarography, AC-Polarography, Controlled Potential Electrolysis, Millicoulometry, Equation for half-wave potentials, for reversible system when oxidant alone, reductant alone and both are present.

Books Suggested

1. P.W. Atkins: Physical Chemistry (ELBS).
2. A.K. Chandra: Introduction to quantum Chemistry (Tata Mc Graw Hill).
3. Ira N. Levine: Quantum Chemistry (Prentice Hall).
4. R. Mcweeny: Coulson's Valence (ELBS).
5. J.O.M. Bockris and A.K.N. Reddy, Modern Electrochemistry, vol. I & II (Plenum).
6. S. Glasstone; An Introduction to Electrochemistry (3rd ed.)(Affiliated East-West).
7. V. Moroi: Micelles, theoretical and applied aspects (Plenum).
8. S. Glasstone: A text Book of physical Chemistry (2nd Ed.) (Macmillan).
9. Maron and prutton: principles of physical Chemistry.
10. Silbey, Alberty, Bawendi. Physical Chemistry. Jhon-Wiley & Sons. 4th edition-2006.
11. V.S. Bagotsky. Fundamental of Electrochemistry. Jhon Wiley & sons. 2nd editions-2006.
12. Jack Simons. An Introduction to theoretical chemistry. The press Syndicate of the University of Cambridge.
13. D.N. Bajpai: Advanced physical Chemistry: S. Chand & Company, 1998.

CHE : 203 B : COMPULSARY FOUNDATION**ADVANCED THERMODYNAMICS AND BIOPHYSICAL CHEMISTRY****UNIT – I**

Protein structure- Primary structure of protein - secondary structure of protein - Tertiary structure of protein- Spectroscopic determination –Franck Condon principle- Electronic Spectroscopy-Absorption and fluorescence- Infrared spectroscopy of proteins.

UNIT – II

Forces in protein folding –Intermolecular interaction- Dipole- Dipole interactions – Hydrogen Bonding - Electrostatic forces –Hydrophobic effect- Protein denaturation- Protein folding pathway- Diffusion-langein equation and Brownian motion - Thermodynamics of protein unfolding.

UNIT – III

Thermodynamics and phase changes –Basic concepts of thermodynamics-First law, Second law and Third law of thermodynamics. Free energy and meaning of phase changes, calculation of phase equilibrium curves, Pressure as a measure of escaping tendency, one components phase diagrams, two component system, and three component systems.

UNIT –IV

Thermodynamics of living systems: Simultaneous coupled reactions, coupled reactions and metabolism free energy utilization, free energy utilization in metabolism, citric acid cycle, Terminal oxidation, Chain aerobic metabolism

Suggested Books

1. Richard E. Dickerson, molecular Thermodynamics
2. S. Glasstone, Theoretical Chemistry, Affiliated East-West Press Pvt. Ltd., New Delhi, 1973.
3. S. Glasstone, Thermodynamics for Chemists, Affiliated East-West Press Pvt. Ltd., New Delhi, 1964.
4. Upadhyay and Upadhyay- Biophysical chemistry.
5. P S Kalsi, Dr Nivedita Mahanta, Biophysical chemistry
6. Puri, Sharma and Pathania, Principles of Physical chemistry.
7. U.N Dash, A Text Book of Biophysical Chemistry, Macmillan India Ltd
8. Gurtu and Gurtu, Biophysical Chemistry, Pragati Prakashan.
9. C. Kalidas and M. V. Sangaranarayan, Non-Equilibrium Thermodynamics, Principles and Applications, McMillan India Ltd., 2002

CHE : 204 A : (ELECTIVE FOUNDATION) GENERAL CHEMISTRY-II

UNIT-I: ELECTRO ANALYTICAL METHODS

15 Hrs

Theory of potentiometry, calculation electrode potential at the equivalence. Finding of equivalence volume, derivative and linear titration plots. Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes, glass electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes, Amperometric titrations - Anodic stripping voltammetry, chronoamperometry, chronopotentiometry, Cyclic Voltammetry, Differential Pulse Polarography, linear sweep voltammetry, square wave voltammetry.

UNIT-II: CHROMATOGRAPHY

15 Hrs

General principles and classifications of chromatographic separations

Thin layer chromatography: Classification, principle, experimental technique, sample application, development of plate, retardation factor.

Gas liquid chromatography: Gas liquid chromatography - instrumentation (columns and detectors), retention time and retention volume. Chromatographic behaviour of solutes, column efficiency and resolution, column processes and band broadening, time of analysis and resolution, Van-Deemter equation.

High performance liquid chromatography: Theory and instrumentation- column performance, gradient elution, delivery system, sample introduction, separation columns, detectors and applications of HPLC.

Unit – III : Biodiversity

15 Hrs

Conservation introduction definition genetic species and ecosystem diversity, hot spots of biodiversity, threats to biodiversity habitat loss poaching of wildlife, man wildlife conflicts. Endangered and endemic species of India, conservation of biodiversity in – situ an ex-situ conservation of biodiversity.

Unit – IV Natural resources and non-renewable resources

15 Hrs

An overview of natural resources and associated problems with references to a) Forest resources b) Water resources c) Mineral resources d) Food resources e) Energy resources f) Land resources.

Books Suggested

1. H.W. Willard, LL. Merrit and J.A. Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (McGraw Hill).
5. D. Midgley and K. Torrance : potentiometric Water Analysis (John Wiley).
6. Silbey, Alberty, Bawendi. Physical chemistry. John-Wiley & sons. 4th edition-2006.

CHE : 204 B : (ELECTIVE FOUNDATION) CHEMISTRY IN CONTEMPORARY SOCIETY

UNIT – I : PHARMACEUTICALS

15 Hrs

Pharmaceuticals : Importance of quality control, drugs and pharmaceuticals, sources of impurities in pharmaceutical chemicals, analytical quality control in finished / final products, common methods of assay.

Common drugs and their uses: Analgesics – aspirin, paracetamol; Anthelmintics – mebendazole ; Antiallergies – chlorpheniramine maleate; Antibiotics-penicillin, chloramphenicol; Anti-inflammatory agents- oxyphenbutazone; **Antimalarials** – primaquine phosphate; Antituberculosists – INH; Narcotics – nicotine, morphine; Expectorants – Benadryl; Sedatives – diazepam; Vitamins – B₁, B₂, B₆, niacin and folic acid.

UNIT – II : FORENSIC AND BIOMEDICALS

15 Hrs

Body fluids: Composition and detection of abnormal level of certain constituents leading to diagnosis, sample collection and preservation of physiological fluids, analytical methods for the constituents of physiological fluids (blood, urine).

Blood: Estimation of glucose, cholesterol, urea, haemoglobin and bilirubin.

Urine: Urea, uric acid, creatinine, calcium phosphate, sodium, potassium and chloride.

Enzymes: Biological significance, assay of enzymes (pepsin, tyrosinase), vitamins (thiamine ascorbic acid, vitamin A) and hormones (progesterone, oxytocin, insulin), chemical, instrumental and biological assays to be discussed wherever necessary.

Forensic : General discussion of poisons with special reference to mode of action of cyanide organophosphates and snake venom, poisonous materials such as lead, mercury and arsenic in biological materials.

UNIT – III : FOOD AND BEVERAGES

15 Hrs

Milk and milk products : Composition, alcohol test, fermentation, dye reduction-methylene blue and resazurin tests, analysis of fat content, minerals in milk and butter, estimation of added water in milk.

Oils and fats: General composition of edible oils, detection of purity, tests for common edible oils and groundnut oil, cottonseed oil and mustard oil, tests for adulterants like argemone oil and mineral oils,

Beverages: Soft drinks, alcoholic drinks, tea, coffee and fruit juice, analysis of caffeine in coffee and tea, detection of chicory in coffee, chloral hydrate in toddy, food preservatives like benzoates, propionates, sorbates, bisulphites, artificial sweeteners, like saccharin, dulcin and sodium cyclamate, flavours – vanillin, esters (fruit flavours) and monosodium glutamate, artificial food colourants-coal tar dyes and non-permitted colours and metallic salts, control of food quality – codex alimentarices, Indian standards.

UNIT – IV : FUEL AND SOIL

15 Hrs

Fuels : Definition, classification and characteristics of fuels, sampling, determination of calorific value. Liquid fuels-determination of flash point, fire point, aniline point. Knocking of petrol and diesel – octane and cetane numbers carbon residue.

Gaseous fuels : Coal gas, waste gas, producer gas, gobar gas and blast furnace gas, calorific value determination by Junker's gas calorimeter, relative merits of solid, liquid and gaseous fuels.

Soil : Ingredients of soil-organic matter, nitrogen, sulphur, sodium, potassium and calcium, analysis of trace elements, copper, molybdenum, zinc and boron.

Reference Books :

1. Pharmaceutical Analysis, T. Higuchi and E.B. Hansen, John Wiley and Sons, New York.
2. Quantitative Analysis of drugs, P.D. Sethi, 3rd edition, CBS Publishers, New Delhi, 1997.
3. Practical Clinical biochemistry methods and interpretations, R. Chawala, J.P. Brothers Medical Publishers (P) Ltd., 1995.
4. Laboratory manual in biochemistry, J. Jayaraman. New Age International Publishers, New Delhi, 1981.

II SEMESTER PRACTICALS

CHE-205 A : PRACTICALS – I : INORGANIC CHEMISTRY

I . Quantitative Analysis:

Separation and determination of two component mixtures:

- (i) Separation of Al(III) and Determination of Fe (III)
- (ii) Separation of Cu(II) and Determination of Zn (II)
- (iii) Separation of Ca(II) and Determination of Mg (II)
- (iv) Separation of Cu(II) and Determination of Ni (II)
- (v) Determination of Ferrocyanide and Ferricyanide

CHE-205 B : PRACTICAL – I : PHYSICAL CHEMISTRY

1. Conductometry:
 - (a) Determination of cell constant
 - (b) Verification of Onsager equation
 - (c) Determination of dissociation constant of a weak acid
 - (d) Titration of a strong acid with a strong base
 - (e) Titration of a weak acid with a strong base
2. Potentiometry:
 - (a) Titration of a strong acid with a strong base
 - (b) Titration of a weak acid with a strong base
 - (c) Redox titration
3. Coulometry: Estimation of Manganese
4. pHmetry: Strong acid, Strong base titrations.

CHE-206 A : PRACTICAL – II : ORGANIC CHEMISTRY

Separation and Identification of two component organic mixture by systematic qualitative analysis.

CHE-206 B : PRACTICALS – II : GENERAL CHEMISTRY

Preparation of Metal Complexes:

- (i) Tetra(ammine) copper (II) sulphate.
- (ii) Mercury tetra(thiocyanato) cobaltate(II).
- (iii) Hexa(ammine) Nickel (II) chloride.
- (iv) Tris(acetylacetonato) Manganese (III) chloride.
- (v) Tris (ethylenediammine) Nickel (II) thiosulpha

CHE 207: (AUDIT COURSE) : Human Values and Professional Ethics – II

Chapter I: Value Education – Definition – Relevance to present day – Concept of human values - Self introspection – Self esteem. Family values-Components, Structure and responsibilities of family Neutralization of anger – Adjustability – Threats of family life – Status of women in family and society – Caring for needy and elderly – Time allotment for sharing ideas and concerns.

Chapter II: Medical ethics – Views of Charaka, Sushruta and Hippocrates on moral responsibility of medical practitioners. Code of ethics for medical and healthcare professionals. Euthanasia, Ethical obligation to animals, Ethical issues in relation to health care professionals and patients. Social justice in health care, human cloning, problem of abortion. Ethical issues in genetic engineering and Ethical issues raised by new biological technology or knowledge.

Chapter III: Social ethics – Organ trade, Human trafficking, Human rights violation and social disparities, Feminist ethics, Surrogacy/pregnancy. Ethics of media – Impact of Newspapers, Television, Movies and Internet, Business ethics – Ethical standards of business – Immoral and illegal practices and their solutions. Characteristics of ethical problems in management, ethical theories, causes of unethical behavior, Ethical abuses and work ethics.

Chapter IV: Environmental ethics – Ethical theory, man and nature - Ecological crisis, Pest control, Pollution and waste, Climate change, Energy and pollution, Justice and environmental health.

Books for study:

1. Johns S Mackenjie: A Manual of ethics
2. “The Ethics of Management” by Larue Tone Hosmer, Richard D. Irwin Inc.
3. Management Ethics – Integrity at work by Joseph A. Petrick and John F. Quinn, Response Books, New Delhi.
4. “Ethics in Management” by S.A. Shelekar, Himalaya Publishing House.
5. Harold H. Titus: Ethics for Today
6. Maitra, S.K: Hindu Ethics
7. William Lilly: Introduction to Ethics
8. Sinha: A Manual of Ethics
9. Manu: Manava Dharma Sastra or the Institute of Manu: Comprising the Indian System of Duties: Religious and Civil (ed) G.C. Haughton.
10. Sasruta Samhita: Tr. KavirajKunjanlal, KunjanlalBrishagratha, Chowkamba Sanskrit Series, Vol I,II and III, Varanasi, Vol I PP, 16-20, 21-32 and 74-77 only.
11. Charaka Samhita: Tr. Dr. Ram Karan Sarma and Vaidya Bhagavan Dash, Chowkambha Sanskrit Series Office. Varanasi I, II, III Vol I PP 183-191.
12. Ethics, Theory and Contemporary Issues. Barbara Mackinnon, Wadsworth/Thomson Learning, 2001.
13. Analyzing Moral Issues, Judith A. Boss, Mayfield Publishing Company, 1999.
14. An Introduction to Applied Ethics (Ed.) John H. Piet and Ayodya Prasad, Cosmo Publications.
15. Text Book for Intermediate First Year Ethics and Human Values, Board of Intermediate Education – Telugu Academy, Hyderabad.
16. I.C. Sharma Ethical Philosophy of India. Nagin& Co Julundhar.

III-SEMESTER
ANALYTICAL CHEMISTRY
(NEP -2020 CBCS syllabus effective from 2021-22)

CHE : AC : 301 (CORE-THEORY) : INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS

UNIT –I: THERMAL METHODS OF ANALYSIS

15 Hrs

Thermo gravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Different thermal analysis – principle, instrumentation, difference between TG and DTA, applications with special reference to the clays and minerals.

Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and perchlorates, ammonium nitrate.

UNIT –II: MOSSBAUER SPECTROSCOPY and NQR

15 Hrs

Mossbauer spectroscopy: Basic principles, Recoil energy, Doppler shift, Chemical shift, Quadrupole effects, Magnetic effects. Instrumentation, spectral parameters and spectrum display.

Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds, (2) Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: Basic principles of NQR spectroscopy, quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant and applications.

UNIT –III: ELECTRON SPIN RESONANCE SPECTROSCOPY

15 Hrs

Basic Principles, Hyper fine splitting, Factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, Hamiltonian and spin densities. Zero field splitting and Kramer's degeneracy, Relaxation process and line widths. Instrumentation and Applications. The EPR spectrum of bis(salicylidimine)-copper(II) complex, study of inorganic free radicals, biological applications of Electron Spin Resonance (Study of free radicals and Iron-sulfur proteins)

UNIT –IV: PHOTO ELECTRON SPECTROSCOPY

15 Hrs

Photoelectric effect, Koopmans's theorem, ionization energy.

X-ray photoelectron spectroscopy (ESCA): Principle, Binding energies, Chemical shift, Applications of XPES to Qualitative analysis, to surface studies and structural analysis.

Ultraviolet photoelectron spectroscopy- Principle, application of UPES in studying the molecular orbitals of O_2 and N_2 molecules.

Block diagram of photoelectron spectrophotometer. Sources of radiation, detectors.

Auger spectra – Principle, Applications of Auger spectra to surface studies and use of Auger spectra as a fingerprint tool.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John Wiley & sons. Inc., New York.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter: Inorganic Chemistry, Principles of Structure and Reactivity (4th Ed.) (Addison-Wesley)
3. Gary Wulfsberg: Inorganic Chemistry (5th Ed. (Viva Books)
4. J.D. Lee: Concise Inorganic Chemistry (Blackwell)
5. W.L. Jolly: Modern Inorganic Chemistry (McGraw-Hill)
6. R.L. Carlin: Magneto-chemistry (Springer-Verlag)
7. R.L. Dutta and A. Syamal: Elements of Magnetochemistry (Affiliate East-West).
8. K. Hussain Reddy – Text book of Bioinorganic chemistry.

CHE : AC : 302: (CORE-THEORY) ORGANIC SPECTROSCOPY AND APPLICATIONS

UNIT-I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

15Hrs

Various electronic transitions (185-800 nm), effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fisher-Woodward rules for conjugated

dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

UNIT – II: INFRARED SPECTROSCOPY

15Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance, FT-IR

UNIT –III: ¹H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ¹H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

¹³C NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimensional NMR spectroscopy-COSY.

UNIT-IV: MASS SPECTROMETRY

15Hrs

Introduction, ion production, type of ionization, EI, CI, FD, and FAB-factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular-ion peak, metastable peak, Mc. Lafferty rearrangement. Nitrogen rule, isotope labeling. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books suggested:

1. Organic spectroscopy, W. Kemp 5th Ed, ELBS
2. Spectroscopy of organic compounds, RM Silversteen and others, 5th Ed, John Wiley
3. Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.
4. NMR in chemistry-A multi nuclear introduction, William Kemp, Mc Millan, 1986.
Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi,

CHE : 303 (A): (GENERIC ELECTIVE) : ORGANIC CHEMISTRY - III

UNIT I: REAGENTS IN ORGANIC SYNTHESIS

15 Hrs

Use of the following reagents in organic synthesis: Anhydrous AlCl₃, Boran trifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexylcarbodiimide, Lead tetraacetate, Ziegler-Natta catalysts, DDQ, Dithianes, Merrifield resin.

UNIT-II: ORGANOMETALLIC REAGENTS

15 Hrs

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydroformylation reactions

UNIT III: ASYMMETRIC SYNTHESIS

15 Hrs

Topocity - Prochirality- Substrate selectivity - Diastereoselectivity and enantioselectivity-Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods-Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines – Stereoselective Diels-Alder reaction

Reagent controlled methods-Use of chiral reagents-Asymmetric oxidation-Sharpless epoxidation-Asymmetric reduction-Use of lithium aluminium hydride and borate reagents.

UNIT IV: METHODS OF ORGANIC SYNTHESIS

15 Hrs

- i. **Oxidations:** (a) Alcohols to carbonyls-Chromium (iv) oxidants-Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, oxidation with silver carbonate (b) Alkenes to epoxides-peroxide induced epoxidations. (c) Alkenes to diols-oxidation with potassium permanganate, osmium tetroxide, Prevost reaction (d) Ketones to esters-Bayer-Villiger oxidation (e)

- Oxidative bond cleavage-cleavage of alkenes by transition metals. (f) Oxidation of alkyl or alkenyl fragments-selenium dioxide and chromium trioxide oxidations.
- ii. **Reductions** : Reduction with lithium aluminium hydride, sodium borohydride, alkoxides, bis-methoxy ethoxy aluminium hydride, Boran aluminium hydride and derivatives-catalytic hydrogenation-dissolving metal reductions, Non-Metallic reducing agents including enzymatic and microbial reductions.

References Books:

1. Advanced Organic Chemistry-Reactions, 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.
4. Structure and Mechanism in Organic Chemistry, C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Name reactions and reagents in organic synthesis, B.P. Muway and M.G Ellord, John Wiley.
7. Modern Organic Reactions, H.O. House, Benjamin.
8. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, Blackie Academic & Professional.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Principles of organometallic chemistry, P. Powell, ELBS.
11. Organo transition metal chemistry-Applications to organic synthesis, S.G. Davis, Pergmon.
12. Stereochemistry to Organic Compounds, E.L. Eliel and others, John Wiley.
13. Stereochemistry to Organic Compounds, D. Nasipuri, New Age International.
14. Stereochemistry, P.S.Kalsi, Wiley Eastern.

CHE : 303 (B):GENERIC ELECTIVE; PHYSICAL CHEMISTRY - III

UNIT-I Applications of Group Theory

15 Hrs

Construction of reducible and irreducible representations, Determination of Character Co ordinate of C_{2v} point group based on 3N Co ordinates. Standard reduction formula, Determination of normal modes of vibrations of SO_2 , NH_3 , $POCl_3$, $PtCl_4^{2-} \cdot H_2O_2$ molecules. Mutual exclusion Principle, Direct Product, Accidental Degeneracy and Fermi resonance **Group Theory and Spectroscopy**: selection rules, symmetry Criteria for optical activity, symmetry restrictions on dipole moments, symmetry and stereo isomerism. Prediction of IR and Raman Spectral activity of H_2O , NH_3 and CO_2

UNIT-II: X-ray Diffraction:

15 Hrs

(A) Solid State Chemistry

Dislocation of Solids, Schottky and Frenkel defects, insulators, a, d semiconductors, Band theory of solids, solid state reactions.

(B) Bragg conditions-Miller Indices- Laue method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals. Index reflections, identification of unit cells from systematic absences in diffraction pattern- structure of simple lattices and X-ray intensities- structure factor and its relation to intensity and electron density- Description of procedure for X-ray structure analysis (NaCl and KCl)

(C) Electron Diffraction: Scattering intensity Vs scattering angle, Wierlequation, and its importance. Measurement techniques, Elucidation of structures of simple gas phase molecules, Low energy electron diffraction (LEED) for the study of surfaces.

UNIT-III: SPECTROSCOPY

15 Hrs

Microwave spectroscopy: classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, intensities- stark effect.

Infrared spectroscopy: Linear harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combinations bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.

Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, pure vibrational Raman spectroscopy, selection rules, mutual exclusion principle, resonance Raman spectroscopy and coherent antistokes Raman spectroscopy. Vibrational- rotational Raman spectroscopy.

UNIT-IV: POLYMER SOLUTIONS

15 Hrs

Thermodynamics of polymer dissolution, effect of molecular weight on solubility, solubility of crystalline and amorphous polymer, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins theory of polymer solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular weight determination by light scattering, ultra centrifugation and sedimentation equilibrium method. Liquid Crystals- synthesis and applications.

Books Suggested

1. F.A.Cotton : Introduction to Group theory for chemists.
2. George Davidson Elsevier : Introductory Group Theory for Chemists.
3. Gurdeep Raj , Ajay Bhagi&Vinod Jain : Group Theory and Symmetry in Chemistry
4. Instrumental methods of analysis – M.H.Willard, Meritt Jr. and J.A.Dean
5. Principles of instrumental analysis – Skoog and West
6. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
7. V. R. Gowariker, N. V. Viswanathan, JayadevSreedhar.: polymer Science. New Age international Publishers.

