Department of Chemistry

The Postgraduate programme in chemistry is designed to give students a good foundation in chemistry and develop in them problem solving and experimental skills so that they are well prepared for further studies in specialized areas of chemistry or for employment in academic institutions and in industry.

Mission statement:

- To promote among our learners the skills of thinking, experimentation and application of the knowledge gained.
- To promote concern for environment and to develop appreciation for green chemistry.
- To prepare our students for life in the larger community.

Benchmark Statements for the Course:

- To instill in students a sense of enthusiasm for chemistry, an appreciation of its application in different contexts, and to involve them in intellectually stimulating and satisfying experience of learning and studying.
- To provide students with a broad and balanced foundation of chemical knowledge and practical skills.

Teaching-Learning:

Although the lecture method is extensively used, the students are also encouraged to do self-study through other activities like assignments, seminars, quiz, viva-voce etc.

Co-curricular Activities:

The Chemical Society for P.G. students provides them with a platform to interact with students of other institutions and also with eminent scientists from universities, other academic institutions and industries.

Course Details:

The course details for the P.G. programme are as follows:

ST. JOSEPH'S COLLEGE (AUTONOMOUS)

BANGALORE

M.Sc. Chemistry
Syllabus
(Analytical Chemistry Specialization)

With effect from 2015

Department of Chemistry
St. Joseph's College
Lalbagh Road
Bangalore – 560 027

M.Sc CHEMISTRY

Scheme of Study and Examination

Code	Title of the Paper 1st Semester	Contact Hours/week	Duration of Examination (hrs)	Max Marks for End-Sem	Internal Assessment	Total Marks	Credits
CH 7115	Inorganic Chemistry-I	4	3	70	30	100	4
CH 7215	Organic Chemistry-I	4	3	70	30	100	4
CH 7315	Physical Chemistry-I	4	3	70	30	100	4
CH 7415	Spectroscopy I	4	3	70	30	100	4
CH $7P_1$	Practical: Inorganic Chemistry I	9	6	35	15	50	2
CH $7P_2$	Practical: Organic Chemistry I	9	6	35	15	50	2

Code	Title of the Paper 2nd Semester	Contact Hours/week	Duration of Examination (hrs)	Max Marks for End-Sem	Internal Assessment	Total Marks	Credits
CH 8115	Inorganic Chemistry-II	4	3	70	30	100	4
CH 8215	Organic Chemistry-II	4	3	70	30	100	4
CH 8315	Physical Chemistry-II	4	3	70	30	100	4
CH 8415	Spectroscopy II	4	3	70	30	100	4
CH $8P_1$	Practical: Physical Chemistry II	9	6	35	15	50	2
CH $8P_2$	Practical: Synthesis and characterization of Compounds	9	6	35	15	50	2

Code	Title of the Paper 3rd Semester	Contact Hours/week	Duration of Examination (hrs)	Max Marks for End-Sem	Internal Assessment	Total Marks	Credits
CH 9115	Principals of Chemical Analysis	4	3	70	30	100	4
CH 9215	Separation and Electrochemical Techniques	4	3	70	30	100	4
CHEL 9315	Synthesis in Organic Chemistry	2	3	35	15	50	2
CHEL 9415	Chemistry of Materials	2	3	35	15	50	2
CBCS	Chemistry of Materials	4	3	70	30	100	4
CH $9P_1$	Practical: Inorganic and Biochemical Analysis	9	6	35	15	50	2
CH $9P_2$	Practical: Instrumental Methods of Analysis	9	6	35	15	50	2

Code	Title of the Paper 4th Semester	Contact Hours/week	Duration of Examination (hrs)	Max Marks for End-Sem	Internal Assessment	Total Marks	Credits
CH 0115	Applied Analysis	4	3	70	30	100	4
CH 0215	Organometallic Chemistry and Inorganic Reaction Mechanisms	4	3	70	30	100	4
CH 0315	Solid State Chemisty	4	3	70	30	100	4
CH 0415	Biological Chemistry	4	3	70	30	100	4
CH $0P_1$	Project Work	18	6	35	15	50	4

* The examination will be for 100 marks, which will be reduced to 50 marks.
** The practical examination will be for 50 marks, which will be reduced to 25 marks.
*** Evaluation of project report.

I SEMESTER

CH 7115: INORGANIC CHEMISTRY – I 60 Hours

1. CHEMICAL BONDING 22hrs

Ionic Bond: Lattice energy, Born-Lande equation (derivation), Kapustinskii equation, Born- Haber cycle and its uses, radius ratio rules, derivation of limiting radius ratios, structures of simple solids- sodium chloride, cesium chloride, zinc blende, wurtzite, flourite, antiflouirte, rutile, β-cristobalite, calcite, spinels, inverse spinels and perovskites. Fajan's rules.Lewis structure and formal charge calculation.Qualitative aspects of resonance and hybridization.VSEPR theory and shapes of molecules. Molecular Orbital Theory:MO diagrams of heteronuclear molecules and ions- CO, HCl, BeH_2, NO_2^-,Walsh diagramsof AH_2 type systems,σ, π and δ molecular orbitals, Quadruple and agostic bonds.Methods of estimating elctronegativity: Mulliken-Jaffe', Pauling and Allred-Rochow methods.Bent's rules.Partial ionic character in covalent bonds.

2. CHEMISTRY OF THE MAIN GROUP ELEMENTS 23 hrs

Polymorphism of carbon, phosphorus and sulphur: Structure-property correlation in diamond and graphite, carbon nanotubes and fullerenes- types and preparation. Differences between white phosphorus, black phosphorous and red phosphorous with special emphasis on structural aspects.Cyclosulphur and polycatenasulphur.

Boranes: Classification, preparation of higher boranes by Stock's method and pyrolysis of diborane, reactions of diboranes with Lewis bases- symmetric and unsymmetric cleavage , types of bonds in higher boranes- the *styx* number, formulae for arriving at the number of 2-centre and 3- centre bonds in boranes, Wade's rules as applied to boranes, Geometrical and Lipscomb's semitopological structures of B_4H_{10}, B_5H_9, B_5H_{11}, B_6H_{10} and $B_{10}H_{14}$.

Carboranes: classification, nomenclature, structures of CB_5H_9, $C_2B_4H_8$, $C_3B_3H_7$ and $C_4B_2H_6$.

Metallacarboranes : Preparation from 1,2-dicarba-closo-dodecaborane, sandwich structure.

Borazines: Preparation, properties and structure. Difference in chemical properties between borazine and benzene, borazine derivatives (N& B substituted). Preparation of boron nitride.

Phosphazenes: Classification, Cyclophosphazenes-$(NPCl_2)_3$ and $(NPCl_2)_4$- preparation and structure, Linear polyphosphazenes- preparation and applications.

Sulphur-nitrogen compounds: $(SN)_x$ as one dimensional conductors.

Silicates: Classification and structures of ortho, pyro, chain, cyclic, sheet and three dimensional silicates, silica gel, isomorphous replacement, aluminosilicates and their types .
Graphitic compounds – intercalation compounds with heavier alkali metals, halides, oxides, oxygen and fluorine; graphite oxides.
Condensed phosphates – linear polyphosphates, long chain polyphosphates and metaphosphates.
Polyhalides – XY_n^- and I_x^- types.

3. ACIDS, BASES AND SOLVENTS 10 hrs

Review of acid- base concepts– Bronsted, Lewis and solvent system definitions of acids and bases, generalized acid-base concept, systematics of Lewis acid- base interactions: Drago - Wayland equation, steric effects, solvation effects.
HSAB concept- Pearson's principle, classification of acids and bases as hard and soft, Bronsted acid-base strength verses hardness and softness, symbiosis, theoretical basis of hardness and softness.
Non-aqueous media – Classification of solvents, levelling effect, Acid-base reactions in HF, BrF_3, N_2O_4 and molten salts, super acids- Hammet acidity function.

4. CHEMISTRY OF METALS 5 hrs

Isopoly and heteropoly anions. Metal clusters: polynuclear halide and oxide complexes, zintl anions and cations.

REFERENCES

1. Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Okhil. K.Medhi, Pearson Education Asia Pvt. Ltd. (2006).
2. Basic Inorganic Chemistry - F.A. Cotton, G. Wilkinson and P. L. Gaus, John-Wiley and Sons, III edition, (1995).
3. Concise Inorganic Chemistry 5th edition, J.D.Lee, Blackwell Science, (1996).
4. Inorganic Chemistry, 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, ELBS (Oxford Univ. Press) (1994).
5. Chemistry of Elements, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann (1997).
6. Fundamentals of Inorganic Chemistry, Jack Barrett and Mounir A. Malati, Harwood (1998).

CH 7215: ORGANIC CHEMISTRY – I 60 Hours

1. STRUCTURE & REACTIVITY 6 hrs

Resonance, field effects, hyperconjugation, steric effects, steric inhibition of resonance.
Quantitative treatment of field and resonance effects – Hammett and Taft treatments.

2. REACTION MECHANISMS 9 hrs

Basic concepts: Thermodynamics and kinetics of reactions, Thermodynamic vs. kinetic control, Hammond postulate, microscopic reversibility, Marcus theory, Curtin – Hammett principle.

Reactive intermediates: Carbocations, carbanions, carbon free radicals, carbenes and nitrenes – generation, structure and stability.

Methods of determining mechanisms: Characterization of intermediates, kinetics, stereochemistry, kinetic isotopic effects, isotopic labeling experiments, catalysis and solvent effects.

3. STEREOCHEMISTRY 17 hrs

Molecules with 2 and 3 stereocenters – Interconversion of perspective, Fischer, sawhorse and Newman structures. R-S and E-Z notation, erythro/threo nomenclature, configuration nomenclature of molecules with 3 chiral centers, mesocompounds, systems with pseudoasymmetric centers. In-out isomerism. Classification of racemic modifications.

Axial chirality – allenes, spiranes, biphenyls – R, S notation of these systems. Planar chirality – ansa compounds, cyclophanes. Helicity – helicenes, end substituted benzphenanthrenes. Topicity, prochirality.

Conformations of substituted ethanes and substituted cyclohexanes.

Fused rings and bridged rings – decalins, nomenclature of bridged systems, norbornanes, bicyclo [2.2.2] octane.

Effect of conformation on physical and chemical properties – acyclic and cyclic compounds.

4. ALIPHATIC NUCLEOPHILIC SUBSTITUTION 11 hrs

Substitution at sp^3 carbon atom – limiting cases, S_N1 and S_N2 mechanisms. Factors influencing S_N1 and S_N2 reactions – substrate, leaving group, nucleophile and solvent effects, ambident substrates and nucleophiles – regioselectivity. Borderline cases: intermediate mechanism, mixed S_N1 and S_N2 mechanism. Neighboring group participation, non-classical carbocations. S_Ni mechanism. Allylic rearrangements.

Substitution at a trigonal carbon atom – the tetrahedral mechanism, formation of acid derivatives, cleavage of esters and N-acylation reactions. Susbtitution at vinyl carbon - tetrahedral and addition-elimination mechanisms.

