

## **Contents:**

### **1) Compulsory Paper: Environmental Chemistry**

**2) Any 3 papers are to be selected out of the set of 5 papers of each branch:**

**a) 5 papers for Inorganic chemistry**

**b) 5 papers for Organic chemistry**

**c) 5 papers for Physical chemistry**

### **Compulsory Paper**

#### **CH-401 Environmental Chemistry (PG 330) 60 Hrs**

##### **1. Environment**

**8 Hrs**

Introduction. Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Biodistribution of elements.

##### **2. Hydrosphere**

**12 Hrs**

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle.

Aquatic pollution - inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters - dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards.

Analytical methods for measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand.

Purification and treatment of water.

### **3. Soils**

**6 Hrs**

Composition, micro and macro nutrients, Pollution - fertilizers, pesticides, plastics and metals. Waste treatment.

### **4. Atmosphere 8 Hrs**

Chemical composition of atmosphere - particles, ions and radicals and their formation.

Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry.

Analytical methods for measuring air pollutants. Continuous monitoring instruments

### **5. Industrial Pollution**

**12 Hrs**

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

### **6. Environmental Toxicology**

**14 Hrs**

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three Mile Island, Sewal D and Minamata disasters.

### **Recommended Texts:**

1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.

3. Environmental Chemistry, A. K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
5. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
7. Elemental Analysis Airborne Particle,. Ed. S. Landsberger, aod M. Cealchmao, GO'doo aod Beach Scleoce
8. Environmental Chemistry, C. Baird, W. H. Freeman.

**5 Special papers of Inorganic Chemistry (any 3 are to be selected)**  
**Inorganic Chemistry Special-I (Special topics in Inorganic Chemistry)**

**1. Advanced inorganic compounds:**

Chemistry of inorganic rings, cages and metal cluster compounds, borazines, phosphazenes, polyhedral boranes, carboranes, metalloboranes and metallocarboranes.

Silicates and aluminosilicates

Classifications, structure, properties and applications of naturally occurring silicates and aluminosilicates.

Syntheses of pillared clays, and zeolites.

Characterization of clays, pillared clays and zeolites from measurement of surface area, surface activity pore size, distribution and interlayer spacing.

Application of clays, pillared clays and zeolites with emphasis of catalyses.

**2. Macrocyclic Complexes:**

Types of macrocyclic ligands-design and synthesis of co-ordination template effect, di- and poly- nuclear macroscopic complexes.

**3. Organotransition metal chemistry:**

General introduction, Structure and bonding, Survey of organometallic complexes according to ligands. p bonded organometallic compounds including carbonyls, nitrosyls, tertiary phosphines, hydrides, alkene, alkyne, cyclobutadiene, cyclopentadiene, arene compounds and their M.O. diagrams. Metal-carbon multiple bonds. Fluxional organometallic compounds including p-allyl complexes and their characterization. Metallocycles,

unsaturated nitrogen ligands including dinitrogen complexes.

Futuristic aspects of organotransition metal chemistry.

#### **4. Molecular Magnetic Materials:**

Basic concepts of molecular magnetism, Types of magnetic interactions, inorganic and organic ferro-magnetic materials, low spin-high spin transitions, isotropic interactions in Cu(II) dinuclear compounds, magnetic chain compounds.

#### **5. Metallomesogens:**

Basic concepts, types of meso-phases synthetic strategies, characterization and applications

#### **Recommended Texts:**

1. Green, M. L. H. Organometallic Compounds Chapman & Hall: U.K. (1968).
2. Coates, G. E., Green, M. L. H. & Powell, P. Principles of Organometallic Chemistry Chapman and Hall: U.K. (1988).
3. Lippard, S. J. & Berg, J. M. Principles of Bioinorganic Chemistry Univ. Science Books (1994).
4. Lippard, S. J. Progress in Inorganic Chemistry Vols. 18 and 38, Wiley-Interscience (1991).
5. Jean-Marie Lehn, Supramolecular Chemistry, VCH, Weinheim (1995)
6. J.L. Sellarno, Metallomesogens, VCH, Weinheim (1996)
7. Oliver Kahn, Molecular Magnetism, VCH, Weinheim (1993)
8. Advanced Inorganic Chemistry, F.A. Cotton, G. Wilkinson, C.A. Murillo and M.Bochmann, 6<sup>th</sup> Edition, John Wiley & Sons (Asia), Singapore (2003)