CHE : AC : 304: PRACTICALS (Core & Gen.) Classical Methods of Analysis.

I. Analysis of ores and alloys:

- a) Brass/Bronze
- b) Cement
- c) Ilmenite/Chalcopyrite
- d) Dolomite
- e) Copper and Nickel alloy

II. Water Analysis:

- a) Determination of dissolved Oxygen
- b) Determination of BOD of Waste water
- c) Determination of COD of Waste water
- d) Hardness of Water
- e) Chloride, sulphates, carbonates and bicarbonates.

CHE : AC : 305 (A) : (SKILL ORIENTED COURSE : THEORY) : CHEMOTHERAPY AND DRUG ANALYSIS

UNIT-I: Chemotherapy

Definition, History, and Evolution of Chemotherapy; Discovery, Classification, Nomenclature, Mode of action and synthesis of the following classes of compounds with special references to specific drugs mentioned under each class

- i) Sulfa drugs- Sulfanilamide and Sulfamethoxazole.
- ii) Antibacterials
 - a) Lactum group of antibiotics – Penicillin, Ampicillin and Amoxycillin.
 - b) Cephalosporin-C and Ciprofloxacin.
- iii) Anticancer drugs – 5-Fluorouracil, Methotrexate.
- iv) Antifungals – Griseofulvin
- v) Antimalarials – Chloroquin

UNIT-II: Chemical and Biochemical analysis of Drugs

Qualitative and Quantitative Analysis of drugs: Uses of IR, UV, GLC and HPLC methods.

Drug Assay by Biochemical Analysis – ELISA (Cortisol, alcohol, opiates).

RadioImmuno Assay (RIA) – Enalapril, Insulin

Kidney, Lungs and Liver function tests; Use of isotopes in the Bioanalysis of drugs and in drug design programmes.

Book Suggested

1. Medicinal Chemistry and Pharmaceutical Chemistry – Harikishan Singh and Kapur
2. Medicinal Chemistry and Biochemistry – R.L.Nath
3. Introduction to Medicinal Chemistry – Patrick
4. The Organic Chemistry of Drug Synthesis Vols. 1-6 - Ledneicer Top drugs top synthetic routes – John Saunders
5. Medicinal Chemistry – Ashutoshkar
6. Synthetic Organic Chemistry and Drugs – Gurideep R Chetwal
7. Biochemistry – Harper, Conn & Stumpf, Lehninger
8. Biochemistry – Western Jodd
9. Biochemistry – Cann & Stumpf

10. Bergers Medicinal Chemistry Vols. 1-5 – Manfred E. Wolf
11. Introduction to drug design – Siverman
12. Biochemical approach to Medicinal Chemistry – Thomas Nogrady
13. Principles of Medicinal chemistry – William Foye
14. Text book of organic medicinal and pharmaceutical chemistry – Delgrado and William A
15. Industrial Microbiology – Casida

CHE : AC 305 (B) : PRACTICALS (SKILL ORIENTED COURSE) : Instrumental methods of analysis

1. Colorimetric Determinations:
 - a. Determination of manganese
 - b. Determination of nickel
 - c. Determination of iron by 1,10 Phenanthroline
 - d. Determination of chromium
 - e. Determination of Phosphate
 - f. Determination of Pesticides
 - g. Determination of Nitrite.

CHE : AC : 306(A): (OPEN ELECTIVE) SPECTRAL TECHNIQUES

UNIT – I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY

15 Hrs

Various electronic transitions (185-800nm.), Beer-Lambert Law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds

UNIT – II : INFRARED SPECTROSCOPY

15 Hrs

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids and anhydrides. Effect of hydrogen bonding.

UNIT – III: ATOMIC ABSORPTION SPECTROSCOPY: FLAME AAS:

15 Hrs

Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences-Physical, Chemical, spectral and background correction, and methods of minimization
GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT –IV: MASS SPECTROMETRY

15 Hrs

Principle, instrumentation, different methods of ionization, EI, CI, FD and FAB, Mass spectra-molecular ion, base peak, meta-stable peak, nitrogen rule and McLafferty rearrangement. Mass spectral fragmentation of organic compounds and common functional groups. Normal and branched alkanes, alkenes, cycloalkanes, benzene and its derivatives, alcohols and phenols, ethers, aldehydes and ketones, carboxylic acids and their derivatives, amines and nitro compounds. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Organic spectroscopy, W.Kemp 5th Ed, ELBS .2.
2. Spectroscopy of organic compounds, RM Silverstein and others 5th Ed, John Wiley 1991
3. Spectroscopy of organic compounds, PS Kalsi, Wiley, 1993
4. NMR in chemistry – A Multi nuclear introduction, William Kemp, Mc Millan 1986
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemmi TMH . 2005

CHE : AC : 306(B): (OPEN ELECTIVE) CHROMATOGRAPHIC TECHNIQUES

Unit –I: Introduction - Classification of Chromatographic methods – Column chromatography-Adsorption phenomenon: Nature of adsorbents-Solvent systems-Differential migration-Separation of mixture of o-/p-nitro anilines (A demonstration experiment).

Unit –II: Thin-Layer Chromatography (TLC)-Coating materials and preparation of TLC plates- Solvents for development-Detection of compounds in TLC- R_f values in TLC-Applications of TLC in chemistry-Preparative TLC – Demonstration experiment in TLC.

Unit –III: High-Performance Liquid Chromatography (HPLC) - Application of HPLC- HPLC instrument- Stationary phases in HPLC-Normal and reversed phase HPLC: A comparison- Normal phase HPLC: Principle- Retention times in Normal and reversed phase HPLC- Reversed phase HPLC: Principle.

Unit –IV: Gas-Liquid Chromatography- Instruments for Gas-Liquid Chromatography- Gas-Chromatographic Columns and the Stationary Phase- Application of Gas-Liquid Chromatography- Gas-Solid Chromatography.

Reference Books:

1. Analytical chemistry: G L David Krupadanam, D.Vijaya prasad, K.Varaprasad Rao, KLN Reddy, C.Sudhakar.
2. . Analytical chemistry: Skoog West Holler.
3. Modern Analytical Chemistry : David Harvey DePauw University.
4. J.G.Dick. Analytical Chemistry, McGraw Hill, New Delhi, (1973).

III-SEMESTER
ENVIRONMENTAL CHEMISTRY
(NEP – 2020 CBCS syllabus effective from 2021-2022)

CHE : EC-301 (CORE-THEORY) : INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS

UNIT –I: THERMAL METHODS OF ANALYSIS

15 Hrs

Thermo gravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Different thermal analysis – principle, instrumentation, difference between TG and DTA, applications with special reference to the clays and minerals.

Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and perchlorates, ammonium nitrate.

UNIT –II: MOSSBAUER SPECTROSCOPY and NQR

15 Hrs

Mossbauer spectroscopy: Basic principles, Recoil energy, Doppler shift, Chemical shift, Quadrupole effects, Magnetic effects. Instrumentation, spectral parameters and spectrum display.

Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds, (2) Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: Basic principles of NQR spectroscopy, quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant and applications.

UNIT –III: ELECTRON SPIN RESONANCE SPECTROSCOPY

15 Hrs

Basic Principles, Hyper fine splitting, Factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, Hamiltonian and spin densities. Zero field splitting and Kramer's degeneracy, Relaxation process and line widths. Instrumentation and Applications. The EPR spectrum of bis(salicylidimine)-copper(II) complex, study of inorganic free radicals, biological applications of Electron Spin Resonance (Study of free radicals and Iron-sulfur proteins)

UNIT –IV: PHOTO ELECTRON SPECTROSCOPY

15 Hrs

Photoelectric effect, Koopmans's theorem, ionization energy.

X-ray photoelectron spectroscopy (ESCA): Principle, Binding energies, Chemical shift, Applications of XPS to Qualitative analysis, to surface studies and structural analysis.

Ultraviolet photoelectron spectroscopy- Principle, application of UPES in studying the molecular orbitals of O_2 and N_2 molecules.

Block diagram of photoelectron spectrophotometer. Sources of radiation, detectors.

Auger spectra – Principle, Applications of Auger spectra to surface studies and use of Auger spectra as a fingerprint tool.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John Wiley & sons. Inc., New York.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter: Inorganic Chemistry, Principles of Structure and Reactivity (4th Ed.) (Addison-Wesley)
3. Gary Wulfsberg: Inorganic Chemistry (5th Ed. (Viva Books)
4. J.D. Lee: Concise Inorganic Chemistry (Blackwell)
5. W.L. Jolly: Modern Inorganic Chemistry (McGraw-Hill)
6. R.L. Carlin: Magneto-chemistry (Springer-Verlag)
7. R.L. Dutta and A. Syamal: Elements of Magnetochemistry (Affiliate East-West).
8. K. Hussain Reddy – Text book of Bioinorganic chemistry

CHE : EC 302: (CORE THEORY) : ORGANIC SPECTROSCOPY AND APPLICATIONS

UNIT-I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

15Hrs

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

UNIT – II: INFRARED SPECTROSCOPY

15Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance, FT-IR

UNIT –III: ¹H NMR SPECTROSCOPY

15Hrs

Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ¹H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

¹³C NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimensional NMR spectroscopy-COSY.

UNIT-IV: MASS SPECTROMETRY

15Hrs

Introduction, ion production, type of ionization, EI, CI, FD, and FAB-factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular-ion peak, metastable peak, Mc. Lafferty rearrangement. Nitrogen rule, isotope labeling. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books suggested:

1. Organic spectroscopy, W. Kemp 5th Ed, ELBS
2. Spectroscopy of organic compounds, RM Silversteen and others, 5th Ed, John Wiley
3. Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.
4. NMR in chemistry-A multi nuclear introduction, William Kemp, Mc Millan, 1986.
5. Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi,

CHE : EC -303 (A): (GENERIC ELECTIVE) - ORGANIC CHEMISTRY - III

UNIT I: REAGENTS IN ORGANIC SYNTHESIS

15 Hrs

Use of the following reagents in organic synthesis: Anhydrous AlCl₃, Boran trifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexylcarbodiimide, Lead tetraacetate, Ziegler-Natta catalysts, DDQ, Dithianes, Merrifield resin.

UNIT-II: ORGANOMETALLIC REAGENTS

15 Hrs

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydroformylation reactions

UNIT III: ASYMMETRIC SYNTHESIS

15 Hrs

Topocity - Prochirality- Substrate selectivity - Diastereoselectivity and enantioselectivity-Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods-Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines – Stereoselective Diels-Alder reaction

Reagent controlled methods-Use of chiral reagents-Asymmetric oxidation-Sharpless epoxidation-Asymmetric reduction-Use of lithium aluminium hydride and borate reagents.

UNIT IV: METHODS OF ORGANIC SYNTHESIS

15 Hrs

- i. **Oxidations:** (a) Alcohols to carbonyls-Chromium (iv) oxidants-Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, oxidation with silver carbonate (b) Alkenes to epoxides-peroxide induced epoxidations. (c) Alkenes to diols-oxidation with potassium permanganate, osmium tetroxide, Prevost reaction (d) Ketones to esters-Bayer-Villiger oxidation (e)

- Oxidative bond cleavage-cleavage of alkenes by transition metals. (f) Oxidation of alkyl or alkenyl fragments-selenium dioxide and chromium trioxide oxidations.
- ii. **Reductions** : Reduction with lithium aluminium hydride, sodium borohydride, alkoxides, bis-methoxy ethoxy aluminium hydride, Boran aluminium hydride and derivatives-catalytic hydrogenation-dissolving metal reductions, Non-Metallic reducing agents including enzymatic and microbial reductions.

Books Suggested :

1. Advanced Organic Chemistry-Reactions, 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.
4. Structure and Mechanism in Organic Chemistry, C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Name reactions and reagents in organic synthesis, B.P. Muway and M.G Ellord, John Wiley.
7. Modern Organic Reactions, H.O. House, Benjamin.
8. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, Blackie Academic & Professional.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Principles of organometallic chemistry, P. Powell, ELBS.
11. Organo transition metal chemistry-Applications to organic synthesis, S.G. Davis, Pergmon.
12. Stereochemistry to Organic Compounds, E.L. Eliel and others, John Wiley.
13. Stereochemistry to Organic Compounds, D. Nasipuri, New Age International.
14. Stereochemistry, P.S.Kalsi, Wiley Eastern.

CHE : EC : 303 (B): (GENERIC ELECTIVE) : PHYSICAL CHEMISTRY - III

UNIT-I Applications of Group Theory

15 Hrs

Construction of reducible and irreducible representations, Determination of Character Co ordinate of C_{2v} point group based on 3N Co ordinates. Standard reduction formula, Determination of normal modes of vibrations of SO_2 , NH_3 , $POCl_3$, $PtCl_4^{2-} \cdot H_2O_2$ molecules. Mutual exclusion Principle, Direct Product, Accidental Degeneracy and Fermi resonance **Group Theory and Spectroscopy**: selection rules, symmetry Criteria for optical activity, symmetry restrictions on dipole moments, symmetry and stereo isomerism. Prediction of IR and Raman Spectral activity of H_2O , NH_3 and CO_2

UNIT-II: X-ray Diffraction:

15 Hrs

(a) Solid State Chemistry

Dislocation of Solids, Schottky and Frenkel defects, insulators, a, d semiconductors, Band theory of solids, solid state reactions.

(b) Bragg conditions-Miller Indices- Laue method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals. Index reflections, identification of unit cells from systematic absences in diffraction pattern-structure of simple lattices and X-ray intensities- structure factor and its relation to intensity and electron density- Description of procedure for X-ray structure analysis ($NaCl$ and KCl)

(c) Electron Diffraction: Scattering intensity Vs scattering angle, Wierlequation, and its importance. Measurement techniques, Elucidation of structures of simple gas phase molecules, Low energy electron diffraction (LEED) for the study of surfaces.

UNIT-III: SPECTROSCOPY

15 Hrs

Microwave spectroscopy: classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, intensities- stark effect.

Infrared spectroscopy: Linear harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combinations bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.

Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, pure vibrational Raman spectroscopy, selection rules, mutual exclusion principle, resonance Raman spectroscopy and coherent antistokes Raman spectroscopy. Vibrational- rotational Raman spectroscopy.

UNIT-IV: POLYMER SOLUTIONS

15 Hrs

Thermodynamics of polymer dissolution, effect of molecular weight on solubility, solubility of crystalline and amorphous polymer, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins theory of polymer solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular weight determination by light scattering, ultra centrifugation and sedimentation equilibrium method. Liquid Crystals- synthesis and applications

Books Suggested

1. F.A.Cotton : Introduction to Group theory for chemists.
2. George Davidson Elsevier : Introductory Group Theory for Chemists.
3. Gurdeep Raj , Ajay Bhagi&Vinod Jain : Group Theory and Symmetry in Chemistry
4. Instrumental methods of analysis – M.H.Willard, Meritt Jr. and J.A.Dean
5. Principles of instrumental analysis – Skoog and West
6. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
7. V. R. Gowariker, N. V. Viswanathan, JayadevSreedhar.: polymer Science. New Age international Publishers.

CHE : EC-304: PRACTICALS (Core & Gen.) :: WATER & SOIL ANALYSIS

Water Analysis

- a. Alkalinity
- b. Acidity
- c. Temporary, Permanent and total hardness
- d. Sulphate
- e. Phosphorus
- f. Nitrites
- g. Chlorides
- h. D.O, BOD and COD
- i. Insecticides

Soil Analysis

Determination Of:

- a) pH
- b) Conductivity
- c) Ca
- d) Mg
- e) Heavy metals like Cr, Pb, Cd, Zn.

CHE : EC : 305 (A) : (SKILL ORIENTED COURSE : THEORY) : CHEMOTHERAPY AND DRUG ANALYSIS

UNIT-I: Chemotherapy

Definition, History, and Evolution of Chemotherapy; Discovery, Classification, Nomenclature, Mode of action and synthesis of the following classes of compounds with special references to specific drugs mentioned under each class

- i) Sulfa drugs- Sulfanilamide and Sulfamethoxazole.
- ii) Antibacterials
 - a) Lactum group of antibiotics – Penicillin, Ampicillin and Amoxycillin.
 - b) Cephalosporin-C and Ciprofloxacin.
- iii) Anticancer drugs – 5-Flurouracil, Methotrexate.
- iv) Antifungals – Griseofulvin
- v) Antimalarials – Chloroquin

UNIT-II: Chemical and Biochemical analysis of Drugs

Qualitative and Quantitative Analysis of drugs: Uses of IR, UV, GLC and HPLC methods.

Drug Assay by Biochemical Analysis – ELISA (Cortisol, alcohol, opiates).

RadioImmuno Assay (RIA) – Enalapril, Insulin

Kidney, Lungs and Liver function tests; Use of isotopes in the Bioanalysis of drugs and in drug design programmes.

Book Suggested

1. Medicinal Chemistry and Pharmaceutical Chemistry – Harikishan Singh and Kapur
2. Medicinal Chemistry and Biochemistry – R.L.Nath
3. Introduction to Medicinal Chemistry – Patrick
4. The Organic Chemistry of Drug Synthesis Vols. 1-6 - Ledneicer Top drugs top synthetic routes – John Saunders
5. Medicinal Chemistry – Ashutoshkar
6. Synthetic Organic Chemistry and Drugs – Gurideep R Chetwal
7. Biochemistry – Harper, Conn & Stumpf, Lehninger
8. Biochemistry – Western Jodd
9. Biochemistry – Cann & Stumpf
10. Bergers Medicinal Chemistry Vols. 1-5 – Manfred E. Wolf
11. Introduction to drug design – Siverman
12. Biochemical approach to Medicinal Chemistry – Thomas Nogrady
13. Principles of Medicinal chemistry – William Foye
14. Text book of organic medicinal and pharmaceutical chemistry – Delgrado and William A
15. Industrial Microbiology – Casida

CHE : EC-305 (B) : PRACTICALS (SKILL ORIENTED COURSE) : INSTRUMENTAL METHODS OF ANALYSIS

- 1) Potentiometry:
 - a) Mixture of Acids
 - b) Mixture of Halides
- 2) Flame Photometry: Determination of Na, K, and Li

CHE : 306(A): (OPEN ELECTIVE) SPECTRAL TECHNIQUES

UNIT – I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY

15 Hrs

Various electronic transitions (185-800nm.), Beer-Lambert Law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds

UNIT – II : INFRARED SPECTROSCOPY

15 Hrs

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids and anhydrides. Effect of hydrogen bonding.

UNIT – III: ATOMIC ABSORPTION SPECTROSCOPY: FLAME AAS:

15 Hrs

Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences-Physical, Chemical, spectral and background correction, and methods of minimization
GF AAS: Principle and technique – Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT – IV: MASS SPECTROMETRY

15 Hrs

Principle, instrumentation, different methods of ionization, EI, CI, FD and FAB, Mass spectra-molecular ion, base peak, meta-stable peak, nitrogen rule and McLafferty rearrangement. Mass spectral fragmentation of organic compounds and common functional groups. Normal and branched alkanes, alkenes, cycloalkanes, benzene and its derivatives, alcohols and phenols, ethers, aldehydes and ketones, carboxylic acids and their

derivatives, amines and nitro compounds. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Organic spectroscopy, W.Kemp 5th Ed, ELBS .2.
2. Spectroscopy of organic compounds, RM Silversteen and others 5th Ed, John Wiley 1991
3. Spectroscopy of organic compounds, PS Kalsi, Wiley, 1993
4. NMR in chemistry – A Multi nuclear introduction, William Kemp, Mc Millan 1986
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemmi TMH . 2005

CHE : 306(B): (OPEN ELECTIVE) CHROMATOGRAPHIC TECHNIQUES

Unit –I: Introduction - Classification of Chromatographic methods – Column chromatography-Adsorption phenomenon: Nature of adsorbents-Solvent systems-Differential migration-Separation of mixture of o-/p-nitro anilines (A demonstration experiment).

Unit –II: Thin-Layer Chromatography (TLC)-Coating materials and preparation of TLC plates- Solvents for development-Detection of compounds in TLC- R_f values in TLC-Applications of TLC in chemistry-Preparative TLC – Demonstration experiment in TLC.

Unit –III: High-Performance Liquid Chromatography (HPLC) - Application of HPLC- HPLC instrument- Stationary phases in HPLC-Normal and reversed phase HPLC: A comparison- Normal phase HPLC: Principle- Retention times in Normal and reversed phase HPLC- Reversed phase HPLC: Principle.

Unit –IV: Gas-Liquid Chromatography- Instruments for Gas-Liquid Chromatography- Gas-Chromatographic Columns and the Stationary Phase- Application of Gas-Liquid Chromatography- Gas-Solid Chromatography.

Reference Books:

1. Analytical chemistry: G L David Krupadanam, D.Vijaya prasad, K.Varaprasad Rao, KLN Reddy, C.Sudhakar.
2. . Analytical chemistry: Skoog West Holler.
3. Modern Analytical Chemistry : David Harvey DePauw University.
4. J.G.Dick. Analytical Chemistry,McGraw Hill,New Delhi, (1973).

M Sc., SEMESTER-III
(INORGANIC CHEMISTRY)
(NEP – 2020 CBCS syllabus effective from 2021-22)

CHE : IC-301- (CORE-THEORY) : INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS

UNIT –I: THERMAL METHODS OF ANALYSIS

15 Hrs

Thermo gravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Different thermal analysis – principle, instrumentation, difference between TG and DTA, applications with special reference to the clays and minerals.

Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and perchlorates, ammonium nitrate.

UNIT –II: MOSSBAUER SPECTROSCOPY and NQR

15 Hrs

Mossbauer spectroscopy: Basic principles, Recoil energy, Doppler shift, Chemical shift, Quadrupole effects, Magnetic effects. Instrumentation, spectral parameters and spectrum display.

Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds, (2) Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: Basic principles of NQR spectroscopy, quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant and applications.

UNIT –III: ELECTRON SPIN RESONANCE SPECTROSCOPY

15 Hrs

Basic Principles, Hyper fine splitting, Factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, Hamiltonian and spin densities. Zero field splitting and Kramer's degeneracy, Relaxation process and line widths. Instrumentation and Applications. The EPR spectrum of bis(salicylidimine)-copper(II) complex, study of inorganic free radicals, biological applications of Electron Spin Resonance (Study of free radicals and Iron-sulfur proteins)

UNIT –IV: PHOTO ELECTRON SPECTROSCOPY

15 Hrs

Photoelectric effect, Koopmans's theorem, ionization energy.