5. ELIMINATION REACTIONS **6 hrs**

The E2, E1, E1cB and E2C mechanisms and the spectrum of elimination mechanisms. Regioselectivity and stereochemistry of E2 and E1 reactions; effect of substrate structure, base, leaving group and medium. Substitution vs.elimination. Pyrolytic eliminations - Hofmann elimination, elimination in esters, xanthates and N–oxides - mechanism and orientaion.

6. **AROMATIC SUBSTITUTION** **11 hrs**

Resonance and molecular orbital interpretation of aromaticity; aromaticity in benzenoid and non-benzenoid systems and ions.

Electrophilic substitution: Mechanistic interpretations of second substitution, orientation and reactivity, the ortho/para ratio, ipso attack, third substitution, orientaion and reactivity of other ring systems like polycylic aromatic hydrocarbons, heterocyclic systems (5 and 6 membered rings containing one and two hetero atoms), diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Nucleophilic substitution: S_NAr, S_N1, benzyne and SR_N1 mechanisms.

Reactivity – effect of substrate structure, leaving group and nucleophile; reactivity of heterocyclic systems containing 1 and 2 hetero atoms. The von Richter and Smiles rearrangements.

REFERENCES:

1. Advanced Organic Chemistry, J. March, 4th Edn., John Wiley, 1999.
2. Advanced Organic Chemistry, Part A, F. A. Carey and J. Sundberg, 2nd Edn., Plenum press, 1999
3. Organic Chemistry, Paula Yurkanis Bruice, 3rd Edn., Pearson Education, Inc., 2001.
4. Organic Chemistry, Seyhan Ege, 3rd Edn., Houghton Miftlin Company, 1999.
5. D. Nasipuri, Stereochemistry of Organic Compounds, Wiley Eastern, New Delhi, 1991.
6. Stereochemistry of Carbon compounds, E.L. Eliel, S.H. Wilen and L.N. Mander, John Wiley, 1994.
7. Organic chemistry, Volumes I and II, I.L. Finar, Longman, 1999.
8. Mechanism and Theory in Organic Chemistry (3rd Edition), Thomas H. Lowry, Kathleen S. Richardson, Harper & Row: New York, 1987.
9. Guidebook to Mechanism in Organic Chemistry (6th Edition), Peter Sykes, Pearson Education Limited, 1986.

CH 7315: PHYSICAL CHEMISTRY – I 60 HOURS

1. QUANTUM MECHANICS FORMALISM 6 hrs

Emergence of quantum mechanics: Black body radiation, photoelectric effect and Bohr's model of H-atom (Recall and review). Matter-wave duality, de Broglie equation; Heisenberg's uncertainty principle; Time independent Schrodinger equation from the equation of a standing wave; Physical meaning of wavefunction, well-behaved wavefunctions; Normalization and orthogonality of wave functions.

Operators and operator algebra; Eigen value equations, eigen functions and eigen values; Hermitian operators and their properties; Postulates of quantum mechanics; Time-dependant Schrodinger equation.

2. QUANTUM MECHANICAL TREATMENT OF SIMPLE SYSTEMS 9 hrs

Quantum mechanical treatment of a free particle and a particle in a 1D/3D potential well; eigen values and normalized eigen functions, nodes, symmetry and antisymmetry of eigen functions; Quantum mechanical degeneracy (cubic well); accidental degeneracy (tetragonal and orthorhombic wells); application of particle in a 1D potential well model to conjugated systems; Quantum mechanical tunneling (no derivation) and examples. Quantum mechanical treatment of Harmonic oscillator, eigen values and normalized eigen functions, zero point energy. Quantum mechanical treatment of rigid rotator; eigenfunction and eigenvalues; quantization of angular momentum. Quantum mechanical treatment of hydrogen atom; eigen values and orbital functions; expressions of orbital functions in atomic units.

3. APPROXIMATE METHODS AND MULTIELECTRON ATOMS 6 hrs

Variation principle and its proof; its application to the ground state of the helium atom.

Perturbation theory (Time-independent); application of first order perturbation method to the ground state of helium atom. Multielectron atoms – Symmetric and antisymmetric wave functions; ground and excited states of helium; spin orbitals and Pauli principle; Slater determinants; Slater orbitals. Effective nuclear charge based on Slater's rules; Self-Consistent Field (SCF) method; Hartree-Fock SCF method.

4. THEORY OF ANGULAR MOMENTUM 4 hrs

Commutation relationship among angular momentum operators; quantum mechanical definition of angular momentum, Ladder operators; deriving eigen values of the generalized angular momentum operators using ladder operators; orbital and spin angular momenta; spin-orbit interaction; coupled and uncoupled representation of angular momenta of composite systems; coupling of several angular momenta; Term Symbols, L-S coupling (Russel –Saunders-Coupling), and j-j coupling, Hund's rule of maximum stability.

5. CHEMICAL BONDING **5 hrs**

Huckel MO treatment for simple systems - ethylene, propenyl systems, butadiene, cyclopropenyl systems, cyclobutadiene, benzene. Inroduction to extended Huckel calculations.

6. ELECTROCHEMISTRY—I **8 hrs**

Debye-Huckel theory of ion-ion interaction, Debye –Huckel limiting law, Debye-Huckel equation for appreciable concentration, Huckel and Bronsted equations.

Qualitative verification of the Debye-Huckel equations, ion association-ion pairs and triple ions and conductance minima.

7. ELECTROCHEMISTRY – II **18 hrs**

The electrified interface—Surface excess, interfacial tension and its determination, Electrocapillarry curves, Thermodynamics of electrified interface—Lippmann equation, Determination of the electrical capacitance of the interface, Determination of surface excess.

Structure of electrical double layer—Helmholtz-Pern model, Gouy-Chapmann diffuse charge model and Stern model

The structure of the semiconductor-electrolyte interface—comparison between semiconductor and electrolytic solutions, The Garrett-Brattain space charge, differential capacity due to the space charge

Electrodics—Electron transfer under an interfacial electric field, equilibrium and exchange current density, overpotential—dependence of current density on overpotential, The Butler-Volmer equation and its special cases, the symmetry factor, influence of current density, pH and temperature on overvoltage, theories of overvoltage—Bubble formation as the slow process, combination of atoms as the slow process, ion discharge as the slow process and proton transfer as the slow process

8. ELECTROCHEMISTRY – III **4 hrs**

Corrosion—local cell theory of corrosion, mechanism of corrosion of ultrapure metals, cathodic reaction in corrosion, thermodynamics and the stability of metals, corrosion in the absence of oxide films, corrosion in terms of Evans diagrams, common example of corrosion or types of corrosion.

REFERENCES

1. Quantum Chemistry, I. N. Levine, Prentice Hall India (2001).
2. Quantum Chemistry, D. A. McQuarrie, Viva Books Pvt Ltd (2003)
3. Quantum Chemistry, R. K. Prasad, New Age International (P) Ltd (1997).
4. Modern electrochemistry 2B by John O'M Bockris , AKN Reddy and others
5. An introduction to Electrochemistry by Samuel Glasstone.

CH 7415: SPECTROSCOPIC METHODS OF ANALYSIS – I 60 Hrs

1. GROUP THEORY IN CHEMISTRY 17 hrs

Symmetry elements and symmetry operations, Definition of groups and subgroups, simple theorems in group theory and group multiplication tables. Conjugate relationships, classes of operations and order of a group.Symmetries with multiple higher order axis-symmetry operations in tetrahedral and octahedral point groups. Improper axis of symmetry-operations generated by S_n axis,symmetry conditions for molecular chirality.Point groups, Schoenflies notations for point groups, representation of symmetry operations as matrices, reducible and irreducible representations, characters of representations, great orthogonality theorem (without proof) and its corollaries, properties of irreducible representations. Mulliken's symbols for irreducible representations. Character tables-character tables of C_{nv}, C_{nh} D_{nh} and C_n point groups (derivation of character table only for C_{nv} point group). Applications of character tables in vibrational and electronic spectroscopy.

Group theory & Quantum mechanics: wave functions as basis for irreducible representations, direct products, time dependent perturbation theory, transition moment integral and selection rules in spectroscopy.

2. MICROWAVE SPECTROSCOPY 8 hrs

Rotations of molecules, rigid diatomic molecule-rotational energy expression, energy level diagram, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor. Rotational spectra of polyatomic molecules- linear, and symmetric top molecules. Calculation of bond length of diatomic and linear triatomic molecules. Stark effect.

3. Infrared Spectroscopy 14 hrs

Vibrations of molecules, harmonic and anharmonic oscillators-vibrational energy expression, energy level diagram, selection rules, expression for the energies of spectral lines, fundamentals, overtones, hot bands, vibrational frequency, force constant effect of isotopic substitution . Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P,Q and R branches, breakdown of the Born-Oppenheimer approximation. Vibrations of polyatomic molecules: Normal coordinate, translations, vibrations and rotations, vibrational energy levels, fundamentals, overtones and combinations. Vibration-rotation spectra of polyatomic molecules, parallel and perpendicular vibrations of linear and symmetric top molecules.

4. RAMAN SPECTROSCOPY **8 hrs**

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of Raman effect, pure rotational Raman spectra of linear and symmetric top molecules, vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure – O and S branches, Polarization of Raman scattered photons, Structure determination from Raman and IR spectroscopy- AB_2 and AB_3 molecules. Techniques and instrumentation.

5. ELECTRON SPECTROSCOPY **13 hrs**

Born – Oppenheimer approximation, vibrational coarse structure, intensities by Frank-Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, Pre-dissociation. Electronic structure of diatomic molecules-basic results of MO theory, Classification of states by electronic angular momentum, molecular orbitals, selection rules, spectra of singlet and triplet molecular hydrogen. Application of group theory and HMO method in the spectra of $CH_2 = CH_2$ and Benzene. Decay of excited states-radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion.

REFERENCES

1. Chemical Applications of Group Theory, F.A. Cotton, Wiley Eastern (1976).
2. Molecular Symmetry, D.S. Schonland, Van Norstand, (1965).
3. Introduction to Molecular Spectroscopy, C.N. Banwell, TMH Edition, (1994).
4. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (Int. Students Edition) (1988).
5. Molecular Spectroscopy, J.D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
6. Spectroscopy, Vol 1- 3, B.P. Straughan and W. Walker, Chapman Hall (1976).
7. Modern Spectroscopy, J.M. Hollas, John Wiley.
8. Vibrational Spectroscopy, D.N. Sathyanarayana, New Age International (P) Ltd. (1996).
9. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, (2001).

CH 7P1: PRACTICAL I – INORGANIC CHEMISTRY

I. QUALITATIVE ANALYSIS: 12 Units

Semi-micro qualitative analysis of a mixture containing two common cations and anions each and one of the less familiar elements: W, Mo, Ce, Th, Zr, V, U and Li.