## **Inorganic Chemistry Special-II**

### **1. Inorganic Materials**

Introduction to the solid state, metallic bond, Band theory (Zone model, Brillouin Zones, Limitations of the Zone model); Defects in solids, p-type and n-type; Inorganic semiconductors (use in transistors, IC, etc.); Electrical, optical, magnetic and thermal properties of inorganic materials.

Superconductors, with special emphasis on the synthesis and structure of high temperature superconductors.

Solid State Lasers (Ruby, YAG and tunable lasers):

Inorganic phosphor materials;

Synthesis and advantages of optical fibres over conducting fibres.

Diffusion in solids, catalysis and Zone refining of metals.

Preparation of nanomaterials and their characteristic differences over bulk materials.

### **2. Inorganic Polymers:**

Classification, types of inorganic polymerization, comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, Silicones.

### **3. Nuclear and Radiochemistry**

Nuclear structure and nuclear stability, Nuclear Models, Radioactivity and nuclear reactions (including nuclear fission and fusion reactions).

Hot atom Chemistry, Nuclear Fission and Fusion Reactors.

The interaction of nuclear radiations with matter. Radiation hazards and therapeutics. Detectors and their principles.

The direction of radioactivity. The counting errors and their corrections.

Tracer techniques and their applications. Isotope dilution and radio-

activation methods of analysis. Fission product analysis (e.g., the technique of isolating two or three different fission products of U or Th and determining the yields).

**Recommended Texts:**

1. Ballhausen C. J. Introduction to Ligand Field Theory McGraw Hill Book Co.: N.Y (1962).
2. Marshal, C. E. The Physical Chemistry and Minerology of Soil Vol. I Soil Materials John Wiley & Sons.
3. Wells, A. F. Structural Inorganic Chemistry Oxford University Press.
4. Adams, D. M. Inorganic Solids. An Introduction to Concepts in Solid-State
5. Structural Chemistry John Wiley & Sons
6. Azaroff, L. V. Introduction to Solids Tata McGraw Hill Publishing Co. Ltd.
7. Breck, D. W. Zeolites Molecular Sieves- Structure, Chemistry and Use. John Wiley & Sons.
8. Harvey, B. C. Introduction to Nuclear Chemistry Prentice-Hall (1969).
9. Friedlander, G. Kennedy, J. W., Marcus, E. S. & Miller, J. M. Nuclear & Radiochemistry, John Wiley & Sons (1981).
10. Keer, H. V. Principles of the Solid State Wiley Eastern Ltd.: New Delhi (1993).
11. West, A. R. Solid State Chemistry and its Applications John Wiley & Sons (1987).
12. Hannay, N. Treatise on Solid State Chemistry Plenum (1976).
13. Cheetham, A. K. & Day, P., Eds. Solid State Chemistry Techniques
14. Clarendon Press, Oxford (1987)
15. Timp, G., Ed. Nanotechnology Springer-Verlag: N. Y. (1999).

## **Inorganic Chemistry Special-III (Advanced Inorganic Chemistry)**

### **1. Introduction to the solution of multi-electron problems:**

The central field approximation, angular momenta, step up and step down operators and their use in atomic spectra. Lande's interval rule. Evaluation of energy matrices using Slater's method. Wave functions forming basis for irreducible representations, direct product. Spherical harmonics and their linear combinations. Operator equivalent technique.