X-ray photoelectron spectroscopy (ESCA): Principle, Binding energies, Chemical shift, Applications of XPES to Qualitative analysis, to surface studies and structural analysis.

Ultraviolet photoelectron spectroscopy- Principle, application of UPES in studying the molecular orbitals of O_2 and N_2 molecules.

Block diagram of photoelectron spectrophotometer. Sources of radiation, detectors.

Auger spectra – Principle, Applications of Auger spectra to surface studies and use of Auger spectra as a fingerprint tool.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John Wiley & sons. Inc., New York.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter: Inorganic Chemistry, Principles of Structure and Reactivity (4th Ed.) (Addison-Wesley)
3. Gary Wulfsberg: Inorganic Chemistry (5th Ed. (Viva Books)
4. J.D. Lee: Concise Inorganic Chemistry (Blackwell)
5. W.L. Jolly: Modern Inorganic Chemistry (McGraw-Hill)
6. R.L. Carlin: Magneto-chemistry (Springer-Verlag)
7. R.L. Dutta and A. Syamal: Elements of Magnetochemistry (Affiliate East-West).
8. K. Hussain Reddy – Text book of Bioinorganic chemistry

CHE : IC-302 (CORE-THEORY) : ORGANIC SPECTROSCOPY AND APPLICATIONS

UNIT-I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

15Hrs

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

UNIT – II: INFRARED SPECTROSCOPY

15Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance, FT-IR

UNIT –III: ^1H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ^1H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

^{13}C NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimensional NMR spectroscopy-COSY.

UNIT-IV: MASS SPECTROMETRY

15Hrs

Introduction, ion production, type of ionization, EI, CI, FD, and FAB-factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular-ion peak, metastable peak, Mc. Lafferty rearrangement. Nitrogen rule, isotope labeling. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books suggested:

1. Organic spectroscopy, W. Kemp 5th Ed, ELBS
2. Spectroscopy of organic compounds, RM Silversteen and others, 5th Ed, John Wiley
3. Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.
4. NMR in chemistry-A multi nuclear introduction, William Kemp, Mc Millan, 1986.
5. Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi,

CHE : IC : 303 (A): (GENERIC ELECTIVE) ORGANIC CHEMISTRY - III

UNIT I: REAGENTS IN ORGANIC SYNTHESIS

15 Hrs

Use of the following reagents in organic synthesis: Anhydrous AlCl_3 , Boran trifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexylcarbodiimide, Lead tetraacetate, Ziegler-Natta catalysts, DDQ, Dithianes, Merrifield resin.

UNIT-II: ORGANOMETALLIC REAGENTS

15 Hrs

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydroformylation reactions

UNIT III: ASYMMETRIC SYNTHESIS

15 Hrs

Topocity - Prochirality- Substrate selectivity - Diastereoselectivity and enantioselectivity-Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods-Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines – Stereoselective Diels-Alder reaction

Reagent controlled methods-Use of chiral reagents-Asymmetric oxidation-Sharpless epoxidation-Asymmetric reduction-Use of lithium aluminium hydride and borate reagents.

UNIT IV: METHODS OF ORGANIC SYNTHESIS

15 Hrs

- Oxidations:** (a) Alcohols to carbonyls-Chromium (iv) oxidants-Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, oxidation with silver carbonate (b) Alkenes to epoxides-peroxide induced epoxidations. (c) Alkenes to diols-oxidation with potassium permanganate, osmium tetroxide, Prevost reaction (d) Ketones to esters-Bayer-Villiger oxidation (e)

- Oxidative bond cleavage-cleavage of alkenes by transition metals. (f) Oxidation of alkyl or alkenyl fragments-selenium dioxide and chromium trioxide oxidations.
- ii. **Reductions** : Reduction with lithium aluminium hydride, sodium borohydride, alkoxides, bis-methoxy ethoxy aluminium hydride, Boran aluminium hydride and derivatives-catalytic hydrogenation-dissolving metal reductions, Non-Metallic reducing agents including enzymatic and microbial reductions.

Books Suggested :

1. Advanced Organic Chemistry-Reactions, 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.
4. Structure and Mechanism in Organic Chemistry, C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Name reactions and reagents in organic synthesis, B.P. Muway and M.G Ellord, John Wiley.
7. Modern Organic Reactions, H.O. House, Benjamin.
8. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, Blackie Academic & Professional.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Principles of organometallic chemistry, P. Powell, ELBS.
11. Organo transition metal chemistry-Applications to organic synthesis, S.G. Davis, Pergmon.
12. Stereochemistry to Organic Compounds, E.L. Eliel and others, John Wiley.
13. Stereochemistry to Organic Compounds, D. Nasipuri, New Age International.
14. Stereochemistry, P.S.Kalsi, Wiley Eastern.

CHE : IC :303 (B): (GENERIC ELECTIVE) : PHYSICAL CHEMISTRY - III

UNIT-I Applications of Group Theory

15 Hrs

Construction of reducible and irreducible representations, Determination of Character Co ordinate of C_{2v} point group based on 3N Co ordinates. Standard reduction formula, Determination of normal modes of vibrations of SO_2 , NH_3 , $POCl_3$, $PtCl_4^{2-} \cdot H_2O_2$ molecules. Mutual exclusion Principle, Direct Product, Accidental Degeneracy and Fermi resonance **Group Theory and Spectroscopy**: selection rules, symmetry Criteria for optical activity, symmetry restrictions on dipole moments, symmetry and stereo isomerism. Prediction of IR and Raman Spectral activity of H_2O , NH_3 and CO_2

UNIT-II: X-ray Diffraction:

15 Hrs

(D) Solid State Chemistry

Dislocation of Solids, Schottky and Frenkel defects, insulators, a, d semiconductors, Band theory of solids, solid state reactions.

(E) Bragg conditions-Miller Indices- Laue method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals. Index reflections, identification of unit cells from systematic absences in diffraction pattern- structure of simple lattices and X-ray intensities- structure factor and its relation to intensity and electron density- Description of procedure for X-ray structure analysis ($NaCl$ and KCl)

(F) Electron Diffraction: Scattering intensity Vs scattering angle, Wierlequation, and its importance. Measurement techniques, Elucidation of structures of simple gas phase molecules, Low energy electron diffraction (LEED) for the study of surfaces.

UNIT-III: SPECTROSCOPY

15 Hrs

Microwave spectroscopy: classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, intensities- stark effect.

Infrared spectroscopy: Linear harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combinations bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.

Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, pure vibrational Raman spectroscopy, selection rules, mutual exclusion principle, resonance Raman spectroscopy and coherent antistokes Raman spectroscopy. Vibrational- rotational Raman spectroscopy.

Thermodynamics of polymer dissolution, effect of molecular weight on solubility, solubility of crystalline and amorphous polymer, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins theory of polymer solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular weight determination by light scattering, ultra centrifugation and sedimentation equilibrium method. Liquid Crystals- synthesis and applications

Books Suggested

1. F.A.Cotton : Introduction to Group theory for chemists.
2. George Davidson Elsevier : Introductory Group Theory for Chemists.
3. Gurdeep Raj , Ajay Bhagi&Vinod Jain : Group Theory and Symmetry in Chemistry
4. Instrumental methods of analysis – M.H.Willard, Meritt Jr. and J.A.Dean
5. Principles of instrumental analysis – Skoog and West
6. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
7. V. R. Gowariker, N. V. Viswanathan, JayadevSreedhar.: polymer Science. New Age international Publishers.

CHE : IC -304: PRACTICALS (Core & Gen.)**Preparation of Inorganic complexes and characterization:**

- a) Tris thiourea Zinc (II) Sulphate
- b) Tris thiourea Copper(I) Sulphate
- c) Hexamine nickel (II) Chloride
- d) Chloropentammine cobalt (III) Chloride
- e) Cis potassium diaquodioxalato chromate (III)
- f) Tris (acetylacetonato) manganese (III)
- g) Mercury tetrakis thiocyanato cobaltate (II)
- h) Sodium trioxalato ferrate (III)
- i) Tetrammine Copper (II) Sulphate
- j) Potassium hexathiocyanato chromate (III) tetrahydrate

CHE : IC - 305 (A) : (SKILL ORIENTED COURSE THEORY) : CHEMOTHERAPY AND DRUG ANALYSIS**UNIT-I: Chemotherapy**

Definition, History, and Evolution of Chemotherapy; Discovery, Classification, Nomenclature, Mode of action and synthesis of the following classes of compounds with special references to specific drugs mentioned under each class

- vi) Sulfa drugs- Sulfanilamide and Sulfamethoxazole.
- vii) Antibacterials
6. Lactam group of antibiotics – Penicillin, Ampicillin and Amoxycillin.
7. Cephalosporin-C and Ciprofloxacin.
- viii) Anticancer drugs – 5-Fluorouracil, Methotrexate.
- ix) Antifungals – Griseofulvin
- x) Antimalarials – Chloroquin

UNIT-II: Chemical and Biochemical analysis of Drugs

Qualitative and Quantitative Analysis of drugs: Uses of IR, UV, GLC and HPLC methods.

Drug Assay by Biochemical Analysis – ELISA (Cortisol, alcohol, opiates).

RadioImmuno Assay (RIA) – Enalapril, Insulin

Kidney, Lungs and Liver function tests; Use of isotopes in the Bioanalysis of drugs and in drug design programmes.

Book Suggested

1. Medicinal Chemistry and Pharmaceutical Chemistry – Harikishan Singh and Kapur
2. Medicinal Chemistry and Biochemistry – R.L.Nath
3. Introduction to Medicinal Chemistry – Patrick

4. The Organic Chemistry of Drug Synthesis Vols. 1-6 - Ledneicer Top drugs top synthetic routes – John Saunders
5. Medicinal Chemistry – Ashutoshkar
6. Synthetic Organic Chemistry and Drugs – Gurideep R Chetwal
7. Biochemistry – Harper, Conn & Stumpf, Lehninger
8. Biochemistry – Western Jodd
9. Biochemistry – Cann & Stumpf
10. Bergers Medicinal Chemistry Vols. 1-5 – Manfred E. Wolf
11. Introduction to drug design – Siverman
12. Biochemical approach to Medicinal Chemistry – Thomas Nogrady
13. Priniciples of Medicinal chemistry – William Foye
14. Text book of organic medicinal and pharmaceutical chemistry – Delgrado and William A

CHE : IC -305 (B) : PRACTICALS (SKILL ORIENTD COURSE) : Instrumental methods of analysis

Colorimetric determinations:

- a) Determination of manganese
- b) Determination of nickel
- c) Determination of iron by 1,10 Pheren-thioline
- d) Determination of chromium
- e) Determination of Phosphate
- f) Determination of Pesticides
- g) Determination of Nitrite.

CHE : IC : 306(A): (OPEN ELECTIVE) SPECTRAL TECHNIQUES

UNIT – I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY

15 Hrs

Various electronic transitions (185-800nm.), Beer-Lambert Law, effect of solvent on electronic transitions , ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds

UNIT – II : INFRARED SPECTROSCOPY

15 Hrs

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids and anhydrides. Effect of hydrogen bonding.

UNIT – III: ATOMIC ABSORPTION SPECTROSCOPY: FLAME AAS:

15 Hrs

Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences-Physical, Chemical, spectral and back ground correction, and methods of minimization
GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT –IV: MASS SPECTROMETRY

15 Hrs

Principle, instrumentation, different methods of ionization, EI, CI, FD and FAB, Mass spectra-molecular ion, base peak, meta-stable peak, nitrogen rule and Mc Lafferty rearrangement. Mass spectral fragmentation of organic compounds and common functional groups. Normal and branched alkanes, alkenes, cycloalkanes, benzene and its derivatives, alcohols and phenols, ethers, aldehydes and ketones, carboxylic acids and their derivatives , amines and nitro compounds. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Organic spectroscopy, W.Kemp 5th Ed, ELBS .2.
2. Spectroscopy of organic compounds, RM Silversteen and others 5th Ed, John Wiley 1991
3. Spectroscopy of organic compounds, PS Kalsi, Wiley, 1993
4. NMR in chemistry – A Multi nuclear introduction, William Kemp, Mc Millan 1986
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemmi TMH . 2005

CHE : IC : 306(B): (OPEN ELECTIVE) CHROMATOGRAPHIC TECHNIQUES

Unit –I: Introduction - Classification of Chromatographic methods – Column chromatography-Adsorption phenomenon: Nature of adsorbents-Solvent systems-Differential migration-Separation of mixture of o-/p-nitro anilines (A demonstration experiment).

Unit –II: Thin-Layer Chromatography (TLC)-Coating materials and preparation of TLC plates- Solvents for development-Detection of compounds in TLC- R_f values in TLC-Applications of TLC in chemistry-Preparative TLC – Demonstration experiment in TLC.

Unit –III: High-Performance Liquid Chromatography (HPLC) - Application of HPLC- HPLC instrument- Stationary phases in HPLC-Normal and reversed phase HPLC: A comparison- Normal phase HPLC: Principle- Retention times in Normal and reversed phase HPLC- Reversed phase HPLC: Principle.

Unit –IV: Gas-Liquid Chromatography- Instruments for Gas-Liquid Chromatography- Gas-Chromatographic Columns and the Stationary Phase- Application of Gas-Liquid Chromatography- Gas-Solid Chromatography.

Reference Books:

1. Analytical chemistry: G L David Krupadanam, D.Vijaya prasad, K.Varaprasad Rao, KLN Reddy, C.Sudhakar.
2. . Analytical chemistry: Skoog West Holler.
3. Modern Analytical Chemistry : David Harvey DePauw University.
4. J.G.Dick. Analytical Chemistry,McGraw Hill,New Delhi, (1973).

SEMESTER-III
(ORGANIC CHEMISTRY)
(NEP – 2020 CBCS syllabus for the students admitted from 2021-22)

CHE : OC-301 (Core-Theory) : Organic Chemistry - III

UNIT I: REAGENTS IN ORGANIC SYNTHESIS

15 Hrs

Use of the following reagents in organic synthesis: Anhydrous AlCl_3 , Boran trifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexylcarbodiimide, Lead tetraacetate, Ziegler-Natta catalysts, DDQ, Dithianes, Merrifield resin.

UNIT-II: ORGANOMETALLIC REAGENTS

15 Hrs

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydroformylation reactions

UNIT III: ASYMMETRIC SYNTHESIS

15 Hrs

Topocity - Prochirality- Substrate selectivity - Diastereoselectivity and enantioselectivity-Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods-Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines – Stereoselective Diels-Alder reaction

Reagent controlled methods-Use of chiral reagents-Asymmetric oxidation-Sharpless epoxidation-Asymmetric reduction-Use of lithium aluminium hydride and borate reagents.

UNIT IV: METHODS OF ORGANIC SYNTHESIS

15 Hrs

i. **Oxidations:** (a) Alcohols to carbonyls-Chromium (iv) oxidants-Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, oxidation with silver carbonate (b) Alkenes to epoxides-peroxide induced epoxidations. (c) Alkenes to diols-oxidation with potassium permanganate, osmium tetroxide, Prevost reaction (d) Ketones to esters-Bayer-Villiger oxidation (e) Oxidative bond cleavage-cleavage of alkenes by transition metals. (f) Oxidation of alkyl or alkenyl fragments-selenium dioxide and chromium trioxide oxidations.

ii. **Reductions :** Reduction with lithium aluminium hydride, sodium borohydride, alkoxides, bis- methoxy ethoxy aluminium hydride, Boran aluminium hydride and derivatives-catalytic hydrogenation-dissolving metal reductions, Non-Metallic reducing agents including enzymatic and microbial reductions.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, 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.
4. Structure and Mechanism in Organic Chemistry, C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Name reactions and reagents in organic synthesis, B.P. Muway and M.G Ellord, John Wiley.
7. Modern Organic Reactions, H.O. House, Benjamin.
8. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, Blackie Academic & Professional.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Principles of organometallic chemistry, P. Powell, ELBS.
11. Organo transition metal chemistry-Applications to organic synthesis, S.G. Davis, Pergmon.
12. Stereochemistry to Organic Compounds, E.L. Eliel and others, John Wiley.
13. Stereochemistry to Organic Compounds, D. Nasipuri, New Age International.
14. Stereochemistry, P.S.Kalsi, Wiley Eastern.

CHE : OC - 302: (CORE THEORY) : ORGANIC SPECTROSCOPY AND APPLICATIONS

UNIT-I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

15Hrs

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

UNIT – II: INFRARED SPECTROSCOPY

15Hrs

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance, FT-IR

UNIT –III: ^1H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ^1H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation. Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

^{13}C NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimensional NMR spectroscopy-COSY.

UNIT-IV: MASS SPECTROMETRY

15Hrs

Introduction, ion production, type of ionization, EI, CI, FD, and FAB-factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular-ion peak, metastable peak, Mc. Lafferty rearrangement. Nitrogen rule, isotope labeling. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books suggested:

1. Organic spectroscopy, W. Kemp 5th Ed, ELBS
2. Spectroscopy of organic compounds, RM Silversteen and others, 5th Ed, John Wiley
3. Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.
4. NMR in chemistry-A multi nuclear introduction, William Kemp, Mc Millan, 1986.
5. Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi,

CHE : OC:303(A) : GENERIC ELECTIVE : INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS

UNIT –I: THERMAL METHODS OF ANALYSIS

15 Hrs

Thermo gravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Different thermal analysis – principle, instrumentation, difference between TG and DTA, applications with special reference to the clays and minerals.

Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and perchlorates, ammonium nitrate.

UNIT –II: MOSSBAUER SPECTROSCOPY and NQR

15 Hrs

Mossbauer spectroscopy: Basic principles, Recoil energy, Doppler shift, Chemical shift, Quadrupole effects, Magnetic effects. Instrumentation, spectral parameters and spectrum display.

Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds, (2) Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: Basic principles of NQR spectroscopy, quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant and applications.

UNIT –III: ELECTRON SPIN RESONANCE SPECTROSCOPY

15 Hrs

Basic Principles, Hyper fine splitting, Factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, Hamiltonian and spin densities. Zero field splitting and Kramer's degeneracy, Relaxation process and line widths. Instrumentation and Applications. The EPR spectrum of bis(salicylidimine)-copper(II) complex, study of inorganic free radicals, biological applications of Electron Spin Resonance (Study of free radicals and Iron-sulfur proteins)

UNIT –IV: PHOTO ELECTRON SPECTROSCOPY**15 Hrs**

Photoelectric effect, Koopmans's theorem, ionization energy.

X-ray photoelectron spectroscopy (ESCA): Principle, Binding energies, Chemical shift, Applications of XPS to Qualitative analysis, to surface studies and structural analysis.

Ultraviolet photoelectron spectroscopy- Principle, application of UPES in studying the molecular orbitals of O_2 and N_2 molecules.

Block diagram of photoelectron spectrophotometer. Sources of radiation, detectors.

Auger spectra – Principle, Applications of Auger spectra to surface studies and use of Auger spectra as a fingerprint tool.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John Wiley & sons. Inc., New York.
2. J.E. Huheey, E.A. Keiter and R.L. Keiter: Inorganic Chemistry, Principles of Structure and Reactivity (4th Ed.) (Addison-Wesley)
3. Gary Wulfsberg: Inorganic Chemistry (5th Ed. (Viva Books)
4. J.D. Lee: Concise Inorganic Chemistry (Blackwell)
5. W.L. Jolly: Modern Inorganic Chemistry (McGraw-Hill)
6. R.L. Carlin: Magneto-chemistry (Springer-Verlag)
7. R.L. Dutta and A. Syamal: Elements of Magnetochemistry (Affiliate East-West).
8. K. Hussain Reddy – Text book of Bioinorganic chemistry

CHE : OC : 303 (B): (GENERIC ELECTIVE) : PHYSICAL CHEMISTRY - III**UNIT-I Applications of Group Theory****15 Hrs**

Construction of reducible and irreducible representations, Determination of Character Co ordinate of C_{2v} point group based on 3N Co ordinates. Standard reduction formula, Determination of normal modes of vibrations of SO_2 , NH_3 , $POCl_3$, $PtCl_4^{2-} \cdot H_2O$ molecules. Mutual exclusion Principle, Direct Product, Accidental Degeneracy and Fermi resonance Group Theory and Spectroscopy: IR Spectral activity of NH_3 molecule, selection rules, symmetry Criteria for optical activity, symmetry restrictions on dipole moments, symmetry and stereo isomerism. Prediction of IR and Raman Spectral activity of H_2O and CO_2 .

UNIT-II: X-ray Diffraction:**15 Hrs****(G) Solid State Chemistry**

Dislocation of Solids, Schottky and Frenkel defects, insulators, a, d semiconductors, Band theory of solids, solid state reactions.

(H) Bragg conditions-Miller Indices- Laue method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals. Index reflections, identification of unit cells from systematic absences in diffraction pattern- structure of simple lattices and X-ray intensities- structure factor and its relation to intensity and electron density- Description of procedure for X-ray structure analysis ($NaCl$ and KCl)

(I) Electron Diffraction: Scattering intensity Vs scattering angle, Wierlequation, and its importance. Measurement techniques, Elucidation of structures of simple gas phase molecules, Low energy electron diffraction (LEED) for the study of surfaces.

UNIT-III: SPECTROSCOPY**15 Hrs**

Microwave spectroscopy: classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, intensities- stark effect.

Infrared spectroscopy: Linear harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combinations bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.

Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, pure vibrational Raman spectroscopy, selection rules, mutual exclusion principle, resonance Raman spectroscopy and coherent antistokes Raman spectroscopy. Vibrational- rotational Raman spectroscopy.

UNIT-IV: POLYMER SOLUTIONS

15 Hrs

Thermodynamics of polymer dissolution, effect of molecular weight on solubility, solubility of crystalline and amorphous polymer, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins theory of polymer solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular weight determination by light scattering, ultra centrifugation and sedimentation equilibrium method. Liquid Crystals- synthesis and applications

Books Suggested

1. F.A.Cotton : Introduction to Group theory for chemists.
2. Geroge Davidson Elsevier : Introductory Group Theory for Chemists.
3. Gurdeep Raj , Ajay Bhagi&Vinod Jain : Group Theory and Symmetry in Chemistry
4. Instrumental methods of analysis – M.H.Willard, Meritt Jr. and J.A.Dean
5. Principles of instrumental analysis – Skoog and West
6. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
7. V. R. Gowariker, N. V. Viswanathan, JayadevSreedhar.: polymer Science. New Age international Publishers.