II. QUANTITATIVE ANALYSIS: 8 Units

Volumetric and gravimetric determination of the following mixtures:

(a) Iron and aluminium (b) Copper and nickel (c) Copper and iron (d) Copper and zinc

(e) Barium and calcium

REFERENCES

1. Vogel's Textbook of Qualitative Chemical Analysis, J Bassett, R C Denny, G H Jeffery and J Mendham, ELBS (1986).
2. Vogel's Textbook of Quantitative Chemical Analysis, 5th edition, G N Jeffery, J Bassett, J Mendham and R C Denny, Longman Scientific and Technical (1999).
3. Inorganic semimicro Qualitative Analysis, V V Ramanujam, The National Publ. Co. (1974).

CH 7P2: PRACTICAL II: ORGANIC CHEMISTRY

I. QUALITATIVE ANALYSIS: 12 Units

Separation, systematic analysis and identification of organic compounds in a binary mixture.

II. QUANTITATIVE ANALYSIS: 8 units

1.Determination of equivalent weight of carboxylic acids.
2.Saponification value of oil/fat.
3.Estimation of glucose.
4.Estimation of phenols by acylation method.
5.Iodine value oil/fat.
6.Estimation of nitro group.
7.Estimation of nitrogen Kjeldhal's method.
8.Estimation of carbonyl group by hydroxylamine- pyridine method.

REFERENCES

1. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari (1996).
2. Practical Organic Chemistry, Mann and Saunders (1980).
3. Textbook of Practical Organic Chemistry, A I Vogel (1996)
4. Textbook of Quantitative Organic Analysis, A I Vogel (1996).
5. A Handbook of Organic Analysis, Clarke and Hayes (1964).

II SEMESTER

CH 8115: INORGANIC CHEMISTRY – II 60 HOURS

1. METAL – LIGAND BONDING 15 hrs

Review of basic concepts of co-ordination chemistry. Stereochemistry of complexes with coordination Nos. 2 to12, crystal field splitting in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal ligand fields, structural and thermodynamic effects of crystal field splitting- octahedral ionic radii, Jahn–Teller distortion in metal complexes and metal chelates, hydration and lattice energies, site preferences in spinels, octahedral versus tetrahedral co-ordination, Iriving-William stability order; spectrochemical series, limitations of crystal field theory, Evidences for metal – ligand orbital overlap from ESR, NMR, electronic spectra and antiferromagnetic coupling, nephelauxetic effect and nephelauxetic series, LFT (ACFT), , MO theory, MO diagrams of octahedral complexes (including π-bonding).

2. METAL – LIGAND EQUILIBRIA IN SOLUTION 9 hrs

Step-wise and overall formation constants and their relationships, trends in step-wise formation constants and exceptions to the trends, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate and macrocyclic effects and their thermodynamic origin, Kinetic and thermodynamic stability of metal complexes.

Determination of composition and stability constants of complexes by spectrophotometry (Job's method) and potentiometry and ion-exchange methods.

3. STRUCTURE AND BONDING IN METAL COMPLEXES 15 hrs

Hydride, dihydrogen, isocyanide complexes; mononuclear and dinuclear metal carbonyls and metal carbonyl clusters, Wades rules as applied to metal carbonyl clusters, Nitrosyl, dinitrogen and tertiary phosphine complexes, ligand cone angle in phosphine complexes; complexes containing SO_2 and CO_2.

Metal complexes as liquid crystals, stereochemical non-rigidity, Stereoisomeriosm – chirality, optical activity, CD, ORD, Cotton effect and absolute configurations.

Supramolecular chemistry– molecular recognition and self assembly, examples of simple supramolecular systems, metal ions as templates.

4. ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES 12 hrs

Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel and Tanabe-Sugano diagrams, Correlation diagram of d^2 configuration, spectra of 3d metal aqua complexes of trivalent V, Cr, divalent Mn, Co, Ni and $[CoCl_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra, spectral behaviour of lanthanide ions.

5. MAGNETIC PROPERTIES OF METAL COMPLEXES 9 hrs

Origin and types of magnetic behaviour- diamagnetism, paramagnetism, ferro and antiferromagnetism, magnetic susceptibility and its measurement by the Guoy method, temperature dependence of magnetism – Curie and Curie-Weiss laws, types of paramagnetic behaviour – spin-orbit coupling, magnetic behaviour of lanthanide ions, quenching of orbital contribution and spin only behaviour (explanation based on A, E and T terms), applications of magnetic data, temperature independent paramagnetism, spin-cross over.

REFERENCES

1. Advanced Inorganic Chemistry, F.A Cotton and G. Wilkinson, John Wiley &SoInc. 6th Edition (1999).
2. Advanced Inorganic Chemistry – A Comprehensive Text, F.A. Cotton and G. Wilkinson, Wiley Eastern limited, III edition, (1984).
3. Inorganic Chemistry – Principles of Structure and Reactivity, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Pearson Education Asia Pvt. Ltd. (2000).
4. Inorganic Chemistry, 4th Edition, D.F. Shriver and P.W. Atkins, ELBS Oxford Univ. Press. (2006).
5. Inorganic Chemistry, G. Wulfsberg, Viva Books Pvt. Ltd. (2002).
6. Inorganic Chemistry, G.L. Miessler and Tarr, 3rd edition, Pearson Education (2004).
7. Coordination Chemistry, 2nd edition, D. Banerjea, Asian Books Pvt. Ltd. (2007).
8. Chemistry of the Elements, N.N. Greenwood and A.E. Earnshaw, Butterworth Heinemann, (1997).

CH 8215: ORGANIC CHEMISTRY – II 60 hours

1. ADDITION REACTIONS 10 hrs

Addition to carbon-carbon multiple bonds: Mechanisms of electrophilic addition reactions; regioselectivity and stereoselectivity; hydrogenation and hydroboration; Nucleophilic addition; Michael addition.

Addition to carbon-hetero atom multiple bonds: Mechanisms of metal hydride reduction of carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents and organolithium reagents to carbonyl compounds; mechanisms of formation of hydrates, acetals, oximes and hydrazones on carbonyl compounds, Wittig reaction.

2. ALIPHATIC ELECTROPHILIC SUBSTITUTION 5 hrs

S_E2, S_E1 and S_Ei mechanisms, hydrogen exchange, migration of double bonds, halogenation of aldehydes, ketones and acids, haloform reaction; aliphatic diazonium coupling; nitrosoation at carbon and nitrogen, diazo transfer reaction, carbene and nitrene insertion, decaboxylation of aliphatic acids; Haller-Bauer reaction.

3. REARRANGEMENTS 15 hrs

Carbon to Carbon Migrations: Wagner-Meerwein, Pinacol-Pinacolone, Benzil-Benzilic acid, Favorskii and Neber rearrangements; Arndt-Eistert synthesis; expansion and contraction of rings.

Carbon to Nitrogen Migrations: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements.

Nitrogen/Oxygen/Sulfur to Carbon Migrations: Stevens and Wittig rearrangements

Carbon to Oxygen Migrations: Baeyer-Villiger rearrangement

Non-1,2 Rearrangements: Fischer indole synthesis, benzidine rearrangement.

4. PERICYCLIC REACTIONS 20 hrs

Molecular orbital symmetry; frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system; classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams; FMO and transition state aromaticity approach; selection rules.

Electro cyclic reactions: conrotatory and disrotatory motions; 4n, 4n+2 and allyl systems.

Cycloadditions: suprafacial and antarafacial additions, 4n and 4n+2 systems; [2+2] addition of ketenes, 1,3-dipolar cycloadditions and chelotropic reactions.

Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 1,3-, 1,5- and 3,3-sigmatropic rearrangements; Cope and Claisen rearrangements; Sommelet-Hauser rearrangement; Ene reaction.

5. FREE RADICAL REACTIONS AND PHOTOCHEMISTRY 10 hrs

Generation of free radicals – thermolysis and photolysis of peroxides, peresters and azo compounds, hydrogen abstraction, chain process.
Addition, substitution, elimination, rearrangement and electron transfer reactions; use of free radicals in organic synthesis.
General principles of photochemistry: singlet and triplet state-differences in reactivity, photosensitisation; quantum efficiency, quantum and chemical yields.
Photochemical reactions: Cis-trans isomerisation, di-π-methane rearrangement; Norish type I and type II cleavages; Paterno-Buchi reaction; photoreduction of ketones; photochemistry of arenes.

REFERENCES

1. Advanced Organic Chemistry, J. March, 4th Edn., John Wiley, 1999
2. Advanced Organic Chemistry, Part A and B, F. A. Carey and J. Sundberg, 2nd Edn., Plenum press, 1999
3. Modern Synthetic Reactions, H.O. House, Benjamin, 1972.
4. Organic Chemistry, Paula Yurkanis Bruice, 3rd Edn., Pearson Education, Inc., 2001.
5. Organic Chemistry, Seyhan Ege, 3rd Edn., Houghton Miftlin Company, 1999.
6. Frontier orbitals and Organic chemical reactions, Ian Fleming, John Wiley, 1980.
7. Radicals in Organic synthesis, B. Giese, Pergamon Press, 1986.
8. Introduction to Organic Photochemistry, J.D. Coyle, John Wiley & Sons.
9. Organic Photochemistry, J.M. Coxon and B. Halton, 1st Edn., Cambridge University Press, London, 1974.
10. Molecular reactions and Photochemistry, C.H. Deputy and D.S. Chapman, 1st Edn. Prentice Hall India, New Delhi, 1972.
11. Mechanism and Theory in Organic Chemistry (3rd Edition), Thomas H. Lowry, Kathleen S. Richardson, Harper & Row: New York,. 1987

CH 8315: PHYSICAL CHEMISTRY – II 60 Hours

1. REACTION KINETICS 20 hrs

Theories of Reaction rates – Review of Arrhenius and Bimolecular Collision theories. Activated complex theory – derivation- Thermodynamic method and partition function method. Reactions in solutions – factors affecting reaction rates in solution.

Diffusion controlled reactions – influence of solvation, internal pressure and dielectric constant on reaction rates. Ionic reactions – double sphere model for effect of solvent on ionic reaction rates. Primary and secondary salt effects.

Kinetic and thermodynamic control of reactions.

Unimolecular Reactions – Quantitative treatment of Lindemann and Hinshelwood theories. Qualitative treatment of RRK and RRKM theories. Comparison of these theories.

Kinetics of Chain reactions – H_2 and O_2 reaction – Explosion limits. Dehydrogenation of ethane, pyrolysis of acetaldehyde – Rice – Herzfeld mechanisms.

Kinetics of fast reactions – Features of fast reactions. Study of fast reactions by flow method, relaxation method, flash photolysis and NMR method.

2. POLYMERISATION AND KINETICS OF POLYMERIZATION 4 hrs

Kinetics and mechanism of free radical polymerization, kinetic chain length and chain transfer.

Kinetics of cationic and anionic polymerization.