### **2. The octahedral potential:**

Contribution of spherical harmonics to the octahedral potential  $V_{xyz}$ . Single electron in a cubic field, quantitative basis (r,  $\theta$ ,  $\phi$ ) for the splitting of d orbital to  $e_g$  and  $t_{2g}$  in terms of  $Dq$ , multielectron systems - the weak and strong field cases. Generation of a secular determinant for  $3F$  term ( $d^2$ ) in weak field. Bethe's method of descending symmetry. Non octahedral fields, tetrahedral (including contribution of odd harmonics), trigonal and tetragonal (including  $D_s$  &  $D_t$  parameters). Spin orbit coupling and its magnitude in comparison to crystal field. Splitting of  $e_g$  and  $t_{2g}$  orbitals due to spin orbit coupling, for a  $d_1$  and  $d_9$  case. The use of double group  $D_4'$  and  $O'$ . Effect of spin orbit coupling on A, E and T terms in octahedral fields.

### **3. Magnetism:**

Types of magnetic behaviour, magnetic susceptibilities, Pascal's constants, paramagnetism in experimental simple systems where  $S = \tilde{A}, \hat{A}^{1/2}$ , van Vleck's equation, its derivation and its applications. Spin-orbit coupling and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms of A, E and T symmetry, T.I.P.,

intramolecular effects, antiferromagnetism and ferromagnetism of metal complexes, super paramagnetism. High and low spin equilibria.

**Recommended Texts:**

1. Cheetham, A. K. & Day, P., Eds. Solid State Chemistry Techniques Clarendon Press, Oxford (1987)
2. Skoog, D. A., West, D. M., Holler, R. J & Nieman, T. A. Principles of Instrumental Analysis Saunders Golden Sunburst Series (1997).
3. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) Instrumental Methods of Analysis - 7th Ed., Wadsworth Publishing (1988) ISBN 0534081428
4. Khopkar, S. M. Concepts in Analytical Chemistry Halsted (1984).

## **Inorganic Chemistry Special-IV (Advanced Spectral Techniques in Inorganic Chemistry)**

### **1. Electronic spectroscopy:**

Vibrational and electronic energy levels in a diatomic molecule, potential energy level diagram. Symmetry requirements for  $n$  to  $p^*$  transitions, oscillator strengths, transition moment integrals (electric dipole and magnetic dipole moment operator), selection rules, spin orbit and vibronic coupling contributions, mixing of  $d$  and  $p$  orbitals in certain symmetries. Polarized absorption spectra. Survey of the electronic spectra of tetragonal complexes. Calculation of  $Dq$  and  $\tilde{\Delta}_f$  for Ni(II) Oh complexes, nephelauxetic effect, effect of  $s$  and  $p$  bonding on the energy of  $t_{2g}$  orbitals and  $Dq$ , spectrochemical series, effect of distortion on the  $d$  orbital energy level ( $T_d$ ,  $D_{2d}$ ,  $D_{4h}$ ), cis and trans isomers and bonding parameters from spectra of tetragonal complexes, bonding parameters, calculation of  $Dq$ ,  $D_s$  and  $D_t$  for tetragonal complexes, intervalence electronic transition, structural evidence from electronic spectra.

### **2. Nuclear magnetic resonance spectroscopy:**

Nuclear spin quantum number and its calculation using the nuclear shell model, spin parity rules. Types of nuclei based on value of nuclear spin angular momentum quantum number, and its relation to classical magnetic moment. Behaviour of a bar magnet in a magnetic field. The NMR transition and NMR experiment, measuring chemical shifts, signal intensities and splitting. Application of chemical shifts, signal intensities and spin-spin coupling to structure determination of inorganic compounds carrying NMR active nuclei like  $^1H$ ,  $^{11}B$ ,  $^{15}N$ ,  $^{19}F$ ,  $^{29}Si$ ,  $^{31}P$ ,  $^{183}W$ ,  $^{195}Pt$ , etc. Effect of fast chemical reactions, coupling to quadrupolar nuclei, NMR of

paramagnetic substances in solution, nuclear and electron relaxation time, the expectation value of  $\sigma_z$ , contact shift, pseudo contact shift, factoring contact and pseudo contact shift for transition metal ions. Contact shift and spin density,  $p$  delocalization, simplified M.O. diagram for Co(II) and Ni(II). Application to planar tetrahedral equilibrium, Contrast agents.