CHE : OC : 304 : Practicals (Core & Gen.) Organic Estimations

- 1) Estimation of phenol
- 2) Estimation of glucose
- 3) Estimation of percentage purity of aspirin
- 4) Estimation of percentage purity of paracetamol.

CHE : OC : 305 (A) : SKILL ORIENTED COURSE (THEORY) : CHEMOTHERPY AND DRUG ANALYSIS

UNIT-I: Chemotherapy

Definition, History, and Evolution of Chemotherapy; Discovery, Classification, Nomenclature, Mode of action and synthesis of the following classes of compounds with special references to specific drugs mentioned under each class

- xi) Sulfa drugs- Sulfanilamide and Sulfamethoxazole.
- xii) Antibacterials
8. Lactum group of antibiotics – Penicillin, Ampicillin and Amoxycillin.
9. Cephalosporin-C and Ciprofloxacin.
- xiii) Anticancer drugs – 5-Fluorouracil, Methotrexate.
- xiv) Antifungals – Griseofulvin
- xv) Antimalarials – Chloroquin

UNIT-II: Chemical and Biochemical analysis of Drugs

Qualitative and Quantitative Analysis of drugs: Uses of IR, UV, GLC and HPLC methods.

Drug Assay by Biochemical Analysis – ELISA (Cortisol, alcohol, opiates).

RadioImmuno Assay (RIA) – Enalapril, Insulin

Kidney, Lungs and Liver function tests; Use of isotopes in the Bioanalysis of drugs and in drug design programmes.

Book Suggested

1. Medicinal Chemistry and Pharmaceutical Chemistry – Harikishan Singh and Kapur
2. Medicinal Chemistry and Biochemistry – R.L.Nath
3. Introduction to Medicinal Chemistry – Patrick
4. The Organic Chemistry of Drug Synthesis Vols. 1-6 - Ledneicer Top drugs top synthetic routes – John Saunders
5. Medicinal Chemistry – Ashutoshkar
6. Synthetic Organic Chemistry and Drugs – Gurideep R Chetwal
7. Biochemistry – Harper, Conn & Stumpf, Lehninger
8. Biochemistry – Western Jodd
9. Biochemistry – Cann & Stumpf

10. Bergers Medicinal Chemistry Vols. 1-5 – Manfred E. Wolf
11. Introduction to drug design – Siverman
12. Biochemical approach to Medicinal Chemistry – Thomas Nogrady
13. Principles of Medicinal chemistry – William Foye
14. Text book of organic medicinal and pharmaceutical chemistry – Delgrado and William A
15. Industrial Microbiology – Casida

CHE : OC: 305 (B) : Practicals (Skill Oriented Course) : Multistep preparations

- 1) Preparation of benzilic acid
- 2) Preparation of benzanilide
- 3) Preparation of o-chlorobenzoic acid
- 4) Preparation of symmetric tribromobenzene

CHE : OC : 306 (A) : (Open Elective) - SPECTRAL TECHNIQUES

UNIT – I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY

15 Hrs

Various electronic transitions (185-800nm.), Beer-Lambert Law, effect of solvent on electronic transitions , ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds

UNIT – II : INFRARED SPECTROSCOPY

15 Hrs

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids and anhydrides. Effect of hydrogen bonding.

UNIT – III: ATOMIC ABSORPTION SPECTROSCOPY: FLAME AAS:

15 Hrs

Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences-Physical, Chemical, spectral and back ground correction, and methods of minimization

GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT –IV: MASS SPECTROMETRY

15 Hrs

Principle, instrumentation, different methods of ionization, EI, CI, FD and FAB, Mass spectra-molecular ion, base peak, meta-stable peak, nitrogen rule and Mc Lafferty rearrangement. Mass spectral fragmentation of organic compounds and common functional groups. Normal and branched alkanes, alkenes, cycloalkanes, benzene and its derivatives, alcohols and phenols, ethers, aldehydes and ketones, carboxylic acids and their derivatives , amines and nitro compounds. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Organic spectroscopy, W.Kemp 5th Ed, ELBS .2.
2. Spectroscopy of organic compounds, RM Silversteen and others 5th Ed, John Wiley 1991
3. Spectroscopy of organic compounds, PS Kalsi, Wiley, 1993
4. NMR in chemistry – A Multi nuclear introduction, William Kemp, Mc Millan 1986
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemmi TMH . 2005

CHE : OC : 306(B): (OPEN ELECTIVE)-CHROMATOGRAPHIC TECHNIQUES

Unit –I: Introduction - Classification of Chromatographic methods – Column chromatography-Adsorption phenomenon: Nature of adsorbents-Solvent systems-Differential migration-Separation of mixture of o-/p-nitro anilines (A demonstration experiment).

Unit –II: Thin-Layer Chromatography (TLC)-Coating materials and preparation of TLC plates- Solvents for development-Detection of compounds in TLC- R_f values in TLC-Applications of TLC in chemistry-Preparative TLC – Demonstration experiment in TLC.

Unit –III: High-Performance Liquid Chromatography (HPLC) - Application of HPLC- HPLC instrument- Stationary phases in HPLC-Normal and reversed phase HPLC: A comparison- Normal phase HPLC: Principle-Retention times in Normal and reversed phase HPLC- Reversed phase HPLC: Principle.

Unit –IV: Gas-Liquid Chromatography- Instruments for Gas-Liquid Chromatography- Gas-Chromatographic Columns and the Stationary Phase- Application of Gas-Liquid Chromatography- Gas-Solid Chromatography.

Reference Books:

1. Analytical chemistry: G L David Krupadanam, D.Vijaya prasad, K.Varaprasad Rao, KLN Reddy, C.Sudhakar.
2. Analytical chemistry: Skoog West Holler.
3. Modern Analytical Chemistry : David Harvey DePauw University.
4. J.G.Dick. Analytical Chemistry, McGraw Hill, New Delhi, (1973).

SEMESTER-III
(PHYSICAL CHEMISTRY)

(NEP – 2020 CBCS syllabus for the students admitted from 2021-22)

CHE : PC : 301 (CORE-THEORY) : PHYSICAL CHEMISTRY III

UNIT-I Applications of Group Theory

15 Hrs

Construction of reducible and irreducible representations, Determination of Character Co ordinate of C_{2v} point group based on 3N Co ordinates. Standard reduction formula, Determination of normal modes of vibrations of SO_2 , NH_3 , $POCl_3$, $PtCl_4^{2-} \cdot H_2O_2$ molecules. Mutual exclusion Principle, Direct Product, Accidental Degeneracy and Fermi resonance Group Theory and Spectroscopy: IR Spectral activity of NH_3 molecule, selection rules, symmetry Criteria for optical activity, symmetry restrictions on dipole moments, symmetry and stereo isomerism. Prediction of IR and Raman Spectral activity of H_2O and CO_2 .

UNIT-II: X-ray Diffraction:

15 Hrs

(J) Solid State Chemistry

Dislocation of Solids, Schottky and Frenkel defects, insulators, a, d semiconductors, Band theory of solids, solid state reactions.

(K) Bragg conditions-Miller Indices- Laue method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals. Index reflections, identification of unit cells from systematic absences in diffraction pattern-

structure of simple lattices and X-ray intensities- structure factor and its relation to intensity and electron density- Description of procedure for X-ray structure analysis ($NaCl$ and KCl)

(L) Electron Diffraction: Scattering intensity Vs scattering angle, Wierlequation, and its importance. Measurement techniques, Elucidation of structures of simple gas phase molecules, Low energy electron diffraction (LEED) for the study of surfaces.

UNIT-III: SPECTROSCOPY

15 Hrs

Microwave spectroscopy: classification of molecules, rigid rotator model, effect of isotopic substitution on the transition frequencies, intensities- stark effect.

Infrared spectroscopy: Linear harmonic oscillator, zero point energy, anharmonicity, Mores potential energy diagram, fundamental and overtone transitions, hot bands and combinations bands. Vibration-rotation spectroscopy, PQR branches, selection rules, factors affecting the band positions and intensities for IR region.

Raman spectroscopy: Classical and quantum theories of Raman effect, pure rotational, pure vibrational Raman spectroscopy, selection rules, mutual exclusion principle, resonance Raman spectroscopy and coherent antistokes Raman spectroscopy. Vibrational- rotational Raman spectroscopy.

UNIT-IV: POLYMER SOLUTIONS

15 Hrs

Thermodynamics of polymer dissolution, effect of molecular weight on solubility, solubility of crystalline and amorphous polymer, heat of dissolution, regular solution theory, Hildebrand solubility parameter, Flory-Huggins theory of polymer solutions, conformational entropy, osmotic pressure and viscosity of polymer solutions. Molecular weight determination by light scattering, ultra centrifugation and sedimentation equilibrium method. Liquid Crystals- synthesis and applications

Books Suggested

1. F.A.Cotton : Introduction to Group theory for chemists.
2. Gerge Davidson Elsevier : Introductory Group Theory for Chemists.
3. Gurdeep Raj , Ajay Bhagi&Vinod Jain : Group Theory and Symmetry in Chemistry
4. Instrumental methods of analysis – M.H.Willard, Meritt Jr. and J.A.Dean
5. Principles of instrumental analysis – Skoog and West
6. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
7. V. R. Gowariker, N. V. Viswanathan, JayadevSreedhar.: polymer Science. New Age international Publishers.

CHE : PC: 302 : (CORE THEORY) : ORGANIC SPECTROSCOPY AND APPLICATIONS

UNIT-I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY:

15Hrs

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

UNIT – II: INFRARED SPECTROSCOPY**15Hrs**

Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ether, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and fermi resonance, FT-IR

UNIT –III: ¹H NMR spectroscopy: Magnetic properties of nuclei, Principles of NMR. Instrumentation, CW and pulsed FT instrumentation, equivalent and non equivalent protons, enantiotopic and diastereotopic protons, Chemical shifts, factors affecting the chemical shifts, electronegativity and anisotropy, shielding and deshielding effects, Signal integration, Spin-spin coupling: vicinal, germinal and long range, Coupling constants and factors affecting coupling constants.

Applications of ¹H NMR spectroscopy: Reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E, Z isomers, conformation of cyclohexane and decalins, keto-enol tautomerism, hydrogen bonding, proton exchange processes (alcohols, amines and carboxylic acids), C-N rotation.

Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, nuclear Overhauser effect (NOE).

¹³C NMR spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimensional NMR spectroscopy-COSY.

UNIT-IV: MASS SPECTROMETRY**15Hrs**

Introduction, ion production, type of ionization, EI, CI, FD, and FAB-factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular-ion peak, metastable peak, Mc. Lafferty rearrangement. Nitrogen rule, isotope labeling. High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books suggested:

1. Organic spectroscopy, W. Kemp 5th Ed, ELBS
2. Spectroscopy of organic compounds, RM Silverstein and others, 5th Ed, John Wiley
3. Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.
4. NMR in chemistry-A multi nuclear introduction, William Kemp, Mc Millan, 1986.
5. Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi,

CHE : PC : 303 (A): (GENERIC ELECTIVE) : ORGANIC CHEMISTRY - III**UNIT I: REAGENTS IN ORGANIC SYNTHESIS****15 Hrs**

Use of the following reagents in organic synthesis: Anhydrous AlCl₃, Boran trifluoride, N-Bromosuccinimide, Diazomethane, Dicyclohexylcarbodiimide, Lead tetraacetate, Ziegler-Natta catalysts, DDQ, Dithianes, Merrifield resin.

UNIT-II: ORGANOMETALLIC REAGENTS**15 Hrs**

Synthesis and applications of Grignard reagents, Organolithium, Zinc, Copper, Mercury, Palladium and Rhodium compounds in Organic Synthesis, Homogeneous catalytic hydrogenation and hydroformylation reactions

UNIT III: ASYMMETRIC SYNTHESIS**15 Hrs**

Topocity - Prochirality- Substrate selectivity - Diastereoselectivity and enantioselectivity-Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods-Use of chiral auxiliaries-Chiral enolates-alkylation of chiral imines – Stereoselective Diels-Alder reaction

Reagent controlled methods-Use of chiral reagents-Asymmetric oxidation-Sharpless epoxidation-Asymmetric reduction-Use of lithium aluminium hydride and borate reagents.

UNIT IV: METHODS OF ORGANIC SYNTHESIS**15 Hrs**

- Oxidations:** (a) Alcohols to carbonyls-Chromium (iv) oxidants-Dimethyl sulfoxide oxidation, periodate oxidation, Oppenauer oxidation, oxidation with manganese dioxide, oxidation with silver carbonate (b) Alkenes to epoxides-peroxide induced epoxidations. (c) Alkenes to diols-oxidation with potassium permanganate, osmium tetroxide, Prevost reaction (d) Ketones to esters-Bayer-Villiger oxidation (e)

- Oxidative bond cleavage-cleavage of alkenes by transition metals. (f) Oxidation of alkyl or alkenyl fragments-selenium dioxide and chromium trioxide oxidations.
- ii. **Reductions** : Reduction with lithium aluminium hydride, sodium borohydride, alkoxides, bis-methoxy ethoxy aluminium hydride, Boran aluminium hydride and derivatives-catalytic hydrogenation-dissolving metal reductions, Non-Metallic reducing agents including enzymatic and microbial reductions.

Books Suggested :

1. Advanced Organic Chemistry-Reactions, 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.
4. Structure and Mechanism in Organic Chemistry, C.K.Inglod, Cornell University Press.
5. Organic Chemistry, R.T Morrison and R.N. Boyd, Prentice - Hall.
6. Name reactions and reagents in organic synthesis, B.P. Muway and M.G Ellord, John Wiley.
7. Modern Organic Reactions, H.O. House, Benjamin.
8. Principles of Organic Synthesis, R.O.C Norman and J.M Coxon, Blackie Academic & Professional.
9. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, New Age International.
10. Principles of organometallic chemistry, P. Powell, ELBS.
11. Organo transition metal chemistry-Applications to organic synthesis, S.G. Davis, Pergmon.
12. Stereochemistry to Organic Compounds, E.L. Eliel and others, John Wiley.
13. Stereochemistry to Organic Compounds, D. Nasipuri, New Age International.
14. Stereochemistry, P.S.Kalsi, Wiley Eastern.

CHE : PC : 303(B) : (GENERIC ELECTIVE) INORGANIC SPECTROSCOPY & THERMAL METHODS OF ANALYSIS

UNIT –I: THERMAL METHODS OF ANALYSIS

15 Hrs

Thermo gravimetry –Principle, Factors affecting the results, instrumentation. Application with special reference to $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CaC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Different thermal analysis – principle, instrumentation, difference between TG and DTA, applications with special reference to the clays and minerals. Different scanning calorimetry –principle, and applications to inorganic materials like chlorates and perchlorates, ammonium nitrate.

UNIT –II: MOSSBAUER SPECTROSCOPY and NQR

15 Hrs

Mossbauer spectroscopy: Basic principles, Recoil energy, Doppler shift, Chemical shift, Quadrupole effects, Magnetic effects. Instrumentation, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{2+} and Fe^{3+} compounds, (2) Sn^{2+} and Sn^{4+} compounds.

NQR spectroscopy: Basic principles of NQR spectroscopy, quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant and applications.

UNIT –III: ELECTRON SPIN RESONANCE SPECTROSCOPY

15 Hrs

Basic Principles, Hyper fine splitting, Factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, Hamiltonian and spin densities. Zero field splitting and Kramer's degeneracy, Relaxation process and line widths. Instrumentation and Applications. The EPR spectrum of bis(salicylidimine)-copper(II) complex, study of inorganic free radicals, biological applications of Electron Spin Resonance (Study of free radicals and Iron-sulfur proteins)

UNIT –IV: PHOTO ELECTRON SPECTROSCOPY

15 Hrs

Photoelectric effect, Koopmans's theorem, ionization energy.

X-ray photoelectron spectroscopy (ESCA): Principle, Binding energies, Chemical shift, Applications of XPES to Qualitative analysis, to surface studies and structural analysis.

Ultraviolet photoelectron spectroscopy- Principle, application of UPES in studying the molecular orbitals of O_2 and N_2 molecules.

Block diagram of photoelectron spectrophotometer. Sources of radiation, detectors.

Auger spectra – Principle, Applications of Auger spectra to surface studies and use of Auger spectra as a finger print tool.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition,1999.John wiley & sons. Inc., New York.
2. J.E. Huheey, E.A.Keiter and R.L.Keiter: Inorganic Chemsitry, Principles of Structure and Reactivity (4th Ed.) (Addison-Wesley)
3. Gary Wulfsberg: Inorganic Chemistry (5th Ed. (Viva Books)
4. J.D.Lee: Concise Inorganic Chemistry (Blackwell)
5. W.L.Jolly: Modern Inorganic Chemsitry (McGraw-Hill)
6. R.L.Carlin: Magneto-chemsitry (Springer-Verlag)
7. R.L.Dutta and A.Syamal: Elements of Magnetochemsitry (Affiliate East-West).
8. K. Hussain Reddy – Text book of Bioinorganic chemistry

CHE : PC-304: Practicals (Core & Gen.)

1. Chemical Kinetics:

- a) Study of the kinetics of halogenations of acetone.
- b) Determination of activation energy of reaction between iodide and Persulphate
- c) Determination rate constant of oxidation of iodide ion by persulphate ion and study the effect of neutral salt (KCl).

2. Flame Photometry:

- a) Determination of Na
- b) Determination of K
- c) Determination of Cu

CHE : PC : 305 (A) : SKILL ORIENTED COURSE THEORY) : CHEMOTHERAPY AND DRUG ANALYSIS

UNIT-I: Chemotherapy

Definition, History, and Evolution of Chemotherapy; Discovery, Classification, Nomenclature, Mode of action and synthesis of the following classes of compounds with special references to specific drugs mentioned under each class

- xvi) Sulfa drugs- Sulfanilamide and Sulfamethoxazole.
- xvii) Antibacterials
10. Lactum group of antibiotics – Penicillin, Ampicillin and Amoxycillin.
11. Cephalosporin-C and Ciprofloxacin.
- xviii) Anticancer drugs – 5-Flurouracil, Methotrexate.
- xix) Antifungals – Griseofulvin
- xx) Antimalarials – Chloroquin

UNIT-II: Chemical and Biochemical analysis of Drugs

Qualitative and Quantitative Analysis of drugs: Uses of IR, UV, GLC and HPLC methods.

Drug Assay by Biochemical Analysis – ELISA (Cortisol, alcohol, opiates).

RadioImmuno Assay (RIA) – Enalapril, Insulin

Kidney, Lungs and Liver function tests; Use of isotopes in the Bioanalysis of drugs and in drug design programmes.

Book Suggested

1. Medicinal Chemistry and Pharmaceutical Chemistry – Harikishan Singh and Kapur
2. Medicinal Chemistry and Biochemistry – R.L.Nath
3. Introduction to Medicinal Chemistry – Patrick
4. The Organic Chemistry of Drug Synthesis Vols. 1-6 - Ledneicer Top drugs top synthetic routes – John Saunders
5. Medicinal Chemistry – Ashutoshkar
6. Synthetic Organic Chemistry and Drugs – Gurideep R Chetwal

7. Biochemistry – Harper, Conn & Stumpf, Lehninger
8. Biochemistry – Western Jodd
9. Biochemistry – Cann & Stumpf
10. Bergers Medicinal Chemistry Vols. 1-5 – Manfred E. Wolf
11. Introduction to drug design – Siverman
12. Biochemical approach to Medicinal Chemistry – Thomas Nogrady
13. Principles of Medicinal chemistry – William Foye
14. Text book of organic medicinal and pharmaceutical chemistry – Delgrado and William A

CHE : PC-305 (B) : Practicals (Skill Oriented Course)

1. Conductometry:
 - a) Titration of mixture of halides
 - b) Titration of mixture of HCl+HOAC
 - c) Saponification of an ester
2. Colorimetry:
 - a) Estimation of Manganese
 - b) Estimation of Iron
 - c) Estimation of Phosphate
 - d) Titration of copper Vs EDTA

CHE : PC : 306(A): (OPEN ELECTIVE) SPECTRAL TECHNIQUES

UNIT – I: ULTRAVIOLET AND VISIBLE SPECTROSCOPY

15 Hrs

Various electronic transitions (185-800nm.), Beer-Lambert Law, effect of solvent on electronic transitions , ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds

UNIT – II : INFRARED SPECTROSCOPY

15 Hrs

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids and anhydrides. Effect of hydrogen bonding.

UNIT – III: ATOMIC ABSORPTION SPECTROSCOPY: FLAME AAS:

15 Hrs

Principle, Instrumentation – Sources of radiation (HCL and EDL), Different types of burners, Interferences-Physical, Chemical, spectral and back ground correction, and methods of minimization
GF AAS: Principle and technique –Comparison between Flame AAS and furnace AAS, Applications of AAS, Comparison between Atomic Absorption & Flame Photometry.

UNIT –IV: MASS SPECTROMETRY

15 Hrs

Principle, instrumentation, different methods of ionization, EI, CI, FD and FAB, Mass spectra-molecular ion, base peak, meta-stable peak, nitrogen rule and Mc Lafferty rearrangement. Mass spectral fragmentation of organic compounds and common functional groups. Normal and branched alkanes, alkenes, cycloalkanes, benzene and its derivatives, alcohols and phenols, ethers, aldehydes and ketones, carboxylic acids and their derivatives , amines and nitro compounds. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Books Suggested:

1. Organic spectroscopy, W.Kemp 5th Ed, ELBS .2.
2. Spectroscopy of organic compounds, RM Silversteen and others 5th Ed, John Wiley 1991
3. Spectroscopy of organic compounds, PS Kalsi, Wiley, 1993
4. NMR in chemistry – A Multi nuclear introduction, William Kemp, Mc Millan 1986
5. Spectroscopic methods in Organic Chemistry, DH Williams & I Flemmi TMH . 2005

CHE : PC : 306(B): (OPEN ELECTIVE) CHROMATOGRAPHIC TECHNIQUES

Unit –I: Introduction - Classification of Chromatographic methods – Column chromatography-Adsorption phenomenon: Nature of adsorbents-Solvent systems-Differential migration-Separation of mixture of o-/p-nitro anilines (A demonstration experiment).

Unit –II: Thin-Layer Chromatography (TLC)-Coating materials and preparation of TLC plates- Solvents for development-Detection of compounds in TLC- R_f values in TLC-Applications of TLC in chemistry-Preparative TLC – Demonstration experiment in TLC.