Co polymerization – free radical mechanism and copolymer composition

3. CHEMICAL THERMODYNAMICS 15 hrs

Introduction –Review of thermodynamic laws. Thermodynamics of open systems-, Partial molal quantities- partial molal volume and its determination-reciprocal density method and apparent molal volume method, Partial molal free energy, Chemical potential, effect of temperature and pressure, Gibbs-Duhem equation, chemical potential of a pure substance, fugacity and its determination—graphical and compressibility factor, chemical potential in ideal gas mixture, Activity and activity coefficients, and determination by solubility and emf methods effect of temperature and pressure on fugacity and activity. Gibbs-Duhem-Margules equation; Application of Gibbs-Duhem-Margules equation-Konovalov's first law and second law.

Chemical potential in ideal solution. Thermodynamic deduction of Henry's law, Raoult's law, Nernst distribution law and its validation. Chemical potential of non-ideal solutions;

thermodynamic functions of mixing of ideal and non-ideal solutions. Excess thermodynamic functions

4. NON-EQUILIBRIUM THERMODYNAMICS 6 hrs

Irreversible processes and Steady State. Conservation of mass and energy in open systems. Entropy production – heat flow in chemical reactions. Entropy production and flow in open systems. Rate of entropy production – generalized forces and fluxes. Phenomenological equations. Onsagar Reciprocity relation – Electro kinetic and thermoelectric phenomena.

5. STATISTICAL THERMODYNAMICS 15 hrs

Introduction:. A review of macroscopic and microscopic properties. Postulates of statistical thermodynamics. Quantum mechanical, spectroscopic , thermodynamic and statistical evaluation of molecular properties .

Different types of ensembles, ensemble averaging, Stirling's approximation, Boltzmann statistics Fermi-Dirac statistics, Bose-Einstein statistics. Introduction to quantum statistics:

Partition function and thermodynamic parameters—energy, heat capacity, free energy, chemical potential, pressure entropy and equilibrium constant translational partition function, monoatomic gases, State functions in terms of partition function—energy, pressure, Sackur-tetrpde equation, free energy functions, rotational partition function and vibrational partition function, electronic partition function, the partition function of system—Thermodynamic properties of molecules from partition function of system, Application of statistical thermodynamics: Equipartition theorem, heat capacity behaviour of crystals.

References:

1. Physical Chemistry, P.W. Atkins, Julio de Paula, ELBS, 7th edition (2002).
2. Chemical Kinetics, K.J. Laidler, Pearson Education (Singapore) Pte. Ltd. 3rd Edition, (2004).
3. Kinetics and mechanism of chemical transformation, J.Rajaram and J. Kuriacose, McMillan (1986).
4. Advanced Physical Chemistry, J.N.Gurtu and A. Gurtu, Pragati Prakashan, 8th edition, (2006).
5. Principles of Physical Chemistry, B.R. Puri, L.R.Sharma and M.S. Pathania
6. Molecular thermodynamics, Donald A. McQuarrie, John D. Simon University Science Books, California, (1999).
7. Polymer Science, V.R. Gowarikar, N.V. Viswanathan & J. Sreedhar, Wiley Eastern

CH 8415: SPECTROSCOPIC METHODS OF ANALYSIS – II 60 Hours

1. UV AND VISIBLE SPECTROSCOPY 7 hrs

Terminology, classification of electronic transitions. Effect of substituent and conjugation on the spectra of alkenes. Woodward – Fieser rules for polyenes. Electronic spectra of carbonyl compounds. Effect of solvent on $\pi - \pi^*$ and $n - \pi^*$ transitions. Woodward's rules for enones. Electronic spectra of benzene and its derivatives.

2. INFRARED SPECTROSCOPY 11 hrs

Technique and instrumentation, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides). Effect of solvent and hydrogen bonding on the vibrational frequencies in alcohols. IR spectra of metal complexes involving ammine, aquo, hydroxo and carbonyl ligands.

3. NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY 15 hrs

Introduction. Nuclear spin and nuclear parameters. NMR nuclei. Nuclear spin states. The mechanism of absorption(resonance condition).Calculation of resonance frequency. Population densities of nuclear spin states. Relaxation processes.

The chemical shift and shielding. Chemical environment and chemical shift. Factors affecting chemical shift. Magnetic anisotropy. Continuous wave and pulsed Fourier methods of recording NMR spectra. Spin – spin coupling and splitting of NMR signals. Spin – spin interactions – AX, AX_2, AX_3, AMX and AB types. The coupling constant. Intensities of multiplets – Pascal's triangle Equivalence of protons – chemical and magnetic equivalence.

Low and high resolution spectra of ethanol – chemical exchange.

Geminal and vicinal coupling. Karplus equation and Karplus curve.

Effect of hindered rotation on the NMR spetrum.

First and second order coupling of AB systems. Spin decoupling methods. Double resonance. Applications in structural elucidation.

4. CARBON–13 NMR SPECTROSCOPY 4 hrs

The carbon – 13 nucleus, carbon – 13 chemical shift. Proton coupled and proton decoupled carbon – 13 spectra. Nuclear overhauser effect. Problems with integration in carbon -13 spectra. Off resonance decoupling. Applications.

5. ADVANCED NMR TECHNIQUES 4 hrs

Pulse sequences, spins and magnetization vectors. The DEPT experiment. Determining the number of attached hydrogens.

Introduction to two – dimensional spectroscopic methods. The COSY technique. An overview of the COSY Experiment.

6. MASS SPECTROMETRY **9 hrs**

Introduction, principle and instrumentation. Ion production – electron impact, chemical ionization, field desorption and fast atom bombardment techniques. High resolution mass spectrometry – base -, molecular ion -, parent ion -, fragmentation ion -, metastable – and isotopic peaks. Factors affecting fragmentation, ion analysis and ion abundance. Mass spectral fragmentation of organic compounds (hydrocarbons, aromatic compounds, alcohols, carbonyl compounds, acids and esters). McLafferty rearrangement. Determination of molecular weight and molecular formula.

7. ELECTRON SPIN RESONANCE SPECTROSCOPY **6 hrs**

Theoretical principles, 'g' factor, hyperfine splitting, Illustration of hyperfine splitting using examples, cyclopentadienyl radical, radical anions of benzene, naphthalene, p-benzo semiquinone. Isotropic spectra of some transition metal complexes and compounds, bis(salicylaldimine)Cu(II), $[VO(glycolate)_2]^{-2}$, $[(NH_3)_5Co\text{-}O\text{-}O\text{-}Co(NH_3)_5]^{5+}$, Mn^{2+} as a substitutional impurity in MgO.

8. MOSSBAUER SPECTROSCOPY **4 hrs**

Mossbauer effect and Mossbauer nuclei, isomer shift, quadrupole splitting and magnetic hyperfine interactions, elucidation of electronic structures of Fe(II) and Fe(III) systems

References:

1. Physical methods in Inorganic chemistry, R.S. Drago, Affiliated East-West Press Pvt. Ltd., New Delhi (1965).
2. Infrared Spectra of Inorganic and co-ordination Compounds, K. Nakamoto, Wiley-Interscience, New York, (1970).
3. Vibrational spectroscopy: theory and Applications, D.N.Sathyanarayana, New-Age International Publishers, New Delhi (2000).
4. Electronic Absorption Spectroscopy and related techniques, D.N.Sathyanarayana, Universities Press, Bangalore, (2001).
5. Applications of absorption Spectroscopy to Organic Compounds, J.R. Dyer, Prentice – Hall, New Delhi, (1969).
6. Organic Spectroscopy, W. Kemp, ELBS London, (1975).
7. Spectrometric Identification of Organic Compounds, R.M. Silverstein and W.P. Webster, Wiley & Sons, (1999).
8. Organic Mass Spectroscopy, K.R. Dass and E.P. James, IBH New Delhi, (1976).
9. Mass Spectrometry of Organic Compounds, H. Budzkiewicz, Djerassi C. and D.H Williams, Holden-Day, New York, (1975).
10. Principles of Instrumental Analysis, D.A. Skoog, S.J. Holler, T.A. Nilman, 5^{th} Edition, Saunders College Publishing, London, (1998).

11. Introduction To Spectroscopy, 2nd Edition, Donald L. Pavia, Gary M. Lampman and George S. Keiz, Harcourt Brace College Publishers, (1996).
12. Physical Methods for Chemists, R.S. Drago, 2nd Edition, Saunders College Publishing New York, (1992).
13. Mass Spectrometry – Analytical Chemistry By Open Learning -, R. Davies, M. Frearson and E. Prichard, John Wiley and Sons, New York, (1987).
14. Modern NMR techniques For Chemistry Research, Vol. 6, A.E. Derome, Oxford Pergamon Press, (1987).
15. Spectroscopic Methods in Organic Chemistry, 4th Edition, D.H. Williams and I. Fleming, Tata-McGraw Hill Publications, New Delhi, (1988).

CH 8P1: Practical III – Physical Chemistry

Chemical Kinetics

1. Determination of the velocity constant, catalytic coefficient, temperature coefficient, energy of activation and Arrhenius parameters for the acid hydrolysis of an ester.
2. Evaluation of Arrhenius parameters for the reaction between potassium persulphate and potassium iodide (I order)
3. Kinetics of reaction between $K_2S_2O_8$ and KI (salt effect).

Colorimetry

4. Determination of the Fe/ Cu in different matrices by colorimetry.
5. Determination of percentage titration error of ferrous ammonium sulphate with potassium permanganate or an acid base titration colorimetrically.
6. Kinetics of reaction between $K_2S_2O_8$ – KI colorimetrically.
7. Determination of pK_a of indicators.
8. Simultaneous estimation of Mn and Cr by spectrophotometric method

Partial Molal Volume

9. Determination of partial molal volume of ethanol by reciprocal density method.
10. Determination of PMV by apparent molar volume method, NaCl-H_2O system.

Conductivity

11. Titration of a mixture of strong and weak acids and salt against a strong base.
12. Determination of dissociation constant of a weak acid or weak base by conductometry.
13. Determination of Onsagar parameters for a strong electrolyte by conductometry.
14. Estimation of weak acid like phenol by dialkali method.
15. Estimation of urea by enzyme hydrolysis using conductance method

Potentiometry.

16. Titration of silver nitrate against potassium chloride/bromide/ iodide, calculation of the solubility product of silver chloride/bromide/iodide.
17. Titration of a weak acid against a strong base using quinhydrone electrode and calculation of pKa values of the weak acid.

18. Titration of a mixture of HCl and CH_3COOH potentiometrically and the determination of the composition of the mixture.
19. Estimation of a weak acid in a given sample using sodium hydroxide by differential potentiometry.
20. Evaluation of I order rate constant by potentiometry.
21. Determination of activity coefficient of an electrolyte by potentiometry.

References

1. Findlay's Practical Physical Chemistry revised by Levitt, Longman's, London (1966).
2. Experiments in Physical Chemistry, Shoemaker and Garland, McGraw Hill International edition. (1996).
3. Advanced Practical Physical Chemistry, J B Yadav, Goel Publication House, Meerut.
4. Experimental Physical Chemistry, Daniel et al.,McGraw Hill (1962).
5. Experimental Physical Chemistry, Wilson, Newcombe and others, Pergamon Press, N.Y. (1962).
6. Practical Physical Chemistry, A M James and D E Pritchard, Longman Group Ltd. (1968).