### **3. Electronic paramagnetic resonance spectroscopy:**

Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. EPR spectrometers, presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Shift operators and the second order effect. Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in  $g$ -value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

### **4. Nuclear Quadrupolar Resonance (NQR) Spectroscopy:**

Quadrupolar moment, energy levels of a quadrupolar nucleus and effect of asymmetry parameters and energy levels. Effect of an external magnetic field, selected examples for elucidation of structural aspects of inorganic compounds using NQR spectroscopy.

#### **Recommended Texts:**

1. Ebsworth, E. A. O. Structural Methods in Inorganic Chemistry Blackwell Scientific Publications (1991).
2. Drago, R. S. Physical Methods in Chemistry W. B. Saunders Co.: U.K. (1977).
3. Carrington, A. & McLachlan, A. D. Introduction to Magnetic Resonance Chapman & Hall: N.Y. (1983).

4. Mabbs, F. E. & Machin, D. J. Magnetism and Transition Metal Complexes  
Chapman and Hall: U.K. (1973).

## **Inorganic Chemistry Special-V (Chemistry of Materials)**

### **I. Multiphase of Materials**

Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

### **II. Glasses, Ceramics, Composites and Nanomaterials**

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications.

Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

### **III. Thin Films and Langmuir-Blodgett Films**

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

### **IV. Liquid Crystals**

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic – nematic transition and clearing temperature-homeotropic, planar and schlieren

textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

## **V. Ionic Conductors**

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

## **VI. High T<sub>c</sub> Materials**

Defect perovskites, high T<sub>c</sub> superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multigap structure in high T<sub>c</sub> materials, applications of high T<sub>c</sub> materials.

## **VII. Materials for Solid State Devices**

Rectifiers, transistors, capacitors-IV-V compounds, low-dimensional quantum structures; optical properties.

### **Recommended Texts:**

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Solid State Physics, H.S. Saxena, R.C. Gupta, P.N. Saxena, Pragati Prakashan.

3. Principles of the Solid State, H.V. Keer, Wiley Eastern.
4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS.
5. Material Science and Engineering, An Introduction, W.D. Cullister, Wiley.

### **Inorganic Chemistry Practicals:**

#### **Note:**

1. Duration of examination: Three days, six hours daily
2. One internal examiner from college and one external examiner from other university are to be appointed.
3. Total section = 05

Total Practicals to be conducted in exam. = 04

One from section A, One from section B and any two from section C, D, E;

But only one from one section.

Total marks = 100

Mixture = 40

Preparation = 15

From C, D, E = 20 (2x10)

Viva-voce = 15

Record = 10

**A: Identifications/ Qualitative Determinations** (all three experiments are to be performed in practice )

1. Qualitative analysis of mixtures of salts including rare element salts (soluble and insoluble) containing eight radicals including interfering.
2. Quantitative analysis of mixtures of metal ions by complexometric titrations

(mixture of two metals) with the use of masking and demasking agents.

3. Determination of concentration of some metal ions, such as iron, nickel, etc. by colourimetric method.

**B: Preparations** (Any three are to be performed in practice)

Preparation of selected inorganic compounds and their study by IF, electronic spectra, Mossbauer, ESR and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines.