Unit –III: High-Performance Liquid Chromatography (HPLC) - Application of HPLC- HPLC instrument- Stationary phases in HPLC-Normal and reversed phase HPLC: A comparison- Normal phase HPLC: Principle-Retention times in Normal and reversed phase HPLC- Reversed phase HPLC: Principle.

Unit –IV: Gas-Liquid Chromatography- Instruments for Gas-Liquid Chromatography- Gas-Chromatographic Columns and the Stationary Phase- Application of Gas-Liquid Chromatography- Gas-Solid Chromatography.

Reference Books:

1. Analytical chemistry: G L David Krupadanam, D.Vijaya prasad, K.Varaprasad Rao, KLN Reddy, C.Sudhakar.
2. . Analytical chemistry: Skoog West Holler.
3. Modern Analytical Chemistry : David Harvey DePauw University.
4. J.G.Dick. Analytical Chemistry,McGraw Hill,New Delhi, (1973).

M. Sc., ANALYTICAL CHEMISTRY
FOURTH SEMESTER
(NEP – 2020 CBCS syllabus of the Academic Year 2021-22)

CHE : AC 401: CORE THEORY : QUALITY CONTROL AND GENERAL PRINCIPLES

UNIT-I: QUALITY CONTROL IN ANALYTICAL CHEMISTRY

15 Hrs

Definition of analytical terms: Accuracy, precision, limit of detection, sensitivity, selectivity and specificity, ruggedness, principles of Ruggedness test, validating the Method as a Standard Method.

Quality assurance and management systems: Elements of quality assurance, Quality and quantity management system, ISO 9000 and ISO 14000 series.

Good laboratory practices (GLP): Elements of Good Laboratory Practice, Laboratory accreditation, GLP status in India.

UNIT-II: ORGANIC REAGENTS IN INORGANIC ANALYSIS

15 Hrs

Theoretical basis for the use of organic reagents in inorganic analysis: Application of the following reagents in inorganic analysis: dimethylglyoxime, salicylaldehyde, cupferron, d-benzoin, 1,10 phenanthroline, 8-hydroxy quinoline, nitron, tannin, pyridine, 8-hydroxyquinoline, dithizone, Acetylacetone, theonyl, trifluoroacetone, 8-hydroxy quinoline, tri-M-octylphosphine oxide.

UNIT – III: KINETIC METHODS OF TRACE ANALYSIS

15 Hrs

Rate laws, Analytical use of reaction rates, First and second order reactions, relative rate of reactions. Determination of reaction rates. Analytical utility of first and pseudo first order reactions. Types of kinetic methods, differential, integral, logarithmic, extrapolation method. Evaluation of kinetic methods – Scale of Operation, Catalyzed reactions, measurement method for catalyzed reaction. Micro determination of Inorganic species like Iodine and Hg in complex materials. Determination of organic species. Kinetics of enzyme, catalyzed reactions. Michael's constant factors affecting the rate of enzyme, Catalyzed reactions, Enzyme characteristics and applications of Kinetic methods of trace analysis.

UNIT-IV:REDOX AND COMPLEXOMETRIC TITRATIONS:

15Hrs

Redox Titrations: Standard reduction potential, equilibrium constants of oxidation-reduction reactions, change of electrode potential during the titration of reductant with an oxidant. Formal potential primary standard substance. Standard solutions. Preparation and storage. Oxidations with cerium (IV) sulphate solutions. Theory and use of (i) acid-base, (ii) Oxidation-reduction (iii) Metal ion indicators.; **Complexometric titrations:** Introduction, complexones, stability constants of EDTA complexes, conditional stability constants, titration curves, types of EDTA titration's, titration of mixtures.

Books Suggested

1. Vogel's Text book of Quantitative Chemical Analysis, Basselt, Denmy, Jaffery and Merdhan, ELBS, Orientlong- Manan, 5th Ed.1990.
2. Analytical Chemistry, Gary D. Christian, John Laliley and Senes, New York, 6th Ed., 2007.
3. Fundamentals of ANALYTICAL CHEMISTRY, Skoog, West, Holler; 7th Editin 2001
4. Fundamentals of Analytical Chemistry, D.A. Skoog & D.M. West, Holf-Saunderrs, 5th Ed., 1991.
5. Principles and Methods Chemical Analysis: H.F. Walton, Prentice Hall, New Delhi.
6. Chemical Analysis, H.A. Laitinan, Mc.Graw Hill Book Company.
7. Technical methods of analysis – Griffin, Mc Graw Hill Book Co.
8. K.V.S.G Murali Krishna, An Introduction ISO 9000, ISO 1400 Series,
9. Environmental Management Quality Assurance and Good Laboratory Practices, Prof. Y. Anjaneyulu, In Now Publication, New York
10. Quality Assurance in Analytical Chemistry – G.Kateman and F.W Pijpers, John Wiley and Sons, New York

CHE : AC 402: CORE THEORY: INSTRUMENTAL METHODS OF ANALYSIS

UNIT –I SPECTROSCOPIC METHODS

15 Hrs

Emission Spectroscopy:

(i) ICP-AES: Principles, instrumentation, AES detectors, applications in the analysis of trace and toxic metals in water, geological and industrial samples.

(ii) ICP-MS: Principles, instrumentation, quadrupole mass spectrometers, applications

Fluorescence Spectroscopy:

i) Molecular Fluorescence Spectroscopy: Principle, Theory of fluorescence, phosphorescence, relation between intensity of fluorescence and concentration, Correlation of fluorescence with molecular structure, Fluorescence quenching, Instrumentation and applications.

ii) X-ray Fluorescence Spectroscopy: Principle, energy dispersive X-ray fluorescence (EDXRF), Wavelength dispersive X-ray fluorescence (WDXRF), applications.

UNIT – II: CHROMATOGRAPHIC METHODS**15 Hrs**

High Performance Liquid Chromatography (HPLC): Principles, Stationary phases, Instrumentation, Solvent delivery system, sample introduction, gradient elution, columns and detectors. Partition Chromatography, adsorption chromatography, Gel permeation chromatography.

Capillary Electrophoresis: Principle, Electroosmotic flow, Instrumentation, Applications to separation of small ions, separation of Molecular Species, DNA sequencing

Supercritical-fluid chromatography: Supercritical-fluids, Instrumentation and Applications

UNIT –III: HYPHENATED TECHNIQUES**15 Hrs**

Mass Spectroscopy: Principle, basic instrumentation, resolution, Ionization sources- Electron impact and Chemical ionization, Mass Analyzers- Quadrupole Mass analyzer and Time- of- Flight Analyzer.

Gas Chromatography- Mass spectrometry: Introduction, GC – MS interface, processing of GC – MS data – ion chromatogram. Quantitative measurement – sample preparation, Selected ion monitoring – Application of GC-MS for Trace constituents. Drugs analysis, Environmental analysis and others.

Liquid chromatography- Mass spectrometry – Introduction – Instrumentation – liquid chromatography – Mass spectrometer Interface – Instrumental details – Processing LC-MS data – ion chromatograms, Sample preparation – selected ion monitoring. Application of LC-MS for Drug analysis, Environmental samples and others.

UNIT- IV: ELECTRO ANALYTICAL METHODS**15 Hrs**

Anodic stripping voltammetry: principle, instrumentation, Hanging mercury drop electrode, application in the analysis of Pb and Cd in environmental samples, principle of cathode stripping voltammetry.

Principals of Adsorptive Stripping voltammetry.

Books Suggested

1. Analytical Chemistry, Gary D. Christian, John Laliley and Senes, New York, 6th Ed., 2007.
2. Fundamentals of ANALYTICAL CHEMISTRY, Skoog, West, Holler; 7th Editin 2001
3. Analytical Chemistry Principles and Techniques, I.G. Harge, Prentice Hall.
4. Principles of Instrumental analysis, D.A. Skoog and J.L. Loacy, W.B. Saunders.
5. Handbook of Instrumental Techniques for Analytical Chemistry, F. Serlie, Prentice Hall.
6. Vogels Text book of Quantitative Chemical Analysis, Basett, Denny Jebbary, 5th Ed. ELBs 1990.
7. Instrumental Methods of Chemical Analysis, Willard Merrit, Dean, Stella Jr 6th Edition.
8. P.W Scott, Techniques and practice of Chromatography, Marel Dekker Inc., New York
9. Separation methods, M.N Sastri, Himalaya Publishing Company, Mumbai
10. E. Helfman, Chromatography, Van Nostrand, Reinhold, New York
11. E. Lederer and M. Lederer, Chromatography, Elsevier, Amsterdam.

CHE : AC 403(A): (GENERIC ELECTIVE) APPLIED AND ENVIRONMENTAL ASPECTS**UNIT-I: SAMPLING AND SEPARATION METHODS****15 Hrs**

Preparing the sample for analysis: Sampling, The effect of sampling uncertainties, Gross sample, determination of the size of the gross sample. Analytical sample. Preparation of laboratory sample from gross sample, Moisture in the sample, Karl-Fisher reagent for the determination of moisture content in samples.

Decomposition and dissolving the sample: Decomposition of sample by fluxes, wet digestion, dry ashing, combustion with oxygen, microwave decomposition.

Separation and pre-concentration: Extractive separation of metal ions as chelates (dithizone, oxine, APDC, NaDDTC), Solid-phase extraction

UNIT-II: ANALYSIS OF AGRO CHEMICALS and MINERALS**15 Hrs**

Soil analysis: Soil moisture, pH, total nitrogen, Phosphorus, silica, boron and metals (Cd, Cu, Fe, Mn, and zinc) in soil.

Fertilizer analysis: Analysis of Ammonical fertilizers, Phosphate fertilizers, Nitrate fertilizers

Pesticide Analysis: Analysis of organo chlorine pesticides by gas chromatography, Determination of DDT residue in vegetable and food grains. Analysis of organo phosphorous pesticides (Malathion, parathion) by spectrophotometric and chromatographic methods.

Analysis of Minerals and Ores: Limestone, Ilmenite, Chalcopyrites and Beryl. Analysis of Cement, Ceramics and glass.

UNIT-III: ANALYSIS OF COMPLEX MATERIALS**15 Hrs**

Analysis of Fuels: Coal, proximate and ultimate analysis, heating values and grading of coal.

Liquid Fuels: Flash point, aniline point, octane number and carbon residue.

Analysis of Gaseous Fuels: Producer gas, Water gas, Calorific values

Analysis of alloys: German Silver, Brass, bronze, Solder, Steels containing elements such as Mo, Co, V, Cr, Si and Ni.

Analysis of Explosives: Introduction, Classification, Deflagrating or low explosives, Characteristics of explosives, Nitrocellulose, PETN or PENTHRT, Di-nitrobenzene (DNB), Trinitrobenzene (TNB), Trinitrotoluene (TNT),

UNIT – IV: ENVIRONMENTAL POLLUTION MONITORING:**15 Hrs**

Water Quality monitoring: Methods of water sample collection, Determination of Dissolved oxygen(D.O), Biochemical Oxygen Demand(BOD) and Chemical Oxygen Demand(COD)

Analytical methods for the determination of the following ions in water:

Anions: F^- , PO_4^{3-} , NO_3^- , NO_2^- Cations: Cr^{6+} , As^{5+} , Pb^{2+} , Hg^{2+} , Cd^{2+}

Air Quality Monitoring: Air sampling methods, Chemical analysis of the following Air pollutants. i) Gaseous pollutants: Carbon monoxide (CO), sulphur dioxide (SO_2), nitrogen dioxide (NO_2), Aliphatic hydrocarbons and polycyclic aromatic hydrocarbons (PAH). (ii) Particulate matter

Books Suggested

1. Analytical Chemistry, Gary D. Christian, John Laliley and Senes, New York, 6th Ed., 2007.
2. Fundamentals of ANALYTICAL CHEMISTRY, Skoog, West, Holler; 7th Editin 2001
3. Analytical Chemistry Principles and Techniques, I.G. Harge, Prentice Hall.
4. Principles of Instrumental analysis, D.A. Skoog and J.L. Loacy, W.B. Saunders.
5. Fundamentals of Air Pollution By A.C. Strem and others, Academic Press, 1975.
6. Standard methods for the examination of water and waste water published by American public health association, 15th Ed.1981.
7. Methods of Soil Analysis, C.A. Black, Part I and II.
8. Handbook of Analytical Control of Iron and Steel Production, Harrison John Weily 1979
9. Standard methods of Chemical Analysis, Welcher
10. Technical Methods of Analysis, Griffin, Mc Graw Hill
11. Environmental Chemistry, Anil Kumar De, Wiley Eastern Ltd.

CHE : AC:403(B):(GENERIC ELECTIVE): BIOINORGANIC, BIOORGANIC, BIOPHYSICAL CHEMISTRY**UNIT-I: BIO-INORGANIC CHEMISTRY- I****15 Hrs**

Metal complexes as oxygen carriers –Heme proteins –Hemoglobin and myoglobin –Non heme proteins – hemerythrin and hemocyanin – model synthetic complexes of iron, cobalt and copper.Co-enzymes Vitamin B_{12} ,carboxy peptidase and superoxidedismutase.

Electron Transfer in Biology: Structure and functions of metalloproteins in electron transfer processes – catalase –peroxidase –cytochromes and iron –sulphur proteins –synthetic models.

UNIT – II: BIOINORGANIC CHEMISTRY- II: Metal ion transport and storage in biological systems, Metal ions in Biology, Molecular mechanism of ion transport across membranes: ionophores, photosynthesis.

Hydrolytic metalloenzymes: Carbonic anyhdrase, carboxy peptidase, calcium in control processes, calcium and muscle contraction, calcium and secretion, calcium in blood clotting mechanisms. Therapeutic uses of enzymes.

Importance of trace metals in biology: Metal ions as chelating agents in medicine, trace metal ions and metal and non-metal deficiency. Biological nitrogen fixation,in-vivo and in-vitro nitrogen fixation.

UNIT-III: BIOORGANIC CHEMISTRY

Carbohydrates: Structure and biological functions of mucopolysaccharides, glycoproteins, and glycolipids- Role of sugars in biological recognition- Blood group substances

Lipids: Essential fatty acids-structure and function of triglycerols, Glycerophospholipids, cholesterol, bile acids prostaglandins- composition and functioning of lipoproteins

Enzymes: Nomenclature and classification, properties, factors affecting enzyme catalysis, enzyme inhibition- reversible and irreversible inhibition. Uses of enzymes in food drink industry and clinical laboratories.

UNIT-IV: BIOPHYSICAL CHEMISTRY:

Standard free energy change in biochemical reactions, exergonic and endergonic reactions, hydrolysis of ATP, thermodynamics of biopolymer solutions, chain configuration of bio polymers, calculation of average dimensions. Membrane equilibrium, ion transport through cell membrane.dialysis and its function. Structure and functions of proteins, enzymes, DNA and RNA in living systems, forces involved in bio polymer interactions, electrostatic forces, hydrophobic forces, molecular expansion, and dispersion forces.

Books Suggested

1. M.N. Hughes, The Inorganic chemistry of Biological Processes, John Wiley and Sons, New York 2nd Edition, 1981.
2. A Text book of Biochemistry , A.V.S.S.Rama Rao
3. Physical chemistry by Atkenes
4. Physical chemistry by Albertz.
5. Bio physical chemistry by Van Holde
6. Bio Physics by Narayanam
7. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
8. Chemistry of Natural Products, P.S.Kalsi, Kalyani Publishers.
9. Chemistry of Organic Natural Products, O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
10. Natural products Chemistry K.B.G. Torssell, John Wiley, 1983.
11. Burger's Medicinal Chemistry, M.E. Wolff, John Wiley
12. Medicinal Chemistry, A. Kar, New Age International

CHE : AC 404: PRACTICALS (CORE & GEN.) I Instrumental methods of analysis- II

1. Flame Photometry: Determination of Na and K, Ca and Li in Water and Soil.
2. TLC/Paper chromatographic separation.
3. Determination of Pesticide residues by gas chromatographic method
4. Polarography: a) Determination of E $\frac{1}{2}$ of Zn and Cd
b) Determination of amounts of Zn and Cd
5. Atomic Absorption Spectroscopy: Determination of transition metal ions (Cd, Cr, Cu, Pb, Zn etc.,) by AAS.
6. Separation of Metal ion by Solvent Extraction /Ion exchange.

II DEMONSTRATION EXPERIMENTS

1. IR – Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard materials
2. AAS: Demonstration of AAS – Determination of Zn, Cd, Pb, Mn, Fe and Ni in effluents using AAS.
3. Spectrofluorimetry – estimation of quinine and fluorescein
4. Ion selective electrodes – estimation of F⁻, S²⁻ and CN⁻ in effluents using ion selective electrode meter.
5. Polarography and Anode stripping voltametry
(a) Polarography and Anode stripping voltametry – behavior of Cd, Zn, Pb in a mixture.
(b) Determination of Pb and Cd in samples using Anode stripping voltametry
6. Gas chromatography- Determination of pesticides
7. HPLC- Determination of pesticides
a) NMR Demonstration of NMR spectrometer and study of hydrogen bonding in a given alcohol or phenol.
B Interpretation of NMR chemical shifts of ethyl benzene, ethyl alcohol
8. TGA, DTA, DSC – Demonstration of TG, DTA and DSC and study of decomposition of calcium oxalate, calcium carbonate, copper sulfate, oxalic acid.
9. pH metry
a) Determination of alkalinity in a colored effluent using pH metric end point.
b) Determination of purity of commercial HCl, H₂SO₄, H₃PO₄ and CH₃COOH using pH metric end point

CHE : AC 405: PROJECT WORK

CHE : AC : 406 (A): (OPEN ELECTIVE) : DRUG CHEMISTRY

UNIT – I: NATURAL PRODUCTS AS LEADS FOR NEW DRUGS

Occurrence, Structure and therapeutic uses of Drugs acting on Central Nervous System
Morphine alkaloids (morphine, codeine, thebaine, heroin, pethidine)
Cannabinoids (9-cannabinol, Tetrahydrocannabinol)
Neuromuscular Blocking Agents (Curare, Decamethonium)
Vinca Alkaloids (Vincristin and Vinblastin), Taxol and Taxotere, podophyllotoxin, Etoposide, Teniposide.

UNIT – II: CARDIOVASCULAR DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.
Cardiac glycosides (ex: Digoxin, Digitoxin);
Antihypertensive drugs (ex: Methyl dopa, Clonidine hydrochloride);
Antiarrhythmic agents (ex: Quinidine sulfate);
Antisymphathetic drugs (ex: Propranolol hydrochloride, Verapamil hydrochloride);
Vasopressor drugs (ex: Prenylamine, Buphenine).

UNIT – III: AUTACOIDS

Definition, Occurrence, Isolation, Nomenclature, Classification, Synthesis, Biosynthesis and Stereochemical structures of Prostaglandins. Structural elucidation of PGE₁, PGE₂; Synthesis and biosynthesis of PGE₂, PGF_{2α}.
Structure and Biosynthesis of Thromboxane A₂ and Prostacyclin (synthesis not expected).

UNIT – IV: ANTI-INFLAMMATORY DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.
Paracetamol, Aspirin (Antipyretic), Salol, Cinchophen, Antipyrine, Phenylbutazone.
Indomethacin, Tolmetin, Ibuprofen, Diclofenac, Naproxen.

Books suggested:

1. Medicinal Chemistry by Ashitosh Kar
2. Medicinal Chemistry by D. Sriram, P. Yogeeswari
3. Medicinal Chemistry by David A. Williams, Thomas L. Lemke
4. Medicinal Chemistry by V. Alagarsamy
5. Biochemistry by U. Satyanarayana
6. Natural Products Chemistry and Applications by Sujata V. Bhat, B.A. Nagasampagi, S. Meenakshi
7. Medicinal Chemistry by V.K. Ahluwalia, Madhu Chopra
8. Medicinal Chemistry by Balkishen Razdar
9. Advanced Practical Medicinal Chemistry by Ashutosh Kar
10. Chemistry of Organic Natural Products by O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
11. Chemistry of Natural Products by S. V. Bhat, B.A. Nagasampagi, M. Sivakumar
12. Natural Products Chemistry by K.B.G. Torrsell, John Wiley, 1983.

CHE : AC : 406(B): (OPEN ELECTIVE) : ELECTRO ANALYTICAL TECHNIQUES

Unit I

Types and Classification of Electro analytical Methods.

- i) **Potentiometry**- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glasselectrodes. Determination of pH. Potentiometric titrations.
ii) **Conductometry** – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

Unit II

D.C Polarography : Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

Unit III

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography (V) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms.

Unit IV

Ion selective electrodes:

Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes.

Books Suggested

1. H.W. Willard, LL.Meritt and J.A.Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (Mc Graw Hill).

M. Sc., INORGANIC CHEMISTRY
FOURTH SEMESTER
(NEP – 2020 CBCS syllabus for the students admitted from 2021-22)

CHE : IC 401: CORE THEORY: Co-ordination compounds, organometallic chemistry and chemistry of non-transition elements

UNIT –I: ORGANOMETALLIC CHEMISTRY OF TRANSITION ELEMENTS **15 Hrs**

1. Dinitrogen complexes of Ru(II), Os(II), Co(I) and Mo(0)
2. Dioxygen complexes of Ir(I) and Rh(I)
3. Cycloheptatriene and Tropylium complexes –Oxidative addition and Reductive Elimination.
Insertion and Elimination reaction –Nucleophilic and Electrophilic attack of coordinated ligands.

UNIT –II: APPLICATIONS OF ORGANOMETALLIC COMPOUNDS **15 Hrs**

Catalytic applications –Fischer –Tropsch synthesis, Olefin hydrogenation (Wilkinson catalyst). Olefin oxygenation (Wacker process or Smidt reaction) Olefin hydroformylation (Ziegler-Natta Catalysis).
Synthetic applications of Organo–Lithium, –Magnesium and Aluminium compounds. Biological applications of organometallic compounds in medicine, agriculture and horticulture.

UNIT –III: METAL-TO METAL BONDS AND METAL ATOM CLUSTERS **15 Hrs**

Introduction, metal carbonyl clusters –low –nuclearity (M and M) clusters, isoelectronic and isolobal relationships, High nuclearity, carbonyl clusters (HNCC'S), Hetero stomes in metal atom clusters, electron counting scheme for HNCC'S, HNCC'S of the Fe, Ru and Os group HNCC'S of the Cu, Rh and Ir group, HNCC'S of the Ni, Pd, and Pt group. Compounds with M-M multiple bonds, Major structural types, quadruple bonds, relation of clusters to multiple bonds and one dimensional solids.