CH 8P2: Practical IV – Synthesis and Characterization of Compounds

Inorganic Compounds:

1. Preparation and quantitative analysis of hexamminecobalt(III) chloride – 2 sessions.
2. Preparation of potassium trioxalatoferrate(III) trihydrate and its characterization by quantitative analysis and IR studies– 2 sessions.
3. Preparation of a variety of complexes (5 Nos.) and their characterization by UV-Visible and IR techniques– 4 sessions.
4. Preparation of a nano materials and their characterization by UV spectroscopy (band gap) and XRD (crystallite size) – 2 sessions.
5. Synthesis of spinels and its characterization by XRD studies– 2 sessions.

Organic Compounds:

6. Preparation of anthrone from anthracene.
7. Preparation of anthranilic acid from phthalic acid.
8. Preparation of benzanilide from benzophenone.
9. Preparation of benzilic acid from benzoin.
10. Preparation of NBS from succcinic acid and its application in allylic bromination.
11. Synthesis of stilbene.
12. Resolution of a racemic mixture by fractional crystallization
13. Preparation of an organic compound (one step preparation) by 2 or 3 different methods and comparison/evaluation of the methods with respect to the following parameters:
    (i) Ease of preparation, problems in handling chemicals, toxicity and flammability of chemicals
    (ii) Yield and cost effectiveness
    (iii) Product purity/quality
    (iv) Environmental costing (from the point of view of Green chemistry)

Characterisation of the organic compounds (experiments 8 –14) by: TLC, column liquid chromatography, fractional crystallization, UV, IR and NMR spectroscopic techniques.

References

1. Handbook of Preparative Inorganic Chemistry, G Brauer, Academic Press (1963).
2. Practical Inorganic Chemistry, Marr and Rocket
3. Laboratory Manual of Organic Chemistry, Day, Sitaraman and Govindachari (1996).
4. Practical Organic Chemistry, Mann and Saunders (1980).
5. Textbook of Practical Organic Chemistry, A I Vogel (1996)
6. A Handbook of Organic Analysis, Clarke and Hayes (1964).

III SEMESTER

CH 9115: PRINCIPLES OF CHEMICAL ANALYSIS 60 HOURS

1. ERRORS IN CHEMICAL ANALYSIS, STATISTICAL DATA TREATMENT AND EVALUATION 10 hrs

Significant Figures: Rounding of numerical expression. Addition and subtraction; multiplication and division- numerical problems on above concepts.

Errors: Some important terms Replicate, outlier, Accuracy and precision. Errors affecting precision and accuracy; Systematic errors: Sources and types of systematic errors with examples. Ways of expressing accuracy: Absolute and relative errors; Constant and proportional errors. Detection of systematic instrument and personal errors. Identification and compensation of systematic method errors. Terms used to describe precision of a set of replicate measurements. Mean and median. Problems. Deviation and average deviation from the mean.

Statistical treatment of random errors; Spread, sample and population; sample mean and population mean. Standard deviation and variance of Population; area under Gausian curve

Sample standard deviation, sample variance, standard error of the mean, Relative standard deviation, coefficient of variation, pooled standard deviation. Confidence interval; Problems.

Student - t statistics; Significance testing, null hypothesis, one and two tailed significance tests. Comparing measured results with a known value.

Comparison of two experimental means. Comparison of standard deviation with the F-test. Error in hypothesis testing. Criteria for rejection of an observation - Q test. Problems.

Calibration curves: Least square method. Finding the least square line. Expression for slope, intercept, standard deviation about regression. Standard deviation of the slope and intercept. Coefficient of determination - Problems.

Method validation. Determination limits, calibration sensitivity. Limit of quantization and Linear dynamic range.

2. ACID – BASE TITRATIONS 5 hrs

Basic principles: K_w pH scale, dissociation of acids and bases Titration curves for mono functional acids and bases, pH calculations, theory of indicators,. Titration curves for di, tri and polybasic acids, polyamines and amino acid systems. Fractions of phosphoric acid

species as a function of pH. Applications to pharmaceutical, environmental and biochemical analysis.

3. REDOX TITRATIONS **8 hrs**

Nernst equation, Standard & formal potentials. Titration curves, end point signals, Indicators, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent system. Adjustment of analyte's oxidation state. Applications: Oxidants such as Permanganate, dichromate, Ce (IV), bromate, Iodates Reductants such as Ferrous ammonium sulphate and Ascorbic acid.

Karl-Fischer titrations: Stoichiometry of the reaction, preparation of the reagent, titration method, standardization of the reagent using water-in-methanol, determination of water in samples, interference and their elimination, application to quantitative analysis of some organic compounds- alcohols, carboxylic acids, acid anhydrides and carbonyl compounds. Applications

4. PRECIPITATION TITRATIONS **4 hrs**

Solubility product. Theoretical principles: Titration curves, end point signals, Mohr, Volhard and adsorption indicators. Applications: Estimation of F^-, K^+, CO_3^{2-}, $C_2O_4^{2-}$, acetylenes and mixture of halides. Applications

5. COMPLEXOMETRIC TITRATIONS **7 hrs**

Complexometric titrations with particular reference to EDTA titrations, suitability of polydentate ligands as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional stability constants, derivation of titration curve, effect of pH and second complexing agent on the conditional stability constant and titration curve. Selectivity by pH control, masking and demasking, metal ion indicators, types of EDTA titrations, titrations involving monodentate ligands. Applications

6. NON-AQUEOUS TITRATIONS **4 hrs**

Acid–base titrations in non-aqueous solvents- classification of solvents, leveling and differentiating solvents, acidic and basic titrants, methods of titration. Titrations in glacial acetic acid and ethylene diamine, applications of non-aqueous titrations.

7. GRAVIMETRIC ANALYSIS **4 hrs**

Formation and treatment of precipitates, co-precipitation, post precipitation homogeneous precipitation, important precipitating agents and their significance in inorganic analysis

8. KINETIC METHODS OF ANALYSIS **4 hrs**

Rate laws, psuedo first order kinetics, types of kinetic methods, fixed time methods. Applications of catalytic and non-catalytic kinetic methods. Applications

9. RADIOCHEMICAL TECHNIQUES **5 hrs**

Measurement of radioactivity, Principle, methodology and applications of isotope dilution analysis, Neutron activation analysis, PGNAA and principle of Radioimmunoassay. Applications

10. ABSORPTION AND EMISSION TECHNIQUES **7 hrs**

Quantitative aspects of spectrochemical Measurements. Nephelometric and turbidimetric methods Instrumentation; turbidimetric titrations.

Molecular luminescence- Quantitative aspects of fluorescence. Fluorescence and structure, Effects of temperature, dissolved oxygen and solvent on quantum efficiency of fluorescence.

Atomic absorption methods- principle and instrumentation (single and double beam) Light sources of AAS; atomization (flame and electrothermal) interferences. Atomic emission method (AES) Plasma – DCP and ICP techniques; Advantages of plasma over flame.

11. THERMAL METHODS OF ANALYSIS **2 hrs**

Thermogravimetric analysis- Differential thermal analysis; differential scanning colorimetry- thermometric analysis. Applications

References:

1. Fundamentals of Analytical Chemistry; Skoog, West. Holler and Crouch 8th edition; Thomson Asia Pvt Lid. (2005).
2. Analytical Chemistry; Gary D Christian; 6th edition; John Wiley and Sons (2007).
3. Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).
4. Analytical Chemistry Principles – John H Kennnedy, 2nd edition, Saunders college Publishing (1990).
5. Principles of Instrumental Analysis, Skoog, Holler and Nieman, 5th edition, Saunders college Publishing, International Limited (1999).

6. Vogel's Text book of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).
7. Quantitative Analysis; R A Day, Jr and A L Underwood ; Prentice-Hall India Pvt Lid. Sixth Edition.
8. Modern methods of Chemical analysis-Pecsok, Shields, Cairns and McWilliams (2nd edition), John Wiley and Sons (1976).
9. Vogel's Textbook of Quantitative Inorganic Analysis, Bassett, Denney, Jeffery and Mendham, (4th edition) ELBS (1985).
10. Hand Book Of Instrumental Techniques For Analytical Chemistry, Frank Settle Prentice Hall PTR (1997).

CH 9215: SEPARATION AND ELECTROCHEMICAL TECHNIQUES

60 Hours

1. SOLVENT EXTRACTION 5 hrs

Partition coefficient-equation for batch extraction & multiple extraction, Extraction efficiency- pH effects, Extraction with metal chelator and crown ethers.

2. CHROMATOGRAPHY 6 hrs

Types of chromatography –Theoretical principles; Retention time, retention volume, adjusted retention time, relative retention, capacity factor (retention factor) –Relation between retention time and partition coefficient –Scaling up, scaling rules-Efficiency of separation, resolution -Ideal chromatographic peaks (Gaussian peak shape)- Factors for Resolution-diffusion, diffusion coefficient - Plate Height- Plate Height as a Measure of Column Efficiency-Number of theoretical plates-asymmetric peaks- Factors Affecting Resolution -Band Spreading- van Deemter equation, Optimum Flow Rate, A Term – multiple paths, longitudinal diffusion, Mass Transport, *Extra column contributions to zone broadening* -advantages of open tubular columns- isotherms and the resulting band shapes.

3. GAS CHROMATOGRAPHY 7 hrs

Separation process in gas chromatography –schematic diagram-open tubular columns, Comparison with packed columns, Effect of column inner diameter and length of the column, choice of liquid stationary phase, chiral phases for separating optical isomers-molecular sieves as stationary pahase-packed columns-Retention index-Temperature and pressure programming -Carrier gas-Guard columns and retention gaps-sample injections, split injection and split less injection, solvent trapping and cold trapping, on column injection- Detectors : thermal conductivity detector, flame ionisation detector, electron capture detector, Mention about other detectors like nitrogen phosphorous detector, flame photometric detector, photoionisation detector, sulphur chemiluminescence detector -GC-MS- Element specific plasma detectors. Sample preparation-solid phase micro extraction, purge and trap, thermal desorption-*Derivatisation in GC*-Method development in GC.

4. LIQUID CHROMATOGRAPHY

4a. HIGH-PERFORMANCE LIQUID CHROMATOGRPHY 8hrs

The chromatographic process-effect of small particles, scaling relation between columns, relation between number of theoretical plates and particle size, column pressure-The column, stationary phase, monolithic silica columns-Bonded stationary phases-solute column interactions-shape selectivity-The elution process, isocratic and gradient elution,

selecting the separation mode, solvents, Maintaining symmetric band shape, dead volume – Injection and detection in HPLC, Detector characteristics, signal to noise ratio, detection limits, Linearity- Spectro photometric detectors, refractive index detector, Evaporative Light scattering detector, Method development in reverse phase separation-Criteria for adequate separation-Optimisation with one solvent, optimization with two or three different solvents-choosing a stationary phase-Gradient separations- Dwell volume and Dwell time-developing a gradient separation. Chiral separation.- derivatives for HPLC.