1. Sodium amide. Inorg. Synth., 1946, 2, 128.
2. Synthesis and thermal analysis of group II metal oxalate hydrate. J. Chem. Ed., 1988, 65, 1024.
3. Trialkylboranes-Preparation, IR and NMR spectra.
4.  $\text{PhBCl}_2$  Dichlorophenylborane-Synthesis in vacuum line.
5. Preparation of Tin(IV) iodide, Pb(IV). Preparation of ammonium hexachlorostannate  $(\text{NH}_4)_2\text{SnCl}_6$ , ammonium hexachloroplumbate  $(\text{NH}_4)_2\text{PbCl}_6$ .
6. Sodium tetra thionate  $\text{Na}_2\text{S}_4\text{O}_6$ .
7. Bromination of  $\text{Cr}(\text{acac})_3$ . J. Chem. Edu., 1986, 63, 90.
8. Separation of optical isomer of  $\text{cis}-[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$ . J. Chem. Soc. 1960, 4369.
9. Determination of Cr(III) complexes.  
 $[\text{Cr}(\text{H}_2\text{O})_6]\text{NO}_3 \cdot 3\text{H}_2\text{O}$ ,  $[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ ,  $[\text{Cr}(\text{en})_3]\text{Cl}_3$ ,  $\text{Cr}(\text{acac})_3$ .  
Inorg. Synth., 1972, 13, 184.

**C: Spectrophotometric Determinations** (Any two are to be performed in practice)

- a) Manganese/Chromium/Vanadium in steel sample
- b) Nickel/molybdenum/tungsten/vanadium/uranium by extractive spectrophotometric method.
- c) Fluoride/nitrate/phosphate.

- d) Iron-phenanthroline complex: Job's Method of continuous variations.
- e) Zirconium-Alizarin Red-S complex: Mole-ratio method
- f) Copper-Ethylene diammine complex: Slope-ratio method.

**D: Flame Photometric Determinations** (Any one is to be performed in practice)

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

**E: Chromatographic Separations** (any two are to be performed in practice)

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

**Recommended Texts:**

1. Inorganic Experiments, J. Derek Woollins, VCH.
2. Microscale Inorganic Chemistry, Z. Szatran, VCH.
3. The Systematic Identification of Organic Compounds, R.L. Shriner and D.Y. Curtin.
4. Organometallic Synthesis, J.J. Fisch and R.B. King. Academic.
5. Practical Inorganic Chemistry, G. Marr and B.W. Rockett. Van Nostrand.

**5 Special papers of Organic Chemistry (any 3 are to be selected)**

**Organic Chemistry Special I**

**CH-402 Organic Synthesis (PG-331) 60Hrs**

**1. Organometallic Reagents: 15 Hrs**

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

**Group I & II metal organic compounds**

Li, Mg, Hg, Cd, Zn and Ce Compounds

**Transition metals**

Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti Compounds.

**Other elements**

S, Si, B and I compounds.

**2. Oxidation: 11 Hrs**

Introduction. Different oxidative processes.

Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated).

Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.

Amines, Hydrazines and sulphides.

Oxidation with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

### **3. Reduction:**

**11 Hrs**

Introduction. Different reductive processes.

Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings.

Carbonyl Compounds- aldehydes, ketones, acids and their derivatives.

Epoxides, nitro, nitroso, azo and oxime groups.

### **4. Rearrangements:**

**15 Hrs**

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

A detailed study of the following rearrangements: Pinacol-Pinnacolone, Wagner-Meerwin, Demjanov, benzyl-Benzilic acid, Favorskii, Arndt-Eistern synthesis, Neber, Beckmann, Hoffman, Curtius, Schmidt, BaeyerVilliger, Shapiro reaction, Barton, Chichibaben, Hoffman-Lofler Freytag reaction, Wittig reaction.

### **5. Metallocenes, Nonbenzenoid Aromatic and Polycyclic Aromatic**

#### **Compounds:**

**8 Hrs**

General considerations, synthesis and reactions of Ferrocene, Chrysene, Azulene.

#### **Recommended Texts:**

1. Modern Synthetic reactions, H. O. House, W.A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
3. Advanced Organic Chemistry, Reaction Mechanisms and Structure, J. March, John Wiley.

4. Principles of Organic Synthesis, R.O.C. Norman and J. M. Coxoxn, Blackie Academic and Professional.
5. Advanced Organic Chemistry Part B, F.A. Carey and R. j. Sundberg, Plenum Press.