UNIT –IV: CHEMISTRY OF NON-TRANSITION ELEMENTS **15 Hrs**

General characteristics of the non-transition elements, special features of individual elements: Synthesis, properties and structure of their Halides and oxides, polymorphism of carbon, Phosphorus and Sulphur. Synthesis, properties and structure of boranes, carboranes, borazines, silicates, carbides, Sulphur-nitrogen compounds, peroxo compounds of boron, carbon and sulphur, oxyacids of nitrogen, phosphorus, sulphur and halogens, inter halogens pseudo halides.

Books Suggested

1. F.A.Cotton and G.Wilkinson, Advanced In-organic chemistry VI Edition, 1999. John Wiley & sons. Inc., New York.
2. James E. Huheey, Inorganic chemistry- Principles of structure and reactivity, IV Edition 1993. Harper Collins College Publishers, New York.
3. J.D.Lee, Concise Inorganic chemistry, V Edition 1996, ELBS, Chapman and Hall, London.
4. Concise Inorganic chemistry by J.D.Lee V Edition ELBS, Chapman and Hall, London.
5. Organometallic Chemistry by R.C.Mehrotra and Singh.

CHE : IC :402: CORE THEORY: INSTRUMENTAL METHODS OF ANALYSIS

UNIT –I SPECTROSCOPIC METHODS **15 Hrs**

Emission Spectroscopy:

(i) ICP-AES: Principles, instrumentation, AES detectors, applications in the analysis of trace and toxic metals in water, geological and industrial samples.

(ii) ICP-MS: Principles, instrumentation, quadrupole mass spectrometers, applications

Fluorescence Spectroscopy:

i) **Molecular Fluorescence Spectroscopy:** Principle, Theory of fluorescence, phosphorescence, relation between intensity of fluorescence and concentration, Correlation of fluorescence with molecular structure, Fluorescence quenching, Instrumentation and applications.

ii) **X-ray Fluorescence Spectroscopy:** Principle, energy dispersive X-ray fluorescence (EDXRF), Wavelength dispersive X-ray fluorescence (WDXRF), applications.

UNIT – II: CHROMATOGRAPHIC METHODS **15 Hrs**

High Performance Liquid Chromatography (HPLC): Principles, Stationary phases, Instrumentation, Solvent delivery system, sample introduction, gradient elution, columns and detectors. Partition Chromatography, adsorption chromatography, Gel permeation chromatography.

Capillary Electrophoresis: Principle, Electroosmotic flow, Instrumentation, Applications to separation of small ions, separation of Molecular Species, DNA sequencing

Supercritical-fluid chromatography: Supercritical-fluids, Instrumentation and Applications

UNIT –III: HYPHENATED TECHNIQUES

15 Hrs

Mass Spectroscopy: Principle, basic instrumentation, resolution, Ionization sources- Electron impact and Chemical ionization, Mass Analyzers- Quadrupole Mass analyzer and Time- of- Flight Analyzer.

Gas Chromatography- Mass spectrometry: Introduction, GC – MS interface, processing of GC – MS data – ion chromatogram. Quantitative measurement – sample preparation, Selected ion monitoring – Application of GC-MS for Trace constituents. Drugs analysis, Environmental analysis and others.

Liquid chromatography- Mass spectrometry – Introduction – Instrumentation – liquid chromatography – Mass spectrometer Interface – Instrumental details – Processing LC-MS data – ion chromatograms, Sample preparation – selected ion monitoring. Application of LC-MS for Drug analysis, Environmental samples and others.

UNIT- IV: ELECTRO ANALYTICAL METHODS

15 Hrs

Anodic stripping voltammetry: principle, instrumentation, Hanging mercury drop electrode, application in the analysis of Pb and Cd in environmental samples, principle of cathode stripping voltammetry.

Principals of Adsorptive Stripping voltammety.

Books Suggested

1. Analytical Chemistry, Gary D. Christian, John Laliley and Senes, New York, 6th Ed., 2007.
2. Fundamentals of Analytical Chemistry, Skoog, West, Holler; 7th Editin 2001
3. Analytical Chemistry Principles and Techniques, I.G. Harge, Prentice Hall.
4. Principles of Instrumental analysis, D.A. Skoog and J.L. Loacy, W.B. Saunders.
5. Handbook of Instrumental Techniques for Analytical Chemistry, F. Serlie, Prentice Hall.
6. Vogels Text book of Quantitative Chemical Analysis, Basett, Denny Jebbary, 5th Ed. ELBs 1990.
7. Instrumental Methods of Chemical Analysis, Willard Merrit, Dean, Stella Jr 6th Edition.
8. P.W Scott, Techniques and practice of Chromatography, Marel Dekker Inc., New York
9. Separation methods, M.N Sastri, Himalaya Publishing Company, Mumbai
10. E. Helfman, Chromatography, Van Nostrand, Reinhold, New York
11. E. Lederer and M. Lederer, Chromatography, Elsevier, Amsterdam.

CHE : IC 403(A): (GENERIC ELECTIVE) INSTRUMENTAL METHODS OF ANALYSIS

UNIT –I SPECTROSCOPIC METHODS

15 Hrs

Emission Spectroscopy:

(i) ICP-AES: Principles, instrumentation, AES detectors, applications in the analysis of trace and toxic metals in water, geological and industrial samples.

(ii) ICP-MS: Principles, instrumentation, quadrupole mass spectrometers, applications

Fluorescence Spectroscopy:

i) **Molecular Fluorescence Spectroscopy:** Principle, Theory of fluorescence, phosphorescence, relation between intensity of fluorescence and concentration, Correlation of fluorescence with molecular structure, Fluorescence quenching, Instrumentation and applications.

ii) **X-ray Fluorescence Spectroscopy:** Principle, energy dispersive X-ray fluorescence (EDXRF), Wavelength dispersive X-ray fluorescence (WDXRF), applications.

UNIT – II: CHROMATOGRAPHIC METHODS

15 Hrs

High Performance Liquid Chromatography (HPLC): Principles, Stationary phases, Instrumentation, Solvent delivery system, sample introduction, gradient elution, columns and detectors.Partition Chromatography, adsorption chromatography, Gel permeation chromatography.

Capillary Electrophoresis: Principle, Electroosmotic flow, Instrumentation, Applications to separation of small ions, separation of Molecular Species, DNA sequencing

Supercritical-fluid chromatography: Supercritical-fluids, Instrumentation and Applications

UNIT –III: HYPHENATED TECHNIQUES

15 Hrs

Mass Spectroscopy: Principle, basic instrumentation, resolution, Ionization sources- Electron impact and Chemical ionization, Mass Analyzers- Quadrupole Mass analyzer and Time- of- Flight Analyzer.

Gas Chromatography- Mass spectrometry: Introduction, GC – MS interface, processing of GC – MS data – ion chromatogram. Quantitative measurement – sample preparation, Selected ion monitoring – Application of GC-MS for Trace constituents. Drugs analysis, Environmental analysis and others.

Liquid chromatography- Mass spectrometry – Introduction – Instrumentation – liquid chromatography – Mass spectrometer Interface – Instrumental details – Processing LC-MS data – ion chromatograms, Sample preparation – selected ion monitoring. Application of LC-MS for Drug analysis, Environmental samples and others.

UNIT- IV: ELECTRO ANALYTICAL METHODS

15 Hrs

Anodic stripping voltametry: principle, instrumentation, Hanging mercury drop electrode, application in the analysis of Pb and Cd in environmental samples, principle of cathode stripping voltametry.

Coulometric analysis: principles of coulometric analysis with constant current, coulometric analysis with controlled potential, applications of coulometric methods for the analysis of cations-As (III), Fe (II) and I- and S₂- by using I₂ liberations and Ce⁴⁺ liberation in solutions

Ion Selective Electrodes: types of ion selective electrodes, basic properties, potentials and construction, calibration of ion selective electrodes, ion selective electrodes with fixed membrane sites, silver, lead, cadmium, sulfide, fluoride, cyanide and glass electrodes, applications in the analysis of air and water pollutants, principles of liquid membrane, gas sensing and enzyme based electrode

Books Suggested

- 1 Analytical Chemistry, Gary D. Christian, John Laliley and Senes, New York, 6th Ed., 2007.
- 2 Fundamentals of Analytical Chemistry, Skoog, West, Holler; 7th Editin 2001
- 3 Analytical Chemistry Principles and Techniques, I.G. Harge, Prentice Hall.
- 4 Principles of Instrumental analysis, D.A. Skoog and J.L. Loacy, W.B. Saunders.
- 5 Handbook of Instrumental Techniques for Analytical Chemistry, F. Serlie, Prentice Hall.
- 6 Vogels Text book of Quantitative Chemical Analysis, Basett, Denny Jebbary, 5th Ed. ELBs 1990.
- 7 Instrumental Methods of Chemical Analysis, Willard Merrit, Dean, Stella Jr 6th Edition.
- 8 P.W Scott, Techniques and practice of Chromatography, Marel Dekker Inc., New York
- 9 Separation methods, M.N Sastri, Himalaya Publishing Company, Mumbai
- 10 E. Helfman, Chromatography, Van Nostrand, Reinhold, New York
- 11 E. Lederer and M. Lederer, Chromatography, Elsevier, Amsterdam.

CHE : IC 403 (B): (GENERIC ELECTIVE) : BIOINORGANIC, BIOORGANIC, BIOPHYSICAL CHEMISTRY

UNIT-I: BIO-INORGANIC CHEMISTRY- I

15 Hrs

Metal complexes as oxygen carriers –Heme proteins –Hemoglobin and myoglobin –Non heme proteins – hemerythrin and hemocyanin – model synthetic complexes of iron, cobalt and copper.Co-enzymes Vitamin B₁₂,carboxy peptidase and superoxidedismutase.

Electron Transfer in Biology: Structure and functions of metalloproteins in electron transfer processes – catalase –peroxidase –cytochromes and iron –sulphur proteins –synthetic models.

UNIT – II: BIOINORGANIC CHEMISTRY- II: Metal ion transport and storage in biological systems, Metal ions in Biology, Molecular mechanism of ion transport across membranes: ionophores, photosynthesis.

Hydrolytic metalloenzymes: Carbonic anyhdrase, carboxy peptidase, calcium in control processes, calcium and muscle contraction, calcium and secretion, calcium in blood clotting mechanisms. Therapeutic uses of enzymes.

Importance of trace metals in biology: Metal ions as chelating agents in medicine, trace metal ions and metal and non-metal deficiency. Biological nitrogen fixation,in-vivo and in-vitro nitrogen fixation.

UNIT-III: BIOORGANIC CHEMISTRY

Carbohydrates: Structure and biological functions of mucopolysaccharides, glycoproteins, and glycolipids- Role of sugars in biological recognition- Blood group substances

Lipids: Essential fatty acids-structure and function of triglycerols, Glycerophospholipids, cholesterol, bile acids prostaglandins- composition and functioning of lipoproteins

Enzymes: Nomenclature and classification, properties, factors affecting enzyme catalysis, enzyme inhibition-reversible and irreversible inhibition. Uses of enzymes in food drink industry and clinical laboratories.

UNIT-IV: BIOPHYSICAL CHEMISTRY:

Standard free energy change in biochemical reactions, exergonic and endergonic reactions, hydrolysis of ATP, thermodynamics of biopolymer solutions, chain configuration of bio polymers, calculation of average dimensions. Membrane equilibrium, ion transport through cell membrane.dialosis and its function. Structure and functions of proteins, enzymes, DNA and RNA in living systems, forces involved in bio polymer interactions, electrostatic forces, hydrophobic forces, molecular expansion, and dispersion forces.

Books Suggested

1. M.N. Hughes, The Inorganic chemistry of Biological Processes, John wiley and Sons, New York 2nd Edition, 1981.
2. A Text book of Biochemistry , A.V.S.S.Rama Rao
3. Physical chemistry by Atkenes
4. Physical chemistry by Albertz.
5. Bio physical chemistry by Van Holde
6. Bio Physics by Narayanam
7. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
8. Chemistry of Natural Products, P.S.Kalsi, Kalyani Publishers.
9. Chemistry of Organic Natural Products, O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
10. Natural products Chemistry K.B.G. Torrsell, John Wiley, 1983.
11. Burger's Medicinal Chemistry, M.E. Wolff, John Wiley
12. Medicinal Chemistry, A. Kar, New Age International

CHE : IC 404: PRACTICALS (CORE & GEN.)

I) Instrumental methods of analysis- II

1. Flame Photometry: Determination of Na and K, Ca and Li in Water and Soil.
2. TLC/Paper chromatographic separation.
3. Determination of Pesticide residues by gas chromatographic method
4. Polarography: a) Determination of E ½ of Zn and Cd; b) Determination of amounts of Zn and Cd
5. Atomic Absorption Spectroscopy: Determination of transition metal ions (Cd, Cr, Cu, Pb, Zn etc.,) by AAS.
6. Separation of Metal ion by Solvent Extraction /Ion exchange.

II DEMONSTRATION EXPERIMENTS

1. IR – Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard materials
2. AAS: Demonstration of AAS – Determination of Zn, Cd, Pb, Mn, Fe and Ni in effluents using AAS.
3. Spectrofluorimetry – estimation of quinine and fluoroscene
4. Ion selective electrodes – estimation of F⁻, S²⁻ and CN⁻ in effluents using ion selective electrode meter.
5. Polarography and Anode stripping voltametry
(a) Polarography and Anode stripping voltametry – behavior of Cd, Zn, Pb in a mixture.
(b) Determination of Pb and Cd in samples using Anode stripping voltametr
6. Gas chromatography- Determination of pesticides
7. HPLC- Determination of pesticides
8. NMR
(a) Demonstration of NMR spectrometer and study of hydrogen bonding in a given alcohol or phenol.
(b) Interpretation of NMR chemical shifts of ethyl benzene, ethyl alcohol
9. TGA, DTA, DSC – Demonstration of TG, DTA and DSC and study of decomposition of calcium oxalate, calcium carbonate, copper sulfate, oxalic acid.
10. pH metry
(a) Determination of alkalinity in a colored effluent using pH metric end point.
(b) Determination of purity of commercial HCl, H₂SO₄, H₃PO₄ and CH₃COOH using pH metric end point

CHE : IC 405: PROJECT WORK

CHE : IC 406 (a): (OPEN ELECTIVE) DRUG CHEMISTRY

UNIT – I: NATURAL PRODUCTS AS LEADS FOR NEW DRUGS

Occurrence, Structure and therapeutic uses of Drugs acting on Central Nervous System

- Morphine alkaloids (morphine, codeine, thebaine, heroin, pethidine)
- Cannabinoids (9-cannabinol, Tetrahydrocannabinol)
- Neuromuscular Blocking Agents (Curare, Decamethonium)
- Vinca Alkaloids (Vincristin and Vinblastin), Taxol and Taxotere, podophyllotoxin, Etoposide, Teniposide.

UNIT – II: CARDIOVASCULAR DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.

- Cardiac glycosides (ex: Digoxin, Digitoxin);
- Antihypertensive drugs (ex: Methyl dopa, Clonidine hydrochloride);
- Antiarrhythmic agents (ex: Quinidine sulfate);
- Antisymphathetic drugs (ex: Propranolol hydrochloride, Verapamil hydrochloride);
- Vasopressor drugs (ex: Prenylamine, Buphenine).

UNIT – III: AUTACOIDS

Definition, Occurrence, Isolation, Nomenclature, Classification, Synthesis, Biosynthesis and Stereochemical structures of Prostaglandins. Structural elucidation of PGE₁, PGE₂; Synthesis and biosynthesis of PGE₂, PGF_{2α}.

Structure and Biosynthesis of Thromboxane A₂ and Prostacyclin (synthesis not expected).

UNIT – IV: ANTI-INFLAMMATORY DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.

- Paracetamol, Aspirin (Antipyretic), Salol, Cinchophen, Antipyrine, Phenylbutazone.
- Indomethacin, Tolmetin, Ibuprofen, Diclofenac, Naproxen.

Books suggested:

- Medicinal Chemistry by Ashitosh Kar
- Medicinal Chemistry by D. Sriram, P. Yogeeswari
- Medicinal Chemistry by David A. Williams, Thomas L. Lemke
- Medicinal Chemistry by V. Alagarsamy
- Biochemistry by U. Satyanarayana
- Natural Products Chemistry and Applications by Sujata V. Bhat, B.A. Nagasampagi, S. Meenakshi
- Medicinal Chemistry by V.K. Ahluwalia, Madhu Chopra
- Medicinal Chemistry by Balkishen Razdar
- Advanced Practical Medicinal Chemistry by Ashutosh Kar
- Chemistry of Organic Natural Products by O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
- Chemistry of Natural Products by S. V. Bhat, B.A. Nagasampagi, M. Sivakumar
- Natural Products Chemistry by K.B.G. Torrsell, John Wiley, 1983.

CHE : IC 406(B): (OPEN ELECTIVE) Electro Analytical Techniques

Unit I

Types and Classification of Electro analytical Methods.

i) **Potentiometry**- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glasselectrodes. Determination of pH. Potentiometric titrations.

ii) **Conductometry** – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

Unit II

D.C Polarography : Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

Unit III

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography (V) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms.

Unit IV

Ion selective electrodes

Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes.

Books Suggested

1. H.W. Willard, LL.Meritt and J.A.Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (Mc Graw Hill).

M. Sc., ORGANIC CHEMISTRY
FOURTH SEMESTER
(NEP – 2020 CBCS syllabus for the students admitted from 2021-22)

CHE : OC-401: CORE THEORY: ORGANIC SYNTHESIS-I

UNIT-I: Chemistry of Organo Boran, Phosphorus, Sulfur and Silicon reagents

15Hrs

Electronic structure and bonding in Boron, Phosphorus, Sulphur and Silicon compounds-Their reactivity and applications in Organic Synthesis.

Boron Reagents-Hydroboration-Organoboranes in the formation of C-C bonds, alcohols, amines, halogen and carbonyl compounds-Free radical reactions of organoboranes.

Phosphorus Reagents- Formation of carbon-carbon double bonds-Functional group transformations – deoxygenation reactions-reactivity as electrophiles- conversion of alcohols to alkyl halides, Wittig reaction and nucleophiles - Corey-Winters reaction, Michaelis-Arbusov reaction-Perkow reaction and Mitsunobu reaction.

Sulphur Reagents- Sulphur ylides, stabilized and non-stabilized – Preparation and reactivity Pummerer reaction – sulphonyl carbanions-Julia reaction

Silicon reagents-Peterson's olefination, influence of trialkyl silyl reagents in electrophilic reactions, aryl silanes, alkenyl silanes, alkynyl silanes, allyl silanes.

UNIT-II: PHOTOCHEMISTRY

15Hrs

Photochemical energy, photochemical excitations, Franck-Condon principle, electronic transitions, Jablonski diagram, singlet and triplet states, energy transfer in photochemical reactions - photosensitization reactions and quantum yield.

Photochemistry of carbonyl compounds - Norrish Type-I and Norrish Type-II reactions, Photo Reduction and Paterno-Buchi reaction. Photochemistry of α,β -unsaturated ketones, enones, dienones and p-benzoquinones.

Photochemistry of unsaturated systems (olefins), cis-trans isomerization and dimerization reactions, Photochemistry of conjugated dienes - 1,3-butadiene, aromatic compounds, Photoaddition (1,2- & 1,4-additions) and Photosubstitution reactions of benzene derivatives. Photo-Fries rearrangement and Barton reaction.

UNIT III: PERICYCLIC REACTIONS

15 Hrs

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3 butadiene, 1,3,5-hexatriene and allyl and pentadienyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO (Möbius Hückel) approach. Electrocyclic reactions-Conrotatory and disrotatory. $4n$, $4n+2$ and allyl systems. Cycloadditions-antarafacial and suprafacial additions, $4n$ and $4n+2$ systems, $2+2$ addition of ketene, 1,3 dipolar cycloadditions 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 Oxy-Cope rearrangements. Ene reaction

UNIT IV: SYNTHETIC POLYMERS

15 Hrs

Polymer Reactions-Addition and condensation polymerization processes- Bulk, Solution, Suspension and Emulsion polymerization.

Stereospecific Polymers-Preparation and significance- classification of polymers based on physical properties- Thermoplastics-Thermosetting plastics-Fibers and elastomers- General applications.

Preparation of Polymers-Preparation of Polymers based on different types of monomers Industrial applications-olefin polymers-Diene polymers-nylons-Glyptal resins-Urea-formaldehyde, phenol-formaldehyde and melamine resins- Epoxy resins - Ion exchange resins.

CHE : OC-402: CORE THEORY: ORGANIC SYNTHESIS-II

UNIT-I: DESIGNING OF ORGANIC SYNTHESIS-I

15 Hrs

Disconnection Approach- Classification of organic reactions. Functionalisation and interconversion of functional groups, formation of carbon-carbon single and double bonds, general strategy, disconnection and synthon approach, retrosynthetic analysis, key intermediates and starting materials in designing a synthesis, linear and convergent synthesis, reconnections. The importance of the order of events in organic synthesis,

Protecting Groups- Principles of protection of alcohol, amine, carbonyl and carboxyl groups. One group C-X and two group C-X disconnections, chemoselectivity, regioselectivity, reversal of polarity, cyclization reactions, amine synthesis.

UNIT-II: DESIGNING OF ORGANIC SYNTHESIS-II**15 Hrs**

One Group C-C Disconnections- Alcohols and carbonyl compounds, Alkene synthesis, use of acetylenic compounds in organic synthesis.

Two Group C-C Disconnections-Diels-Alder reaction, 1,3-difunctionalised compounds, unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Retrosynthesis- Retrosynthetic analysis of Longifolene, Taxol, Juvabione and Fediricamycine A.

UNIT-III: NEWER METHODS IN ORGANIC SYNTHESIS**15 Hrs**

Phase- transfer catalysis – Solid – Solid, Solid – Liquids systems – Mechanism of catalytic action, types of catalysts, application in few important reactions

Enamine mediated reactions – Formation, role of enamines as synthons for the synthesis of organic molecules.

Bio-transformations – Enzyme catalyzed reactions.

Microwave induced reactions – Principle, conditions, advantages over conventional heating methods – Applications.

Ionic liquids– Definition- Types of Ionic Liquids- Synthesis of Ionic Liquids- Selection of ionic liquids- physical properties- Application in organic synthesis- alkylation, allylation, oxidation, reduction, polymerization, hydrogenation, hydroformylation, alkoxycarbonylation, carbon-carbon bond forming reactions, alkene metathesis.