4b. LIQUID CHROMATOGRAPHIC METHODS 12hrs

(i) Reversed phase chromatography for neutral samples. Reverse phase retention process-selectivity- Solvent type selectivity and column selectivity-isomer separations.

(ii) Normal phase Chromatography- Retention mechanism -solvent strength-use of TLC data for predicting NPC retention- Solvent type selectivity and column selectivity-isomer separations.

(iii) Ion Exchange chromatography- ion exchangers, resins-ion exchange selectivity, selectivity coefficient, Donnan Equilibrium- Conducting ion exchange chromatography, Gradient elution, Application of ion exchange.

(iv) Ion Chromatography-Suppressed ion –anion and Cation chromatography-Ion chromatography without suppression-detectors-ion pair chromatography

(v) Molecular exclusion chromatography - The elution equation, stationary phase, molecular mass determination.

(vi) Affinity chromatography - Principle-Matrix, ligand, spacer arm-properties required for efficient and effective chromatographic matrix-partial structure of agarose-Types of ligands- need of spacer arm. Immobilized metal affinity chromatography.

(vii) Hydrophilic interaction chromatography (HILIC).

Sample Preparation: 2 hrs

Statistics of sampling-choosing a sample size-choosing the number of replicates. dissolving samples for analysis., dissolving inorganic material, dissolving organic material, decomposition of organic substances, sample preparation techniques and derivatisation.

5. ELECTROANALYTICAL TECHNIQUES 20 hrs

Electrophoresis and Electrochromatography 3 hrs

General introduction to electrophoresis. Important terms- Basis of electrophoretic separation. Expression for distance traveled on application of electrode potential. Role of buffer in electrophoresis.

Classical gel electrophoresis, High performance capillary electrophoresis – advantages. Instrumentation set up; sample injection. Comparison of classical and capillary electrophoresis. Electroosmotic flow. Modes of electrophoresis.

Capillary gel electrophoresis, capillary isoelectric focusing; capillary isotachophoresis. Capillary electrochromatography (basic principle) Micellar electrokinetic capillary electophoresis.

Ion Selective Electrodes **4 hrs**

Brief Introduction- Potentiometry- electrodes used: Metallic indicator electrodes: types with one example for each. Metallic redox indicator electrodes. Ion selective electrodes ISE: Classification of membranes. Properties of ISE.

Glass membrane electrodes. Composition and structure of glass membrane. Hygroscopicity of glass membrane. Electrical conductance across the glass membrane. Membrane and boundary potential Expression for E_b. Alkaline error. Crystalline membrane electrode. Conductivity of a crystalline membrane.

Fluoride electrode. Electrodes based on silver salts. Liquid membrane electrode for Ca^{+2}

Molecular selective electrode systems. Gas sensing probe for CO_2. Two types of gas sensing membrane materials.

Voltammetric Techniques*:* **13 hrs**

Introduction to voltammetric techniques. Polarization – Ideal polarized and ideal non polarized electrodes: Sources of polarization. Reaction and concentration polarization. Mechanism of mass transport. The current response to applied potential (in terms of Fermi and molecular orbitals) Faradaic and non- Faradaic currents. Charging and residual currents.

Polarography: Advantages of Hg over other solid electrodes. Types : DME, SMDE, HMDE and MFE. Instrumentation-Polarographic convention. Polarographic experiment. Polarographic parameters (diffusion current, half wave potential). Analysis of a polarogram. Effect of dissolved oxygen on electrochemical reduction process. Ilkovic equation (derivation). Quantitative and qualitative aspects of voltammetry: Determination of concentration and standard state potentials. Determination of electrochemical reversibility and number of electrons. Effect of complex formation on polarographic waves. Potential excitation signal and response and different voltammetric techniques. Normal pulse (NPP/V) and differential pulse polarography (DPP/V). Applications of polarography. Amperometric titrations at DME (four types).

Cyclic voltammetry: Excitation signal and current response in CV. Important parameters of CV. Instrumentation. Reversible, irreversible and quasireversible charge transfer. A cyclic voltammetric experiment-Analysis of a cyclic voltammogram. Cathodic and anodic

processes. Electrode materials in voltammetry (glassy carbon, carbon paste, gold, platinum and modified electrodes.) Coupled chemical reactions

References for separation techniques:

1. **Quantitative Chemical Analysis, Daniel C.Harris,7th edition., (W. H. Freeman and Company, New York, 2006).**
2. Principles of Instrumental Methods of Analysis- Skoog, Holler And Nieman, 5thedition, Saunders College Publishing, International Ltd. (1998).
3. Hand Book of Instrumental Techniques For Analytical Chemistry, Frank Settle, Prentice Hall PTR, (1997).
4. Unified Separation Science-J. Calvin Giddings –John Willy& Sons (1991).
5. Chromatography –Concepts And Contrasts -James M Miller- John Wiley& Sons (1988).
6. Analytical Chemistry: Principles –John H Kennedy, Second Edition, Saunders College Publishing (1990).
7. Experimental Organic Chemistry, Daniel R. Palleros, John Willy& Sons (1999).
8. Fundamentals of Analytical Toxicology, Robert J Flanagan et.al. John Willy& Sons (2007).
9. Fundementals of Analytical toxicology , Robert J Flanagan, Andrew Taylor et al John Wiley & Sons Ltd (2007).
10. Introduction to modern liquid chromatography –Lloyd R.Synder, Joseph J. Kirkland et al ; third edn; John Wiley & Sons Ltd (2010).

References for electroanalytical techniques:

11. Principles of Instrumental Analysis, Skoog, Holler and Nieman, 5th edition, Saunders college Publishing, International Limited (1999).
12. Analytical Chemistry Principles – John H Kennnedy, 2nd edition, Saunders College Publishing (1990).
13. Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).
14. Vogel's Text book of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).
15. Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).
16. Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers

CH 9315A: Organic Synthesis – The Disconnection Approach

30 Hours

Basic principles: introduction to synthons, synthetic equivalents and the Disconnection approach.

Synthesis of aromatic compounds; One-Group C-X disconnections; Two-Group C-X disconnections; Amine synthesis; One-Group C-C disconnections; carbonyl condensations; Alkene synthesis; Use of acetylenes; Two-Group C-C disconnections – Diels-Alder reactions, 1,2-, 1,3-, 1,4-, 1,5- & 1,6- Difunctionalised compounds; Ring synthesis of 3 to 6 membered rings.

References:

1. Advanced Organic Chemistry, Part B, F. A. Carey and J. Sundberg, 2nd Edition., Plenum press, (1999).
2. Organic Synthesis: The Disconnection approach, S. Warren, John Wiley & Sons, (2004).
3. Organic synthesis, R.E. Ireland, Prentice-Hall India, New Delhi, (1975).
4. Organic Synthesis, Michael B. Smith, 1st Edition., McGraw-Hill, Inc., (1994).
5. Some Modern Methods of Organic Syntheis, W. Caruthers, 2nd Edition., Cambridge University Press, London, (1998).
6. Organic Synthesis, C. Willis and M. Wills, Oxford University Press, (1995).
7. Principles of Organic synthesis, R.O.C. Norman, J.M. Coxon, 3rd Edition., Chapman & Hall, (1993).

CH 9315B: CHEMISTRY OF MATERIALS **30 Hours**

1. Scope of materials science: Types of materials based on structure (i) layered materials (clays, MoS_2, LDH) (ii) Porous materials: Microporous (zeolites), Mesoporous materials (MCM-41) (iii) Metal Organic Frameworks and dendrimers. (structure and applications in each case need to be discussed) **6 Hrs**
2. Synthesis of bulk materials: Principle and applications: (i) Precipitation methods (ii) Sol – gel method (iii) solid state synthesis (iv) template technique (ALPOs and MCM-41) **6 Hrs**
3. Characterisation techniques: Principle, technique and specific applications of Electron microscopy (TEM and SEM), Atomic Force Microscopy, Photoelectron spectroscopy (XPS and Auger spectroscopic techniques), BET surface area, porosity, solid state NMR (introduction) **10 Hrs**
4. Nanomaterials: Introduction, properties of nanomaterials: (electronic, mechanical, superconducting, magnetic). Synthesis of nanomaterials: Top down methods (ball milling and exfoliation – thermal, solvent and interlayer modification) and bottom up methods (solution synthesis – La Mer principle, Ostwald ripening, role of capping agents, inverse micelle synthesis). Applications of Nanomaterials in medicine and biology – sensing and targeted drug delivery. **8 Hrs**

CH 9P1: Practical V – Analysis of Inorganic and Biochemical Materials

Experiments in Inorganic Chemistry **11 sessions**

1. Estimation of metal acetates using perchloric acid in glacial acetic acid medium.
2. Analysis of steel (2 sessions)
3. Analysis of dolomite (2 sessions)
4. Analysis of soil (2 sessions)
5. Separation and estimation of mixture of metal ions by ion exchange chromatography (2 sessions)
6. Determination of metal to ligand ratio by Job's method.
7. Separation of Fe(III) ion by solvent extraction and estimation.

Experiments in Biochemistry **14 sessions**

1. Estimation of rancidity in a sample of butter.
2. Estimation of BOD and COD of a sample.
3. Extraction of caffeine from tea leaves and characterization using IR, NMR and Mass spectrometer.
4. Estimation of glucose in serum.
5. Estimation of sulpha drug using spectrophotometer.
6. Estimation of RNA using spectrophotometer.
7. Estimation of cholesterol in serum.
8. Gel electrophoresis- separation of proteins. (2 sessions)
9. Agarose gel electrophoresis-separation of RNA/DNA
10. Separation, purification and characterization of protein from plant sample(3 sessions)
11. Any other suitable experiments.

References:

1. Text book of Quantitative Inorganic Analysis by A.I. Vogel, ELBS (1978).
2. Advanced Physicochemical Experiments by Rose, Isaac Pitman (1964).
3. Methods of Soil Analysis Part I & II, C.A. Black et al (Edition) American Society of Agronomy, Inc. (1965).

4. Analytical Chemistry-An introduction; Skoog, West, Holler and Crouch; seventh edition Saunders College Publishing, (1999).
5. Experiments in Environmental chemistry, P.D. Vowels and D.W. Connel, Pergamon (1980).
6. Textbook of Practical Organic Chemistry, A I Vogel, ELBS (1973).
7. Practical Clinical Biochemistry, H. Varley, 4th edition, CBS Indian edition (1988).
8. An Introduction to Practical Biochemistry, David Plummer, Tata McGraw Hill (1979).
9. Laboratory Manual in Biochemistry, J. Jayaraman, Wiley Eastern (1981).
10. Chromatography, C.G. Sharma Krishna Prakashana Media (1997).

CH 9P2: Practical VI – Instrumental Methods of Analysis

(Qualitative and Quantitative Methods)

Gas Chromatography

1. Qualitative identification of organic compounds in a given mixture using gas chromatography.
2. Estimation of organic compounds in a given mixture using gas chromatography.
3. Estimation of percentage esterification in esterification reaction using gas chromatography.

Atomic Absorption Spectroscopy

4. Estimation of iron in a given sample using atomic absorption spectroscopy.
5. Estimation of an alloy (Cu, Zn and lead) using atomic absorption spectroscopy.