## **Organic Chemistry Special II**

**CH-403 Medicinal Chemistry (PG-333)**

**60Hrs**

### **1. Introduction to Medicinal Chemistry:**

**2 Hrs**

Introduction to important functional groups in medicinal chemistry, a century of drug research.

### **2. Drug design:**

**6 Hrs**

Strategies for drug research including various targets, lead generation/ sources for drugs, receptor and drug receptor interactions; enzymes and design of inhibitors; concept of Prodrugs, hard and soft drugs.

### **3. Combinatorial Chemistry:**

**7 Hrs**

Introduction; solid support and linkers; combinatorial synthesis of compounds on solid phase, split and mix method, premix method, spatially addressable parallel chemical synthesis, multiple synthesis; Identification of active compounds from combinatorial libraries; Analytical methods for characterization of combinatorial libraries;

Application of combinatorial libraries using solid phase chemistry.

**4. Computational approaches:****7 Hrs**

Structure activity relationship, concept of QSAR, physicochemical parameters lipophilicity, partition coefficient, electronic-ionization constants, H-bonding, steric parameters, Hammett equation. Isosterism, bioisosterism.

**5. Biodisposition and implications:****10 Hrs**

Pharmacokinetics; concepts including absorption, distribution, metabolism and excretion of the drug, pharmacokinetic parameters; drug metabolism including phase I and phase II biotransformations; mention of the uses of pharmacokinetics in drug development process. Molecular toxicology, avoidance of toxic intermediates,

**6. Neuroactive agents:****10 Hrs**

The chemotherapy of the mind: Introduction, neurotransmitters, CNS depressants, General anaesthetics, mode of action of hypnotics, sedatives, antianxiety agents, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs the neuroleptics, antidepressants, butyrophenone, serendipity and drug development, stereochemical aspects of neuroactive drugs. Synthesis of Diazepam, Oxazepam, Chlorazepam, barbiturates.

**7. Cardiovascular agents:****5 Hrs**

Introduction, cardiovascular diseases, drug inhibitors of the peripheral sympathetic function, central intervention of the cardiovascular output, direct acting arteriolar dilators, synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxeprenolol.

**8. Antineoplastic agents:****7 Hrs**

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

inhibitors; synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, 6- mercaptopurine. Recent development in cancer chemotherapy, the hormones and natural products.

**9. Local anti-infective drugs:**

**6 Hrs**

Introduction and general mode of action, synthesis of sulphonamide, furazolidone, naxilidic acid, eiprofloxacin, dapsone, aminosalicylic acid, isoniazid, ethionamide, ethambutol, fluconazole, econozole, gresiofulvin, chloroquin, primaquin.

**Recommended Texts:**

1. Comprehensive Medicinal Chemistry, Vols. 1-6, Corvin Hansch (editor) 1990.
2. Burger's Medicinal Chemistry, 4th edition, 3 parts; M.E. Wolff, Ed. (RS 403.B8-1979-pt. 1,2 &3).
3. Principles of Medicinal Chemistry, W.O. Foye (editor), 4th edition, 1995.
4. Molecular Mechanism of Drug Action, C. J. Coulson, 1998.
5. Medicinal Chemistry : A Biochemical Approach, Thomas Nogrady, 2nd edition, 1998.
6. Wilson and Gisvold's Textbook of Organic, Medicinal and Pharmaceutical Chemistry, J.N. delago and W.A. Remers (editors) 9th edition 1991.
7. Organic Chemistry of Drug Synthesis, Vol. I, Daniel Lednicer and Lester A., Mitscher (RS 403.L38-Vols. 1,2 and 3).
8. The Pharmacological Basis of Therapeutics, Louis S. Goodman and Alfred Gilman (RM 101.G63-1970).

## **Organic Chemistry Special III**

### **CH-404 Polymers**

**60Hrs**

#### **1. Basics**

**8 Hrs**

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers.

Polymerization: condensation, addition, radical chain-ionic and co-ordination and copolymerization.

Polymerization conditions and polymer reaction. Polymerization in homogeneous and heterogeneous systems.