UNITIV: ANTIMALARIALS AND ANTIBIOTICS**15Hrs**

Antimalarials: Synthesis and activity of Quinoline group–Quinine, Plasmoquine and Chloroquine – Acridine group – Quinacrine – Guanidine group– Paludrine.

Antibiotics: Synthesis and activity of Penicillin, Chloramphenicol and Streptomycin–Broad spectrum antibiotics – Tetracyclines, Novobiocin.

Chemotherapy: Structure–activity relationships.

Reference Books:

1. Designing of organic synthesis. S. Warren, Wiley.
2. Organic synthesis – Concept, Methods and starting materials, J. Fuhrhop and G. Perzillin, Verlage VCH.
3. Modern Synthetic Reactions, H.O.House, W.A Benjamin.
4. Some Modern Methods of Organic Synthesis, W.Carruthers, Cambridge University Press.
5. Advanced Organic Chemistry, F.A.Carey and R.J Sundberg, Plenum.
6. Advanced Organic Chemistry, Reactions Mechanisms and Structure J. March, JohnWiley.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Blackie
8. Advanced Organic Chemistry Part A & B, F.A Carey and R.J Sunderg, Plenum Press.
9. Reaction Mechanism in Organic Chemistry, P.S.Kalsi, New Age International.
10. Text book of organic chemistry Vol.2, I.L. Finar, ELBS.
11. New Trends in Green Chemistry by V.K.Ahluwalia, M.Kidwai.
12. Green Chemistry: Environment Friendly Alternatives by Rashmi Sanghi, M M Srivastava
13. Green Solvents for Organic Synthesis by V.K. Ahluwalia, Rajender S.Varma
14. Green Analytical Chemistry by Mihkel Koel and Mihkel Kaljurand

CHE : OC-403(A) : (GENERIC ELECTIVE): HETEROCYCLES AND NATURAL PRODUCTS**UNIT-I: NOMENCLATURE AND FIVE MEMBERED HETEROCYCLES****15 HRS**

Systematic nomenclature (Hantzsch-Widman nomenclature) for fused and bridged heterocycles, Five membered heterocycles with two heteroatoms: Synthesis and reactions of pyrazole, imidazole, isoxazole, oxazole, isothiazole and thiazole

UNIT-II: BENZOFUSED FIVE MEMBERED AND SIX MEMBERED HETEROCYCLES 15 HRS

Benzofused five membered heterocycles: Synthesis and reactions of Benzopyrazoles, Benzimidazoles and Benzoxazoles

Six Membered heterocycles with two or more heteroatoms: Synthesis and reactions of diazines (pyridazine, pyrimidine & pyrazine) and triazines (1,2,3-, 1,2,4- 1,3,5- triazines)

UNIT-III: STEROIDS AND HORMONES 15 HRS

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol (total synthesis not expected), Bile acids, Androsterone, Testosterone, Estrone, Progesterone. Biosynthesis of steroids.

UNIT-IV: FLAVONOIDS AND ISOFLAVONIDS 15 Hrs

Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin, Kaempferol, Quercetin, Butein, Daidzein, Biosynthesis of flavonoids and isoflavonoids: Acetate Pathway and Shikimic acid Pathway. Biological importance of flavonoids and isoflavonoids.

Reference Books:

1. Heterocyclic chemistry Vol. 1-3, R.R. Gupta, M.Kumar and V. Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon Press.
8. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
9. Introduction to Flavonoids TA Geissman

CHE : OC 403 (B): (GENERIC ELECTIVE): BIOINORGANIC, BIOORGANIC, BIOPHYSICAL CHEMISTRY

UNIT-I: BIO-INORGANIC CHEMISTRY- I 15 Hrs

Metal complexes as oxygen carriers –Heme proteins –Hemoglobin and myoglobin –Non heme proteins – hemerythrin and hemocyanin – model synthetic complexes of iron, cobalt and copper. Co-enzymes Vitamin B₁₂, carboxy peptidase and superoxidedismutase.

Electron Transfer in Biology: Structure and functions of metalloproteins in electron transfer processes – catalase –peroxidase –cytochromes and iron –sulphur proteins –synthetic models.

UNIT – II: BIOINORGANIC CHEMISTRY- II 15 Hrs

Metal ion transport and storage in biological systems, Metal ions in Biology, Molecular mechanism of ion transport across membranes: ionophores, photosynthesis.

Hydrolytic metalloenzymes: Carbonic anhydrase, carboxy peptidase, calcium in control processes, calcium and muscle contraction, calcium and secretion, calcium in blood clotting mechanisms. Therapeutic uses of enzymes.

Importance of trace metals in biology: Metal ions as chelating agents in medicine, trace metal ions and metal and non-metal deficiency. Biological nitrogen fixation, in-vivo and in-vitro nitrogen fixation.

UNIT-III: BIOORGANIC CHEMISTRY 15 Hrs

Carbohydrates: Structure and biological functions of mucopolysaccharides, glycoproteins, and glycolipids- Role of sugars in biological recognition- Blood group substances

Lipids: Essential fatty acids-structure and function of triglycerols, Glycerophospholipids, cholesterol, bile acids prostaglandins- composition and functioning of lipoproteins

Enzymes: Nomenclature and classification, properties, factors affecting enzyme catalysis, enzyme inhibition- reversible and irreversible inhibition. Uses of enzymes in food drink industry and clinical laboratories.

UNIT-IV: BIOPHYSICAL CHEMISTRY 15 Hrs

Standard free energy change in biochemical reactions, exergonic and endergonic reactions, hydrolysis of ATP, thermodynamics of biopolymer solutions, chain configuration of bio polymers, calculation of average dimensions. Membrane equilibrium, ion transport through cell membrane, dialysis and its function. Structure and functions of proteins, enzymes, DNA and RNA in living systems, forces involved in bio polymer interactions, electrostatic forces, hydrophobic forces, molecular expansion, and dispersion forces.

Books Suggested

- 1.M.N. Hughes, The Inorganic chemistry of Biological Processes, John Wiley and Sons, New York 2nd Edition, 1981.
- 2.A Text book of Biochemistry , A.V.S.S.Rama Rao
- 3.Physical chemistry by Atkenes
- 4.Physical chemistry by Albertz.
- 5.Bio physical chemistry by Van Holde
- 6.Bio Physics by Narayanam
- 7.Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
- 8.Chemistry of Natural Products, P.S.Kalsi, Kalyani Publishers.
- 9.Chemistry of Organic Natural Products, O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
- 10.Natural products Chemistry K.B.G. Torssell, John Wiley, 1983.
- 11.Burger's Medicinal Chemistry, M.E. Wolff, John Wiley
- 12.Medicinal Chemistry, A. Kar, New Age International

CHE : OC 404: PRACTICALS (CORE & GEN.)

Spectral identification of organic compounds by UV, IR, NMR (^1H & ^{13}C) & Mass spectroscopy.

DEMONSTRATION EXPERIMENTS

- 1 IR – Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard materials
- 2 AAS: Demonstration of AAS – Determination of Zn, Cd, Pb, Mn, Fe and Ni in effluents using AAS.
- 3 Spectrofluorimetry – estimation of quinine and fluorescein
- 4 Ion selective electrodes – estimation of F^- , S^{2-} and CN^- in effluents using ion selective electrode meter.
- 5 Polarography and Anode stripping voltammetry
 - (a) Polarography and Anode stripping voltammetry – behavior of Cd, Zn, Pb in a mixture.
 - (b) Determination of Pb and Cd in samples using Anode stripping voltammetry
- 6 Gas chromatography- Determination of pesticides
- 7 HPLC- Determination of pesticides
- 8 NMR
 - (a) Demonstration of NMR spectrometer and study of hydrogen bonding in a given alcohol or phenol.
 - (b) Interpretation of NMR chemical shifts of ethyl benzene, ethyl alcohol
- 9 TGA, DTA, DSC – Demonstration of TG, DTA and DSC and study of decomposition of calcium oxalate, calcium carbonate, copper sulfate, oxalic acid.
- 10 pH metry
 - (a) Determination of alkalinity in a colored effluent using pH metric end point.
 - (b) Determination of purity of commercial HCl, H_2SO_4 , H_3PO_4 and CH_3COOH using pH metric end point

CHE : OC 405: PROJECT WORK**CHE : OC : 406 (A): OPEN ELECTIVE: DRUG CHEMISTRY****UNIT – I: NATURAL PRODUCTS AS LEADS FOR NEW DRUGS****15 Hrs**

Occurrence, Structure and therapeutic uses of Drugs acting on Central Nervous System
Morphine alkaloids (morphine, codeine, thebaine, heroin, pethidine)
Cannabinoids (9-cannabinol, Tetrahydrocannabinol)
Neuromuscular Blocking Agents (Curare, Decamethonium)
Vinca Alkaloids (Vincristin and Vinblastin), Taxol and Taxotere, podophyllotoxin, Etoposide, Teniposide.

UNIT – II: CARDIOVASCULAR DRUGS**15 Hrs**

Definition, Classification, Nomenclature, Structure and Synthesis.
Cardiac glycosides (ex: Digoxin, Digitoxin);
Antihypertensive drugs (ex: Methyl dopa, Clonidine hydrochloride);
Antiarrhythmic agents (ex: Quinidine sulfate);
Antisymphathetic drugs (ex: Propranolol hydrochloride, Verapamil hydrochloride);
Vasopressor drugs (ex: Prenylamine, Buphenine).

UNIT – III: AUTACOIDS**15 Hrs**

Definition, Occurrence, Isolation, Nomenclature, Classification, Synthesis, Biosynthesis and Stereochemical structures of Prostaglandins. Structural elucidation of PGE₁, PGE₂; Synthesis and biosynthesis of PGE₂, PGF_{2α}. Structure and Biosynthesis of Thromboxane A₂ and Prostacyclin (synthesis not expected).

UNIT – IV: ANTI-INFLAMMATORY DRUGS

15 Hrs

Definition, Classification, Nomenclature, Structure and Synthesis.

Paracetamol, Aspirin (Antipyretic), Salol, Cinchophen, Antipyrine, Phenylbutazone.

Indomethacin, Tolmetin, Ibuprofen, Diclofenac, Naproxen.

Books suggested:

1. Medicinal Chemistry by Ashitosh Kar
2. Medicinal Chemistry by D. Sriram, P. Yogeeswari
3. Medicinal Chemistry by David A. Williams, Thomas L. Lemke
4. Medicinal Chemistry by V. Alagarsamy
5. Biochemistry by U. Satyanarayana
6. Natural Products Chemistry and Applications by Sujata V. Bhat, B.A. Nagasampagi, S. Meenakshi
7. Medicinal Chemistry by V.K. Ahluwalia, Madhu Chopra
8. Medicinal Chemistry by Balkishen Razdar
9. Advanced Practical Medicinal Chemistry by Ashutosh Kar
10. Chemistry of Organic Natural Products by O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
11. Chemistry of Natural Products by S. V. Bhat, B.A. Nagasampagi, M. Sivakumar
12. Natural Products Chemistry by K.B.G. Torrsell, John Wiley, 1983.

CHE : OC : 406(B): OPEN ELECTIVE:ELECTRO ANALYTICAL TECHNIQUES

Unit I

15 Hrs

Types and Classification of Electro analytical Methods.

i) **Potentiometry**- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of pH. Potentiometric titrations.

ii) **Conductometry** – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

Unit II

15 Hrs

D.C Polarography : Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

Unit III

15 Hrs

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography(V) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms.

Unit IV

15 Hrs

Ion selective electrodes

Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes.

Books Suggested

1. H.W. Willard, LL.Merrit and J.A.Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (Mc Graw Hill).

M. Sc., ENVIRONMENTAL CHEMISTRY
FOURTH SEMESTER
(NEP – 2020 CBCS syllabus for the students admitted from 2021-22)

CHE : EC-401: CORE THEORY: ENERGY, ENVIRONMENT AND SOILS

UNIT-I: Sources of Energy

15 Hrs

Fossil fuels- Nuclear fission and fusion- Solar energy-use of solar energy in space heating and water heating- production of electricity using solar energy- solar trough collectors- power tower- solar pond- solar energy for driving vehicles- power from indirect solar energy – Hydropower- wind power- Biomass energy- production of ethanol from biomass- production of methane from biomass- photosynthesis- photo electro chemistry- Geothermal energy.

UNIT-II: Water Resources and Air

15Hrs

Hydrological cycle- physical and chemical properties of water-complexation in natural and waste water,- Anomalous properties-water pollutants-Types-Sources- Heavy metals- metalloids- organic –Inorganic – Biological and Radio active-Types of reactions in various water bodies including marine environment- Eutrophication- Ground water- Potable water standards.Treatment for portable water.

Air:Chemical reactions in the atmosphere – Aerosols types- Production and distribution – Aerosols and Radiation – structure and composition of atmosphere- temperature inversion – Global warning- Ozone depletion – Green house effect, “CFC”s- Acid rain.

UNIT-III: Soil and Green Chemistry

15 Hrs

Soil: Composition of soil- lithosphere- inorganic and organic contaminants in the soil- Biodegradation- Nondegradable waste and its effect on the environment- Bioremediation –of surface soils- Fate and transport of contaminants on soil system– Bioindicators- Soil parameters- soil destruction- Erosion- Soil conservation – Nitrogen pathways and NPK in soil .

Green Chemistry: Goals of Green chemistry- Significance and basic components of Green chemistry research - industrial applications of Green chemistry-products from natural materials- Green fuels and E-Green propellants- Zeolites- Biocatalysts.

UNIT IV: Soil pollution:

15Hrs

Introduction – soil pollution by industrial wastes. soil pollution by urban wastes, Radio active pollutants and Agricultural waste- chemical and metallic pollutants-Biological agents – mining - Detrimental effects of soil pollutants – Effects of industrial pollutants- Effects of sewage and domestic wastes- Effects of heavy metals- Effects of radio active pollutants- Effects of modern agro- technology – Diseases caused by soil pollution – solid waste management – sources and classification -public Health Aspects – methods of collection- Disposal methods – potential methods of disposal.

Books Suggested:

1. Daniel D.Chiras (1994), Environmental Science, 4th Ed.
2. Environmental Chemistry by W. Moore and J.Moore
3. Environmental chemistry by J.O.M. Bockariss
4. Environmental by BK Sharma
5. Environmental chemistry by SS Dara
6. Environmental chemistry by Mahajan
7. Environmental chemistry by a.K.De

CHE : EC-402: CORE THEORY: WATER POLLUTION MONITORING AND ENVIRONMENT LAWS

UNIT-I: Water pollution

15 Hrs

Basic aspects of water-general principles of water(physical and chemical)-criteria of water quality.Types of water pollutants: sewage and domestic wastes-industrial wastes-agriculture discharges- toxic metals-oxygen demanding wastes-disease causing agents-oils- detergents and phosphates. Sampling: Basics of Sampling, sampling procedure, statistics, sampling and physical state, crushing and grinding, hazards waste of sampling, pre-concentration methods

UNIT-II: Waste water treatment:

15 Hrs

Basic process of water treatment- primary treatment pretreatment – sedimentation – Flotation- secondary (Biological) Treatment – Active sludge process – Trickling filters – sludge Treatment and disposal – Advanced waste water Treatment – Removal of suspended solids – Removal of dissolved solids – Nitrogen removal – phosphorous removal – Advanced Biological systems – chemical oxidation .

UNIT III: Biotechnology and its application in Environmental protection**15 Hrs**

Introduction- Bio-informatics- Bio-Technology and pollution control,-Bioremediation- Biological de-odourisation- Biological purification of contaminated air-microorganisms and energy of mankind-use of microorganisms role in petroleum augmentation and recovery.

UNIT IV: Environmental Management and Important Environmental Laws:**15 Hrs**

Environmental Management: Introduction-objectives-components-environmental impact assessment (EIA)-historical background-elements of EIA process-participants in EIA processes-contents of EIS-design of EIA.

Important Environmental Laws: the world life act-the forest conservation act-the water and control pollution act-air prevention& control act—the environment act-environmental quality management standard-ISO 14000 series.

Books Suggested

1. Environmental Chemistry by W. Moore and J.Moore
2. Environmental chemistry by J.O.M. Bokriss
3. Environmental by BK Sharma
4. Environmental chemistry by SS Dara
5. Environmental chemistry by Mahajan
6. Environmental chemistry by a.K.De
7. Lodge (1994) Methods of air sampling and analysis.Publications, Jaipur
8. Kudesia, V.P. (1985) Water Pollution, Pragati Prakashan
9. Elements of biotechnology by PK Gupta and Rastogi

CHE : EC-403 (A): (GENERIC ELECTIVE): AIR POLLUTION, CONTROL METHODS-NOISE AND THERMAL POLLUTION**UNIT-I: Air Pollution****15 Hrs**

Classification and properties of air pollutants-emission sources-major emissions from global sources-importance of anthropogenic sources-behavior and fate of air pollutants photochemical smog and its effects on health-vegetation-material damage in India.

Air pollution sampling and measurement-ambient air sampling-collection of gaseous air pollutants-collection of particulate pollutants-stack sampling-analysis of air pollutants-sulphur dioxide-carbon monoxide-nitrogen dioxide-oxidants-ozone-hydro carbons and particulate matter

UNIT- II: Control methods**15 Hrs**

Sources-correction methods-particulate emission control-gravitational settling chambers-cyclone separators-fabric filters-electrostatic precipitator-wet scrubbers-control of gaseous emissions by adsorption of solids and liquids-control methods of sulphur dioxide emission , flue gasesanalysis-control method, nitrogen oxides, carbon monoxide and hydrocarbon-mobile sources.

UNIT-III: Vehicular Air Pollution:**15 Hrs**

Genesis of vehicular emissions standard- natural pollution-gasification of vehicles-point sources of air pollution – mechanism of air pollution from automobiles -automobile pollution- Indian scenario population and pollution loads of vehicles-automobile air pollution control-exhaust gas controlling treatment devices-thermal reactor-catalytic converter from automobiles-fuel tank carbonator. Air pollution from Portland cement plants-steel mills and petroleum refineries.

UNIT-IV:Noise and Thermal Pollution**15 Hrs**

Noise pollution: sources-measurement of noise and indices-effect of meteorological parameters on noise propagation-noise exposure levels and standards –measurement of noise-impact of noise on human health

Thermal pollution: Introduction-definition-sources-harmful effects-toxic compounds in traces-prevention and control of thermal pollution –thermal power projects in India.

Books Suggested:

1. Environmental Chemistry by W. Moore and J.Moore
2. Environmental chemistry by J.O.M. Bockeriss
4. Environmental chemistry by Sharmar and Kaur, Krishna Publishers
6. Environmental chemistry by a.K.De
8. Henry C perkins (1974) Air Pollution, McGraw-Hill
- 9 .Kudesia, V.P. (1985) Water Pollution, Pragati Prakashan.
- 10 . Environmental Engineering by CS Rao
11. Environmental by BK Sharma
12. Environmental chemistry by SS Dara

CHE : EC 403 (B): (GENERIC ELECTIVE): BIOINORGANIC, BIOORGANIC, BIOPHYSICAL CHEMISTRY

UNIT-I: BIO-INORGANIC CHEMISTRY- I

15 Hrs

Metal complexes as oxygen carriers –Heme proteins –Hemoglobin and myoglobin –Non heme proteins – hemerythrin and hemocyanin – model synthetic complexes of iron, cobalt and copper. Co-enzymes Vitamin B₁₂, carboxy peptidase and superoxidedismutase.

Electron Transfer in Biology: Structure and functions of metalloproteins in electron transfer processes – catalase –peroxidase –cytochromes and iron –sulphur proteins –synthetic models.

UNIT – II: BIOINORGANIC CHEMISTRY- II: Metal ion transport and storage in biological systems, Metal ions in Biology, Molecular mechanism of ion transport across membranes: ionophores, photosynthesis.

Hydrolytic metalloenzymes: Carbonic anhydrase, carboxy peptidase, calcium in control processes, calcium and muscle contraction, calcium and secretion, calcium in blood clotting mechanisms. Therapeutic uses of enzymes.

Importance of trace metals in biology: Metal ions as chelating agents in medicine, trace metal ions and metal and non-metal deficiency. Biological nitrogen fixation, in-vivo and in-vitro nitrogen fixation.

UNIT-III: BIOORGANIC CHEMISTRY

Carbohydrates: Structure and biological functions of mucopolysaccharides, glycoproteins, and glycolipids- Role of sugars in biological recognition- Blood group substances

Lipids: Essential fatty acids-structure and function of triglycerols, Glycerophospholipids, cholesterol, bile acids prostaglandins- composition and functioning of lipoproteins

Enzymes: Nomenclature and classification, properties, factors affecting enzyme catalysis, enzyme inhibition- reversible and irreversible inhibition. Uses of enzymes in food drink industry and clinical laboratories.

UNIT-IV: BIOPHYSICAL CHEMISTRY:

Standard free energy change in biochemical reactions, exergonic and endergonic reactions, hydrolysis of ATP, thermodynamics of biopolymer solutions, chain configuration of bio polymers, calculation of average dimensions. Membrane equilibrium, ion transport through cell membrane, dialysis and its function. Structure and functions of proteins, enzymes, DNA and RNA in living systems, forces involved in bio polymer interactions, electrostatic forces, hydrophobic forces, molecular expansion, and dispersion forces.

Books Suggested

1. M.N. Hughes, The Inorganic chemistry of Biological Processes, John Wiley and Sons, New York 2nd Edition, 1981.
2. A Text book of Biochemistry, A.V.S.S. Rama Rao
3. Physical chemistry by Atkins
4. Physical chemistry by Albertz.
5. Bio physical chemistry by Van Holde
6. Bio Physics by Narayanam
7. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
8. Chemistry of Natural Products, P.S. Kalsi, Kalyani Publishers.
9. Chemistry of Organic Natural Products, O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
10. Natural products Chemistry K.B.G. Torrsell, John Wiley, 1983.
11. Burger's Medicinal Chemistry, M.E. Wolff, John Wiley
12. Medicinal Chemistry, A. Kar, New Age International

CHE : EC-404: PRACTICALS (CORE & GEN.) : INSTRUMENTAL METHODS OF ANALYSIS -II

1) Conductometry:

- a) Mixture of Acids
- b) Mixture of Halides

2) Colorimetry:

- a) Estimation of Iron
- b) Manganese
- c) Phosphate
- d) Titration of copper Vs EDTA

DEMONSTRATION EXPERIMENTS

- 1 IR – Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard materials
- 2 AAS: Demonstration of AAS – Determination of Zn, Cd, Pb, Mn, Fe and Ni in effluents using AAS.
- 3 Spectrofluorimetry – estimation of quinine and fluorescein

- 4 Ion selective electrodes – estimation of F^- , S^{2-} and CN^- in effluents using ion selective electrode meter.
- 5 Polarography and Anode stripping voltametry
 - (a) Polarography and Anode stripping voltametry – behavior of Cd, Zn, Pb in a mixture.
 - (b) Determination of Pb and Cd in samples using Anode stripping voltametry
- 6 Gas chromatography- Determination of pesticides
- 7 HPLC- Determination of pesticides
- 8 pH metry
 - (a) Determination of alkalinity in a colored effluent using pH metric end point.
 - (b) Determination of purity of commercial HCl, H_2SO_4 , H_3PO_4 and CH_3COOH using pH metric end point.