Liquid Chromatography

6. Estimation of halide ions in a mixture using ion chromatography.
7. Estimation of alkali metalions in a mixture using ion chromatography.
8. Separation and identification of organic compounds using HPLC.

Powder X-ray Diffraction

9. Powder X-ray diffraction analysis of a mixture of two cubic solids.

Atomic Force Microscopy

10. AFM imaging of a polymer film.

Fluorescence Spectroscopy

11. Estimation of a dye by fluorescence spectroscopy.
12. PL emission of semiconductors (bulk and nanoparticles).

Flame Photometry

13. Estimation of sodium by flame photometer.

Spectrophotometry

14. Estimation of caffeine in a given sample using UV spectrophotometer.
15. Estimation of Ni in tea powder.
16. Estimation of chloride in pharmaceutical products.

Electroanalytical Methods

17. Estimation of copper by potentiometry.
18. Estimation of a mixture of chloride and iodide by potentiometry.
19. Standardizing cyclic voltammetry using ferrocyanide-ferricyanide system.
20. Estimation of ascorbic acid by voltammetry.

21. Estimation of organic compounds by differential pulse polarography.

Any other experiments involving one or more of the techniques mentioned above.

References:

1. Analytical Chemistry-An introduction; Skoog, West, Holler and Crouch; seventh edition Saunders College Publishing, (1999).
2. Chromatography, C.G. Sharma, Krishna Prakashana Media (1997).

IV SEMESTER

CH 0115: APPLIED ANALYSIS **60 Hours**

1. BIOPOLYMERS **3 hrs**

Determination of size, shape, molecular weight, hydrodynamic methods, sedimentation,diffusion, viscosity.

2. PROTEIN ANALYSIS **15 hrs**

Protein Purification: Protein isolation, solubility's of proteins, chromatographic separations, electrophoresis and ultracentrifugation. Analysis and determination of protein structure: Primary structure, protein modification, secondary structure, globular and fibrous proteins, tertiary structure, quaternary structure and prediction of protein structure; Techniques for study of biomolecules – only principle and interpretation of data to characterize the biomolecule by: MS (MALDI / SELDI), Confocal microscopy, Microarrays, Flow Cytometry, Microcalorimetry, Differential Scanning Calorimetry, ELISA, RIA, FACS, Northern, Southern, Western blots, NMR, Electrophoresis, CD, ORD, X-Ray crystallography.

3. NUCLEIC ACID ANALYSIS **5 hrs**

Analysis and Determination of structure of Nucleic acids: Primary structure, Secondary structures, Denaturation, renaturation, Tertiary structure, Chemical synthesis of polynucleotides. Recombinant DNA: Cloning, DNA libraries, PCR and recombinant DNA technology. A brief mention of the application of recombinant technology in different disciplines - industry, medicine and forensics.

4. FOOD ANALYSIS **7 hrs**

Analysis of common adulterants in foods. Food additives: monosodium glutamate. Food preservatives: sodium benzoate, sodium sulphite. Edible oils - qualitative tests for purity, estimation of rancidity, tests for common adulterants in lipids. Milk and milk products- alcohol test, fermentation test, dye reduction tests (methylene blue and resazurin), phosphatase test for pasteurisation, estimation of added water in milk; Beverages- caffeine and chicory in coffee, methanol in alcoholic drinks; Estimation of saccharin, coal tar dyes, aflatoxins in foods; Pesticide analysis in food products: phosphates, chlorinated pesticides.

5. ANALYSIS OF DRUGS AND POISONS **3 hrs**

Classification of drugs, Characterisation of common drugs: Analgesics-aspirin; Expectorants – Benadryl; Vitamins - vitamin C; Sedatives- diazepam; Antibiotics - penicillin, chloramphenicol; Cardiovascular – sorbitrate.

6. CLINICAL CHEMISTRY **3 hrs**

Blood analysis: serum electrolytes, serum proteins, blood glucose, blood urea nitrogen, uric acid, and blood gas analysis. Enzyme analysis: Assay of alkaline phosphatase, isoenzymes of lactate dehydrogenase, aldolase,. Metal deficiency and disease; Estimation of calcium, iron, and copper.

7. FORENSIC CHEMISTRY **7 hrs**

Introduction to Forensic Science, Forensic chemistry – physical and chemical properties – scientific methodology – identification of sample – presumptive and confirmatory analysis, Theory of Forensic Analysis, Fingerprint Development – ink print latent print – use of developers – ninhydrin, iodine vapour, silver nitrate reaction, Objectives of testing, Testing for evidence – presence of paints, soil samples, tyres, shoes, heavy metals. Presumptive Drug Analysis – colour (spot) test for common drugs of abuse cocaine, marijuana, amphetamines, LSD, Barbiturates, opium, methamphetamines. Secondary fluid analysis for toxins and drugs. Analysis of metabolites of toxins and drugs – pharmacokinetic intermediates, pharmacodynamic interactions eg DDT, paracetamol, arsenic, CO, cyanide, snake venom. Estimation of drug residues in bioloigical samples. Soil Analysis – size, density, pH, quality of soil, Thin Layer Chromatography and Ink Analysis

8. POLLUTION ANALYSIS **10 hrs**

Air Pollution: Principles and methods of sampling; A survey of reactions and methods involved in the determination of carbon monoxide, sulphur oxides, nitrogen oxides, hydrocarbons and particulates. Tolerance limits. Fuel Analysis and emissions: Ultimate and proximate analysis of coal, Liquid fuels: octane number and cetane number, carbon residue.

Water Pollution: Objectives of analysis; Parameters of analysis: colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen; Heavy metal pollution: public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic, general survey of instrumental techniques for the analysis of heavy metals in aqueous systems.

9. SOIL ANALYSIS 4 hrs

Chemical properties of soil-types of soil colloids, types of clays and their swelling and adsorption properties, cation exchange capacity and its determination, acid soils-types of soil acidity, liming, measurement of pH and conductivity of soil- saline and alkaline soils, analysis of major constituents of soil-organic matter, nitrogen, sulphur, sodium, potassium and calcium.

10. RADIOACTIVE POLLUTION 4 hrs

Detection and monitoring of radioactive pollutants; Methods for the safe disposal of radioactive wastes, dosimetry, analysis of data, advantages and restrictions of radiotracer experiments, safety aspects.

References:

1. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern (1993).
2. Experiments in Environmental Chemistry, P.D. Vowels and D.W. Connel, Pergamon (1980).
3. Measurement of Air Pollutants, M. Katz., WHO (1969).
4. Handbook on Air Pollution, Stern, APHA (1980)
5. Fundamentals of Analytical Chemistry, Skoog, West and Holler. Saunders College (1992).
6. Principles of Instrumental Analysis, D.A . Skoog and West. Saunders College (1980).
7. Quantitative Analysis, R.A. Day and A.L. Underwood, Prentice Hall (1980).
8. Food Analysis, A. G. Woodman, McGraw Hill (1971).
9. Foods: Facts and Principles, Shadaksharaswamy and Manay, Wiley Easter], (1987).
10. Analysis of Food and Food Products, Morris Jacobs

11. Milk and Milk Products, C.H. Eckles, W.B. Combs and H.Macy, Tata McGraw Hill (1976).
12. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, Ed. R.F. Dorge
13. The Essentials of Forensic Medicine and Toxicology, K.S. Narayan Reddy, Suguna Devi, Hyderabad (2002).
14. Hawk's Physiological Chemistry, Edition. B.I. Oser, Tata McGraw Hill (1976).
15. Practical Clinical Biochemistry, H. Varley, 4th edition [CBS] Indian edition (1988).
16. Lynch's Medical Laboratory Technology, S.S.Rapher, Itaku-Shoin edition Saunders (1983).
17. A Biologist's Guide to Principles and Techniques of Practical Biochemistry, K Wilson and K Goulding Edward Arnold (1986).
18. Analytical Biochemistry, Holmes and Peck, Longmans (1983).
19. Separation Techniques in Chemistry and Biochemistry, Roy Keller, Marcel. Dekker (1967).
20. Chemistry: Principles and Applications, Miller, Wadsworth Publishing Co (1976).
21. Methods of Soil Analysis Part I & II, C.A. Black et al (Edition), American Society of Agronomy (1965).
22. A Text book of Soil Chemical Analysis – P.R. Hesse, CBS Publishers (1994).

CH 0215: ORGANOMETALLIC CHEMISTRY AND INORGANIC REACTION MECHANISMS 60 HOURS

1. Organometallic Compounds 8 hrs

Nomenclature of organometallic compounds; classification based on the hapticity of ligands and the polarity of C-M bond; 18- electron rule, electron counting – covalent and ionic models; thermal, thermodynamic and kinetic stability and decomposition pathways; general methods of synthesis of organo metallics of representative elements.

2. Organometallic compounds of main group elements: 6 hrs

Group trends; Structure and bonding in Li, Be, Mg and Al alkyls.

3. Organometallic Compounds of Transition Metals: 14 hrs

Classification, structure, bonding, general methods of preparation and important classes of reactions of transition metal alkyls, carbenes and carbynes ; structure and bonding in transition metal complexes with dihapto to octahapto π-donor ligands - alkene, allyl, 1,3-butadiene, cyclopentadienyl, arene, cycloheptatrienyl and cyclooctatetraenyl complexes, metallocenes with special reference to ferrocene, cyclometallation and ring slippage reactions, activation of small molecules (CO and alkanes), Isolobal analogy and its applications.

4. Organometallic compounds in Organic Synthesis: 16 hrs

General introduction; rhodium complexes in hydrogenation, hydroformylation, decarbonylation reactions; Monsanto Acetic acid process; Palladium complexes in the synthesis of carbonyl compounds; Heck reaction; Wacker process; applications of zinc dialkyls, Grignard reagents, lithium alkyls, Gilman reagents (lithium dialkyl cuprates), organocadmium, organoselenium, organoaluminium, Zeigler-Natta catalysts - Growth reaction, polymerization of olefins; organosilicon, organotin and organomercurials in organic synthesis; Greens' rules; use of iron and chromium carbonyls in the synthesis of aromatic compounds;

5. Inorganic Reaction Mechanisms: 16 hrs

Kinetic lability and inertness, classification of metal ions based on lability; types of nucleophilic substitution reactions; kinetics and mechanism of nucleophilic substitution in square planar and octahedral complexes - trans effect; ligand field effects and reaction rates; reaction rates influenced by acids and bases, S_N1CB mechanism; racemization and isomerization; mechanisms of redox

reactions - outer sphere mechanism, Marcus equation for outer sphere cross reactions, excited state outer sphere electron transfer reactions, photochemical reactions of ruthenium complexes, inner sphere mechanism; oxidative addition and reductive elimination; migratory insertion; nucleophilic and electrophilic attack on coordinated ligands; template reactions.