#### **2. Polymer characterization**

**14 Hrs**

Polydispersion-average molecular weight concept. Number, Weight and Viscosity average molecular weight. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weight. End group, viscosity light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers and chemical analysis of polymers, spectroscopic methods, physical testing – tensile strength, fatigue, impact. Tear resistance. Hardness and abrasion resistance

### **3. Structure and Properties**

**14 Hrs**

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point  $T_m$ -melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature,  $T_g$  relationship between  $T_m$  &  $T_g$ , effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

### **4. Polymer Processing**

**12 Hrs**

Plastics, elastomers and fibers. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fiber spinning.

### **5. Properties of Commercial Polymers**

**12 Hrs**

Polyethylene, Polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicon polymers. Functional Polymers- Fire retarding polymers and electrically conducting polymers. Biomedical polymers- contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

#### **Recommended Texts:**

1. Text Book of Polymer Science, F.W. Billmeyer Jr, Willey.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-  
Eastern

3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and RM. Otanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymers, J. M. G Cowie, Blackie Academic and Professional.

### **Organic Chemistry Special IV (Chemistry of Natural Products)**

- I. **Terpenoids and Carotenoids :** Classification, nomenclature, occurrence, isolation, general methods of structure, determination, isoprene rule, Structure determination, stereochemistry biosynthesis and synthesis of the following representative molecules : Citral, Geraniol,  $\alpha$  termpeneol Menthol, Farnesol, Zingiberen.
  
- II. **Alkaloids:** Definition, nomenclature and physiological action, occurrence, isolation, general methods or structure elucidation, degradation, classification based on nitrogen heterocyclic rings, role of alkaloids in plants, Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+) Coniline, Nicoline, Atropine, Quinine and Morphine.
  
- III. **Steroids :** Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, Isolation, Structure determination and synthesis of Cholestrol, Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Aldosterone, Biosynthesis of steroids.

**IV. Plant Pigments :** Occurrence, nomenclature and general methods of structure determination, Isolation and synthesis of Apigenin, Luteolin, Quercetin, myricetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cyanidin -7- arabinoside, Cyanidin, Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

**V. Prophyris :** Structure and synthesis of Haemoglobin and Chlorophyll.

**VI. Prostaglandins :** Occurrence, biogenesis and physiological effects  
Synthesis of PGE<sub>2</sub> and PGF<sub>2a</sub>.

**Recommended Texts:**

1. Natural Products: Chemistry and Biological Significance. J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
2. Organic Chemistry, Vol. 2, I.L. Finar, E.L.B.S.
3. Stereoselective Synthesis: A Practical Approach, M.Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed.S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt hostettmann, M.P. gupta and A.Marston, Harwood Academic Publishers.

## **Organic Chemistry Special V (Heterocyclic Chemistry)**

### **1. Nomenclature of Heterocycles**

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

### **2. Aromatic Heterocycles**

General chemical behavior of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in  $^1\text{H}$ ) NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations).

Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

### **3. Non-aromatic Heterocycles**

#### **4. Heterocyclic Synthesis**

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

#### **5. Small Rings Heterocycles**

Three-membered and four membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and theitanes.

#### **6. Benzo-Fused Five-Membered Heterocycles**

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.

#### **7. Meso-ionic Heterocycles**

General classification, chemistry of some important meso-ionic heterocycles of type-A and type-B and their applicatios.

#### **8. Six-Membered heterocycles with One Heteroatom**

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium and thiopyrylium salts and pyridines.

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

#### **9. Six-membered Heterocycles with two of More Heteroatoms**

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

#### **Recommended Texts:**

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. M. 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.

### **Organic Chemistry Practicals:**

#### **Note:**

1. Duration of examination: Three days, six hours daily
2. One internal examiner from college and one external examiner from other university are to be appointed.