CHE : EC- 405: PROJECT WORK

CHE : EC : 406 (A): OPEN ELECTIVE: DRUG CHEMISTRY

UNIT – I: NATURAL PRODUCTS AS LEADS FOR NEW DRUGS

Occurrence, Structure and therapeutic uses of Drugs acting on Central Nervous System. Morphine alkaloids (morphine, codeine, thebaine, heroin, pethidine) Cannabinoids (9-cannabinol, Tetrahydrocannabinol) Neuromuscular Blocking Agents (Curare, Decamethonium) Vinca Alkaloids (Vincristin and Vinblastin), Taxol and Taxotere, podophyllotoxin, Etoposide, Teniposide.

UNIT – II: CARDIOVASCULAR DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.

Cardiac glycosides (ex: Digoxin, Digitoxin);

Antihypertensive drugs (ex: Methyl dopa, Clonidine hydrochloride);

Antiarrhythmic agents (ex: Quinidine sulfate);

Antisymphetic drugs (ex: Propranolol hydrochloride, Verapamil hydrochloride);

Vasopressor drugs (ex: Prenylamine, Buphenine).

UNIT – III: AUTACOIDS

Definition, Occurrence, Isolation, Nomenclature, Classification, Synthesis, Biosynthesis and Stereochemical structures of Prostaglandins. Structural elucidation of PGE_1 , PGE_2 ; Synthesis and biosynthesis of PGE_2 , $PGF_{2\alpha}$. Structure and Biosynthesis of Thromboxane A₂ and Prostacyclin (synthesis not expected).

UNIT – IV: ANTI-INFLAMMATORY DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.

Paracetamol, Aspirin (Antipyretic), Salol, Cinchophen, Antipyrine, Phenylbutazone.

Indomethacin, Tolmetin, Ibuprofen, Diclofenac, Naproxen.

Books suggested:

- 1 Medicinal Chemistry by Ashitosh Kar
- 2 Medicinal Chemistry by D. Sriram, P. Yogeeswari
- 3 Medicinal Chemistry by David A. Williams, Thomas L. Lemke
- 4 Medicinal Chemistry by V. Alagarsamy
- 5 Biochemistry by U. Satyanarayana
- 6 Natural Products Chemistry and Applications by Sujata V. Bhat, B.A. Nagasampagi, S. Meenakshi
- 7 Medicinal Chemistry by V.K. Ahluwalia, Madhu Chopra
- 8 Medicinal Chemistry by Balkishen Razdar
- 9 Advanced Practical Medicinal Chemistry by Ashutosh Kar
- 10 Chemistry of Organic Natural Products by O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
- 11 Chemistry of Natural Products by S. V. Bhat, B.A. Nagasampagi, M. Sivakumar
- 12 Natural Products Chemistry by K.B.G. Torrsell, John Wiley, 1983.

CHE : EC : 406(B): OPEN ELECTIVE: ELECTRO ANALYTICAL TECHNIQUES

Unit I Types and Classification of Electro analytical Methods.

i) Potentiometry- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of pH. Potentiometric titrations.

ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

Unit II D.C Polarography :. Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

Unit III (i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography(V) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms.

Unit IV Ion selective electrodes

Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes.

Books Suggested

1. H.W. Willard, LL.Meritt and J.A.Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (Mc Graw Hill).

M. Sc., PHYSICAL CHEMISTRY
FOURTH SEMESTER
(NEP – 2020 CBCS syllabus effective from 2021-2022)

CHE : PC-401: CORE THEORY: ELECTROCHEMISTRY

UNIT-I: Industrial Electrochemistry

15 Hrs

Deposition of metals, Factors influencing physical nature of electrodeposited metals – current density, concentration of electrolyte, temperature, colloidal matter, electrolyte and basis metal. Throwing power, simultaneous discharge of cations. Separation of metals by electrolysis. Electrochemical passivity. Passivity and current density. Chemical passivity. Theories of passivity. Mechanical passivity.

The corrosion of metals. Hydrogen evolution type of corrosion, corrosion in presence of depolarizer. Differential oxygenation corrosion. Methods of corrosion protection.

UNIT- II: Electrochemical Devices:

15 Hrs

Batteries- their performance – characteristics – considerations in the selection and applications, Chemistry of primary batteries – Zinc – Carbon, Mercuric oxide, silver oxide and lithium cells – Solid electrolyte cells.

Chemistry of secondary batteries – Lead acid, Nickel cadmium batteries, Water activated batteries, Fuel cells – Their thermodynamics- performance. Advantages of fuel cells.

UNIT-III: Electrokinetic's and Electro capillary phenomena:

15 Hrs

Electrical double layer, Helmholtz – Perrin, Gouy – Chapman and Stern theories of electrical double layer. Lipmann equation.

Electrokinetic effect: Electro osmosis, Electrophoresis, streaming potential, sedimentation potential and their relation to zeta potential. Determination of zeta potential from electrophoresis measurements. Tiselius apparatus.

Electro capillary curves, Null points of metals and their experimental determination.

UNIT-IV: Electrochemical Oxidation-Reduction:

(A) Oxidation-Reduction systems

15 Hrs

Oxidation-Reduction potentials, types of reversible Oxidation-Reduction systems, determination of standard Oxidation-Reduction potentials, Oxidation-Reduction Indicators, Indicators of Biological systems, Indicator for volumetric analysis.

(B) Electrolytic Oxidation-Reductions

Electrolytic Oxidation-Reduction, Reversible oxidation-reduction process, Non-Reversible process, Oxidation of Fatty acids: The Kolbe reaction, The Brown-Walker Electrosynthesis, Formation of Chromate and Periodate.

Books suggested:

1. S. Glasstone. An introduction to Electrochemistry. Affiliated East-West Press Pvt. Ltd.
2. P.T.K.Kissinger, W.R.Heinemann. Laboratory Techniques in Electro analytical Chemistry, Marsal Debber, Inc.
3. Willard, Merit. Instrumental methods of analysis, Welowarth Publishing Co.,
4. L.Antropov. Theoretical Electrochemistry. Mir Publications.
5. Silbey, Alberty, Bawendi. Physical chemistry. Jhon-Wiley & sons. 4th edition-2006.
6. V.S. Bagotsky. Fundamental of Electrochemistry. Jhon Wiley & Sons. 2nd editions-2006.
7. Introduction to polarography and allied Technique by Dr.K. Zutshi

CHE : PC-402: CORE THEORY: THERMODYNAMICS, POLYMERS AND SOLID STATE CHEMISTRY

UNIT-I: Thermodynamic properties of fluids:

15 Hrs

Thermodynamic relationship residual properties – systems of variable composition- ideal and non-ideal behaviour – fugacity-fugacity coefficient in solutions- Phase equilibrium of low to moderate pressures- dew point-bubble point and flash calculations.

UNIT – II: Thermodynamic properties of ‘Liquid Mixtures:

15 Hrs

Activity and activity coefficients-excess free energy-excess enthalpy-excess volume-excess entropy-relation between excess functions and activity coefficients –Application of Gibbs-Deuhem equation-regular solutions –van Laar theory and Scachard-Hildebrand theory.

UNIT-III: Polymers- structure and properties**15 Hrs**

Morphology and order in crystalline polymers, configuration of Polymer chains, crystal structures and polymers, Stain induced morphology, morphology of chrystalline polymers, crystallisation and melting-polymer structure and physical properties, crystalline melting point, T_m -melting point of homogeneous series, effect of chain flexibility and other steric factors- entropy and heat of fusion, the glass transition temperature, T_g , relationship between T_m and T_g effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking.

UNIT-IV: Solid State Chemistry**15 Hrs**

Magnetic properties of solids- Classification of magnetic materials, Magnetic Susceptibility, Langevin diamagnetism, Weiss theory of para magnetism.

Electronic properties of metals, insulators and semi conductors: Electronic Structure of solids, Band theory, band Structure of metals, insulators and semiconductors. Electrons, holes and Excitons. The temperature dependence of conductivity of extrinsic semi conductors. Photo conductivity and photovoltaic effect –P-n-Junctions.

Super conductivity: Occurrence of superconductivity. Destruction of Superconductivity by magnetic fields- Meisner effect. Types of superconductors. Theories of super conductivity BCS theory.

Books suggested:

1. J.M.Pransnitz. Molecular Thermodynamics of Fluid Phase Equilibrium. Prentice. Hall
2. Kuriocose and Rajram. Thermodynamics
3. Smith and Van Ners. Chemical Thermodynamics.
4. R.C. Srivastava, Subi.K.saha. Thermodynamics-A care course. Prentice-Hall of India Pvt, Ltd, 3rd edition-2007.
5. Silbey, Alberty, Bawendi. Physical chemistry. Jhon-Wiley & sons. 4th edition-2006.
6. F. W. Billmeyer, Jr.: Text Book of Polymer Science. Wiley Interscience.
7. V. R. Gowariker, N. V. Viswanathan, Jayadev Sreedhar.: polymer Science. New Age international Publishers.
8. Solid State chemistry by M.G.Arora
9. Solid State Chemistry by Wiley.

CHE : PC-403(A) : (GENERIC ELECTIVE): CHEMICAL KINETICS**UNIT – I: Catalysis****15 Hrs**

Homogeneous catalysis: Steady state and equilibrium treatments of acid-base catalysis. Skrabal P^H diagrams, Protolytic and Prototropic mechanism. Acidity functions, Zucker, Hammett, Bunnett and Yates hypothesis in the elucidation of the mechanism. Enzyme catalysis – influence of concentration, P^H and temperature. **Heterogeneous Catalysis:** Mechanism of interface reactions, application of transition state theories to unimolecular and bimolecular surface reactions

UNIT – II: Photochemistry:**15 Hrs**

Interaction of electromagnetic radiation with matter, laws of photochemistry, Quantum yield, types of excitations, Fate of excited molecule, transfer of excitation energy, kinetics of unimolecular and bimolecular photophysical process, Stern-Volmer equation, Kinetics of photochemical reaction rate constants and life times of reactive energy states, determination of rate constants of reactions, effect of light intensity on the rate of photochemical reactions.

UNIT-III: Electrochemical relaxation methods, Photochemical methods, Isotopic effect**15 Hrs**

Electrochemical relaxation methods: Introduction , advantages of Electrochemical transient (or) relaxation techniques, application of these methods, various types of perturbation of a system, pulse polarography, chronopotentiometry, investigation of kinetic currents by chronopotentiometry.

Photochemical methods: Introduction , phenomena of ISC, fluorescence and phosphorescence, experimental arrangement of fluorescence measurements. Example of quenching reactions.

Isotopic Effects: Equilibrium isotope effects, equilibria in solution, primary kinetic isotopic effects semiclassical treatments, Quantum-mechanical Tunneling, Reactions of the Type $H+H_2$, Transfer of H^+ , H and H^- reactions of Huonium, Isotope effect with Havier atoms.

Unit-IV: Photo Chemical and Radiation Chemical Reactions**15 Hrs**

Photochemical reactions photochemical primary process, reactions of electronically excited states of species, photo chemical thresholds, laws of photochemical equivalence, rotating-sector technique, multi photon excitation, photosensitization, radiation chemical primary process, chemiluminescence.

Books suggested:

1. K.K.Rohatgi Mukerjee. Fundamentals of Photochemistry
2. B. Viswanathan, S. Sivasankar, A.V. Ramaswamy Catalysis principals and Applications. Narosa Publications House, 2007.
3. C. Kalidas. Principles of fast reactions techniques and Applications.
4. V. Yegnaramam,C.A. Basha And G. Prabhakar Rao : Applications of Electrochemistry.
5. Keith J.Laidler: Chemical Kinetics
6. J.Dalton: A New System of Chemical Philosophy.
7. Chemical Kinetics:Keith J.Laider

CHE : PC : 403 (B): (GENERIC ELECTIVE): BIOINORGANIC, BIOORGANIC, BIOPHYSICAL CHEMISTRY**UNIT-I: BIO-INORGANIC CHEMISTRY- I****15 Hrs**

Metal complexes as oxygen carriers –Heme proteins –Hemoglobin and myoglobin –Non heme proteins – hemerythrin and hemocyanin – model synthetic complexes of iron, cobalt and copper.Co-enzymes Vitamin B₁₂,carboxy peptidase and superoxidedismutase.

Electron Transfer in Biology: Structure and functions of metalloproteins in electron transfer processes – catalase –peroxidase –cytochromes and iron –sulphur proteins –synthetic models.

UNIT – II: BIOINORGANIC CHEMISTRY- II: Metal ion transport and storage in biological systems, Metal ions in Biology, Molecular mechanism of ion transport across membranes: ionophores, photosynthesis.

Hydrolytic metalloenzymes: Carbonic anhydrase, carboxy peptidase, calcium in control processes, calcium and muscle contraction, calcium and secretion, calcium in blood clotting mechanisms. Therapeutic uses of enzymes.

Importance of trace metals in biology: Metal ions as chelating agents in medicine, trace metal ions and metal and non-metal deficiency. Biological nitrogen fixation,in-vivo and in-vitro nitrogen fixation.

UNIT-III: BIOORGANIC CHEMISTRY

Carbohydrates: Structure and biological functions of mucopolysaccharides, glycoproteins, and glycolipids- Role of sugars in biological recognition- Blood group substances

Lipids: Essential fatty acids-structure and function of triglycerols, Glycerophospholipids, cholesterol, bile acids prostaglandins- composition and functioning of lipoproteins

Enzymes: Nomenclature and classification, properties, factors affecting enzyme catalysis, enzyme inhibition-reversible and irreversible inhibition. Uses of enzymes in food drink industry and clinical laboratories.

UNIT-IV: BIOPHYSICAL CHEMISTRY:

Standard free energy change in biochemical reactions, exergonic and endergonic reactions, hydrolysis of ATP, thermodynamics of biopolymer solutions, chain configuration of bio polymers, calculation of average dimensions. Membrane equilibrium, ion transport through cell membrane.dialysis and its function. Structure and functions of proteins, enzymes, DNA and RNA in living systems, forces involved in bio polymer interactions, electrostatic forces, hydrophobic forces, molecular expansion, and dispersion forces.

Books Suggested

1. M.N. Hughes, The Inorganic chemistry of Biological Processes, John wiley and Sons, New York 2nd Edition, 1981.
2. A Text book of Biochemistry , A.V.S.S.Rama Rao
3. Physical chemistry by Atkenes
4. Physical chemistry by Albertz.
5. Bio physical chemistry by Van Holde
6. Bio Physics by Narayanam
7. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
8. Chemistry of Natural Products, P.S.Kalsi, Kalyani Publishers.
9. Chemistry of Organic Natural Products, O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
10. Natural products Chemistry K.B.G. Torrsell, John Wiley, 1983.
11. Burger's Medicinal Chemistry, M.E. Wolff, John Wiley
12. Medicinal Chemistry, A. Kar, New Age International

CHE : PC-404: PRACTICALS (CORE & GEN.) INSTRUMENTAL METHODS OF ANALYSIS

1. Potentiometry: a) Titration of mixture of acids

- b) Titration of mixture of halides
- c) Titration of ferrous ammonium sulphate with potassium dichromate
- d) Redox titrations
- e) Solubility of Sparingly soluble salt.
- f) Formula and instability constant of a complex
- g) Dissociation constant of acetic acid

Polarography: a) Determination of $E_{1/2}$ of Zn and Cd

- b) Determination of Zn and Cd in mixture
- c) Amperometric titration

DEMONSTRATION EXPERIMENTS

1. IR – Interpretation of IR spectrum of alcohols, ketones, aldehydes and other standard materials
2. AAS: Demonstration of AAS – Determination of Zn, Cd, Pb, Mn, Fe and Ni in effluents using AAS.
3. Spectrofluorimetry – estimation of quinine and fluoresceine
4. Ion selective electrodes – estimation of F^- , S^{2-} and CN^- in effluents using ion selective electrode meter.
5. Polarography and Anode stripping voltametry
 - (a) Polarography and Anode stripping voltametry – behavior of Cd, Zn, Pb in a mixture.
 - (b) Determination of Pb and Cd in samples using Anode stripping voltametr
6. Gas chromatography- Determination of pesticides
7. HPLC- Determination of pesticides
8. pH metry
 - (a) Determination of alkalinity in a colored effluent using pH metric end point.
 - (b) Determination of purity of commercial HCl, H_2SO_4 , H_3PO_4 and CH_3COOH using pH metric end point.

CHE : PC-405 :PROJECT WORK

CHE : PC : 406 (A): OPEN ELECTIVE: DRUG CHEMISTRY

UNIT – I: NATURAL PRODUCTS AS LEADS FOR NEW DRUGS

Occurrence, Structure and therapeutic uses of Drugs acting on Central Nervous System

Morphine alkaloids (morphine, codeine, thebaine, heroin, pethidine)

Cannabinoids (9-cannabinol, Tetrahydrocannabinol)

Neuromuscular Blocking Agents (Curare, Decamethonium)

Vinca Alkaloids (Vincristin and Vinblastin), Taxol and Taxotere, podophyllotoxin, Etoposide, Teniposide.

UNIT – II: CARDIOVASCULAR DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.

Cardiac glycosides (ex: Digoxin, Digitoxin);

Antihypertensive drugs (ex: Methyl dopa, Clonidine hydrochloride);

Antiarrhythmic agents (ex: Quinidine sulfate);

Antisymphathetic drugs (ex: Propranolol hydrochloride, Verapamil hydrochloride);

Vasopressor drugs (ex: Prenylamine, Buphenine).

UNIT – III: AUTACOIDS

Definition, Occurrence, Isolation, Nomenclature, Classification, Synthesis, Biosynthesis and Stereochemical structures of Prostaglandins. Structural elucidation of PGE_1 , PGE_2 ; Synthesis and biosynthesis of PGE_2 , $PGF_{2\alpha}$.

Structure and Biosynthesis of Thromboxane A₂ and Prostacyclin (synthesis not expected).

UNIT – IV: ANTI-INFLAMMATORY DRUGS

Definition, Classification, Nomenclature, Structure and Synthesis.

Paracetamol, Aspirin (Antipyretic), Salol, Cinchophen, Antipyrine, Phenylbutazone.

Indomethacin, Tolmetin, Ibuprofen, Diclofenac, Naproxen.

Books suggested:

1. Medicinal Chemistry by Ashitosh Kar
2. Medicinal Chemistry by D. Sriram, P. Yogeeswari
3. Medicinal Chemistry by David A. Williams, Thomas L. Lemke
4. Medicinal Chemistry by V. Alagarsamy

5. Biochemistry by U. Satyanarayana
6. Natural Products Chemistry and Applications by Sujata V. Bhat, B.A. Nagasampagi, S. Meenakshi
7. Medicinal Chemistry by V.K. Ahluwalia, Madhu Chopra
8. Medicinal Chemistry by Balkishen Razdar
9. Advanced Practical Medicinal Chemistry by Ashutosh Kar
10. Chemistry of Organic Natural Products by O. P. Agarwal, Vols., 1 & 2, Geol Pubs.
11. Chemistry of Natural Products by S. V. Bhat, B.A. Nagasampagi, M. Sivakumar
12. Natural Products Chemistry by K.B.G. Torrsell, John Wiley, 1983.

CHE : PC : 406(B): OPEN ELECTIVE: ELECTRO ANALYTICAL TECHNIQUES

Unit I

Types and Classification of Electro analytical Methods.

i) Potentiometry- Types of electrodes, Hydrogen gas, Calomel, Quin hydrone and glass electrodes. Determination of pH. Potentiometric titrations.

ii) Conductometry – Definition of terms – conductivity, specific conductivity, cell constant. Mobility of ions, Conductometric titrations.

Unit II

D.C Polarography : Dropping mercury electrode- Instrumentation-polarogram. Types of Currents : Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not necessary) and its consequences. Types of limiting Currents: Adsorption, Diffusion, Kinetic. Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

Unit III

(i) A.C.polarography (ii) Square-wave polarography (iii) Pulse polarography (iv) Differential pulse polarography(V) Cyclic Voltammetry: Principle, instrumentation, reversible and irreversible cyclic voltammograms.

Unit IV

Ion selective electrodes

Ion-sensitive electrodes –types of ion sensitive electrodes –metal based cation and anion sensitive electrodes, solid membrane electrodes. Liquid ion-exchange electrodes, gas sensing membrane electrodes.

Books Suggested

1. H.W. Willard, LL.Merrit and J.A.Dean: Instrumental Methods of Analysis. Affiliated East-West).
2. G.H. Jeffery J. Bassett, J. Mendham and R.C. Denny. Vogel's Text Book of Quantitative Chemical Analysis (ELBS).
3. D.A. Skoog and D.M. West: Principles of Instrumental Analysis (Holt, Rinehart and Wilson).
4. J.G. Dick : Analytical Chemistry (Mc Graw Hill).

IV SEMESTER CHEMISTRY INFORMATICS AND DRUGY DELIVERY

UNIT – I : Basic Principles of Pharmacology

Introduction, definitions

ii. Pharmacokinetics (ADME)

Routes of drug administration

Absorption, distribution, metabolism and excretion of drugs Bioavailability

iii. Pharmacodynamics

Principles of drug action

Theories of drug action

(Occupancy theory, rate theory, induced fit theory and macro molecular perturbation theory)

Mechanism of drug action

Drug synergism and antagonism

Drug toxicity.

UNIT – II : Drug design And Lead Modifications

Introduction, Lead discovery, Folklore drugs, Lead modifications, Structure Pruning techniques taking morphine (naturally occurring alkaloid) as a pharmacophore. Uses of physiochemical properties in drug designing like Lipophilic barrier to drugs pKa, pH Partition theory Ionisation, hydrogen bonding Stereochemical properties, Bio-isosterism and its applications Structure activity relationship (SAR) in drug desing SAR of Barbiturates, Benzodiazepines and sulpha drugs. QSAR methods and parameters in drug desing Prodrug, classification of prodrugs.