References

1. Organometallic Chemistry, R.C. Mehrotra and A. Singh, Wiley Eastern, (1991).
2. Basic Organometallic Chemistry-Concepts, Syntheses and Applications, B D Gupta and A J Elias, University Press, India Pvt Ltd. (2011).
3. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley & sons (1988).
4. Organometallics, Vol 1 & 2, M. Bochmann, Oxford Chemistry Primers, Oxford University Press, (1994).
5. Organometallic Reagents in Synthesis, Paul R Jerkins, Oxford Chemistry Primers, Oxford University Press, (1992).
6. Advanced Organic Chemistry, J. March, 4th Edition. John Wiley, (1999).
7. Advanced Organic Chemistry, Part A, F. A. Carey and J. Sundberg, 2nd Edition., Plenum press (1999).
8. Principles of Organic Synthesis, Sir Richard Norman and James M Coxon, Third Edition., Chapman & Hall (1993).
9. Modern Synthetic Reactions, H.O. House, Benjamin, (1972).
10. Reaction Mechanisms of Inorganic and Organometallic Systems, J.B. Jordan, Oxford University Press, 2nd edition (1998).
11. Inorganic Chemistry, G.L. Miessler and Tarr, 3rd edition, Pearson Education (2004).
12. Inorganic Chemistry, 4th edition, J.E. Huheey, E.A. Keiter and R.L. Keiter, Addison-Wesley (1993).
13. Coordination chemistry, 2nd edition, D Banerjea, Asian Books pvt. Ltd.(2007)

CH 0315: SOLID STATE CHEMISTRY 60 Hours

1. ELECTRICAL AND MAGNETIC PROPERTIES OF SOLIDS 16 hrs

Band theory – electron in periodic potential, Bloch theorem,Kronig–Penny model (no derivation), Band structure – extended, reduced and repeat zone representation, Brilloin zones, DOS plots,metals, semiconductors and insulators.Properties of metals –metal-metal junction, thermoelectricity. Semiconductors – intrinsic and extrinsic semiconductors, Fermi levels of intrinsic, n-type and p-type semiconductors, concept of electron and hole, metal-semiconductor junction, p-n junction. Insulators –dielectric properties, piezoelectric effect,ferroelectricity, ferroelectric transitions in $BaTiO_3$, ionic conduction.Magnetic properties of solids – paramagnetism, diamagnetism, ferromagnetism and anti-ferro magnetism – M vs H and χvs T curves.

2. DEFECTS IN SOLIDS 4hrs

Point defects – Schotky and Frenkel defects, colour centers and non-stoichiometry, Line defects – edge dislocation and screw dislocation, Plane defects – grain boundary and stacking faults.Diffusion in solids,Fick's law.

3. PHASE TRANSITIONS IN SOLID 2 hrs

Definition and classification; first and second order phase transitions with examples.

4. SUPERCONDUCTIVITY 6 hrs

Definition, Meissner effect, type I and type II superconductors, features of superconductors, Frolich diagram, Cooper pairs, theory of low temperature superconductivity, high T_c superconductors.

5. GEOMETRIC CRYSTALLOGRAPHY 14hrs

Crystalline and amorphous states of matter. Periodicity in crystals. Symmetry elements and symmetry operations. Axis of symmetry, plane of symmetry, centre of symmetry; derivation of non-occurrence of five-fold rotation axis. Pure rotation axis, roto- inversion, roto-reflection axes, screw axes, glide planes; combination of symmetry operations – Euler's construction (interaxial angles) and its application to the general formula of the type A.B = C. Plane lattices, space lattices, point groups and space groups. Seven crystal systems with unit cell parameters and essential symmetry elements. Number of point groups in each crystal system, crystal classes. Stereographic

projections of the following point groups: 222, 32, 422, 622, 23, 432 (Supporting the interfacial angles Euler's Construction); Space group representation – Hermann-Maugin symbols of some selected space groups.

6. CRYSTAL STRUCTURES OF SOME REPRESENTATIVE SYSTEMS: 3hrs

AB (NaCl, CsCl, wurtzite and zinc blende types), AB_2 (rutile, fluorite and antiflourite, CdI_2 types), AB_3 (ReO_3 and related structures), ABO_3 (corundum, perovskite types).

7. X-RAY DIFFRACTION 13hrs

X-rays, Bragg's equation and Bragg's method, Miller indices, unit cell parameters and (Mentioninig of crystal systems whenever required). X-ray structural analysis of solid substances: powder diffraction pattern of primitive, face- centered and body centered cubic lattices, indexing of reflections, identification of space groups from systematic absences (space group extinctions). The concept of reciprocal lattice and construction of Ewald's sphere, derivation of Bragg's law from reciprocal lattice, structure factor(s) and its relation to intensity, intensities from atomic positions for BCC and FCC lattices. Phase problem- heavy atom (Patterson's) method and introduction to the principle of direct methods of phase determination. Electron density function and Fourier synthesis, electron density map(s).

8. ELECTRON AND NEUTRON DIFFRACTION 2hrs

Principle comparison with X-ray diffraction and applications

References :

1.Introduction to solids - L.V. Azaroff , Tata-McGraw Hill Publishing Company , New Delhi (1977)

2.Fundamentals of Crystallography - edited by C. Giacovazzo , International Union of Crystallography , Oxford University Press (2002).

3.The basics of crystallography and diffraction - C. Hammond , International Union of Crystallography , Oxford University press (2001)

4.Solid state Chemistry and its applications - A.R. West , John Wiley and Sons (1984)

5.A basic Course in Crystallography - J. Tareen and TRN Kutty , Universities Press (2001)

6.Principles of Solid State - H.V. Keer , Wiley Eastern Ltd. (1993).

7.Solid State Chemistry - D.K. Chakraborty , New Age International Publishers (2000).

8.An introduction to X -ray crystallography - M.M. Wolfson , Cambridge University Press (1997).

9. Crystal Structure Analysis for Chemists and Biologists, J.P. Glusker, M. Levis and M. Ross, Wiley-VCH (1994).

10. X-ray Structure determination – G.H. Stout and L.H. Jensen, McMillan Publishing Co, (1968).

11. SolidState physics- S. L. Gupta and V. Kumar, K. Nath and Co, Meerut, (2003).

CH 0415: BIOLOGICAL CHEMISTRY 60 HOURS

1. ESSENTIAL AND TRACE ELEMENTS IN BIOLOGICAL SYSTEMS 3 hrs

Role of metal ions in biological processes. Metal ion toxicity and detoxification - chelation therapy. Metal complexes in medicine: gold complexes and Platinum complexes.

2. METAL ION STORAGE AND TRANSPORT 6 hrs

Ferritin, transferrin, ceruloplasmin, siderophores. Transport and storage of dioxygen: hemoglobin, myoglobin, phenomenon of cooperativity, model systems (picket fence porphyrins), hemocyanin and hemerythrin.

3. TRANSPORT OF IONS ACROSS MEMBRANES 6 hrs

Thermodynamic treatment, active and passive transport, ionophores, Na^+/K^+ pump. Chemistry of vision and nerve conduction

4. ELECTRON TRANSPORT PROTEINS 6 hrs

Rubredoxin, ferredoxins, cytochromes. Photosynthesis: chlorophyll, PS I, PS II, role of manganese-protein complex in electron transfer in photosynthesis Nitrogen fixation: bacterial nitrogenase system. Biochemical importance of NO, role of Ca in signal transduction.

5. ENZYMES 7 hrs

Mechanism of enzyme action. Examples of some typical enzyme mechanisms - chymotrypsin, lysozyme, Michaelis-Menten kinetics and derivation of the equation, modifications and extensions of Michaelis-Menten equation, significance of Michaelis-Menten parameters, graphical representation of data - Lineweaver-Burke and Eddie Hoftsee plots, enzyme inhibition kinetics (competitive, non-competetive, uncompetitive and mixed) Non-productive binding, Competing substrates, Reversibility – Haldane Equation, Breakdown of Michaelis-Menten equation. Multisubstrate systems – brief description of different mechanisms (ordered, sequential and random

6. METALLOENZYMES 9 hrs

Non-redox enzymes – Carboxypeptidase A and Carbonic anhydrase, Redox enzymes- Superoxide dismutase (mono and binuclear) Peroxidase, Catalase, Cytochrome Oxidase, Cyt P_{450}, ascorbic acid oxidase, cobalamine, alcohol dehydrogenase.(Coordination environment around the metal and mechanism of action of each enzyme to be discussed)

7. COENZYMES **7 hrs**

Structure and biological function of Coenzyme A, Thiamine pyrophosphate, Pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, Lipoic acid. Mechanism of reactions involving the above coenzymes (one representative mechanism for each).

8. BIOSYNTHESIS OF MACROMOLECULES **7 hrs**

Pseudocycles - gluconeogenic pathway and its regulation. Biosynthesis of cholesterol and its regulation. Protein synthesis: Genetic code, wobble hypothesis, five stages of translation – i) activation(including idea of regulation of aminoacylt-RNA synthesis ii)Initiation process(including significance of Shine Delgarno sequence) iii)Elongation iv) Termination and v) post translation modification

9. BIOENERGETICS **5 hrs**

Standard free energy change in biochemical reactions. Methods for overcoming non-spontaneous reactions, ATP hydrolysis and synthesis, Energy generation in mechano-chemical systems: muscle contraction.

10. BIOPOLYMER INTERACTIONS **4 hrs**

Electrostatic charges, Hydrophobic forces, Dispersion force interactions, various types of binding processes in biological systems.

References:

1. Principles of Biochemistry, A. L. Lehninger, CBS, New Delhi (1993).
2. Biochemistry, L. Stryer, 2nd edition, CBS, New Delhi (1986).
3. Biochemistry, G. Zubay 4th Edition, WCB, Mcgraw Hill (1998).
4. Biochemistry, Voet and Voet, 2nd edition, John Wiley (1995).
5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpf, Wiley Eastern (1976).
6. Biochemistry: The Chemical Reactions of Living Cells, D. E. Metzler, Academic Press (1997).
7. Organic Chemistry, Paula Bruice (Pearson)
8. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima Publishers, (1997).
9. Biocoordination Chemistry, Fenton, Oxford University Primer Series (1995).
10. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine, Viva Books Pvt. Ltd., (1998).
11. Bioinorganic Chemistry, Robert W. Hay, Ellis Harwood, (1984).

12. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
13. Enzymes: Structure and Function, S Blackburn Marcel Dekker, (1976).
14. Enzyme Chemistry: Impact and Applications, Edition. Collin J. Suckling, Chapman and Hall.
15. Enzyme Mechanisms, Edition. M. I. Page and A. Williams,Royal Society of Chemistry.
16. Enzymes, M Dixon and Webb, 3rd edition, Longmans (1979).
17. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman (1979).
18. Enzyme Structure and Mechanism, A. Fersht, W. H. Freeman (1977).
19. Macromolecules: Structure and Function, F. Wold, Prentice Hall.
20. Physical Chemistry with Applications to Biological Systems, Raymond Chang, Mcmillan (1977).

CH 10PJ: RESEARCH PROJECT

The student is expected to carry out independent research putting in 18 hours of work per week and submit a project report, which will be evaluated.

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