3. Total section-4

Total practicals to be conducted in the exam-4 (One from each section)

4. Marks distribution:

<b>Total marks</b>	<b>=100</b>
Mixture	= 30 marks,
Preparation	=15 marks,

Estimation of aniline	=10 marks,
Estimation of sulphur	=20 marks
Viva	=15 marks,
Record	=10 marks

**Each section is to be covered in practice.**

1. Analysis of ternary organic mixtures.

- Separation with  $\text{NaHCO}_3$  and water
- Separation with  $\text{NaOH}$  and water.
- Separation with  $\text{HCl}$  and water
- Separation with organic solvents.

2. Three step organic preparations.

- To prepare o-chlorobenzoic acid from phthalic anhydride.
- To prepare benzilic acid from benzaldehyde.
- To prepare dibenzil from benzaldehyde.
- To prepare benzoic acid from benzophenone.

3. To determine the strength of the given aniline/phenol solution (estimation of Aniline/phenol).

4. To determine the percentage of sulphur in the given organic compound by messenger's method.

## **5 Special papers of Physical Chemistry (any 3 are to be selected)**

### **Physical Chemistry Special-I (Solid State Chemistry)**

#### **I. Solid State Reactions**

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

#### **II. Crystal Defects and Non-Stoichiometry**

Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects. Thermodynamics of schottky and

### **III. Electronic Properties and Band Theory**

Metals, insulators and semiconductors, electronic structure of solids-band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, superconductors.

Optical Properties- Optical reflectance, photoconduction-photoelectric effects.

Magnetic properties-Classification of materials : Quantum theory of paramagnetics- cooperative phenomena- magnetic domains, hysteresis

### **IV. Organic Solids**

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

### **V. LASERS**

Luminescence and lasers

### **VI. Recent trends in solid state chemistry**

#### **Recommended Texts:**

1. Solid State Chemistry and its applications, A.R. West, Plenum.
2. Principles of the Solid States, H.V. Keer, Wiley Eastern.
3. Solid State Chemistry, N.B. Hannay.
4. Solid state Chemistry, D.K. Chakrabarty, New Age International

## **Physical Chemistry Special-II (Advanced Quantum Chemistry)**

### **I. Theoretical and Computational Treatment of Atoms, Molecules**

Hartree-Fock Theory    Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussian basis sets.

### **II. Configuration Interaction of MC-SCF**

Introduction to CI, full and truncated CI theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods

### **III. Semi-Empirical Theories**

A review of Huckel, EHT and PPP treatments, ZDO approximations, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MOPAC and AMI with hands on experience on personal computers

#### **IV. Density Functional theory**

Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulations, N- and V- representabilities; review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functional, treatment of chemical concepts with the density functional theory.

#### **V. Computer Experiments**

Computer experiments using quantum chemistry- software packages such as GAUSSIAN/GAMESS/MOPAC and modeling software e.g. MM2/AMBER/CHARM etc.

#### **Recommended Texts:**

1. Modern Quantum Chemistry, N.S. Ostlund and A.Szabo, Mcgraw Hill.
2. Methods of Molecular Quantum Mechanics, R.McWeeny and B.T. Sutcliffe, Academic Press
3. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford.
4. Exploring Chemistry with Electron structure Methods, JI.B. Foresman and E.Frish, Goussian inc.
5. Semi-empirical MO Theory, J. Popie and D.L. Beveridge.

## **Physical Chemistry Special-III (Liquid State)**

### **I. General Properties of Liquids**

- (a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations, internal pressure and its significance in liquids, Equation of state, critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids, additivity of pair potential approximation.
- (b) A classical partition function for liquids, correspondence principle, configuration integral, configurational properties

### **II. Theory of Liquids**

Theory of liquids, partition function method or model approach; single cell models, communal energy and entropy, LTD model, significant structure model.

### **III. Distribution Function and related Equations**

Radial distribution function method, equation of state in terms of RDF. Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.

### **IV. Methods for Structure Determination and Computational Techniques**

Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy.

Computation Techniques- Monte Carlo and molecular dynamics methods

### **V. Supercooled and Ionic Liquids**

Supercooled and ionic liquids, theories of transport properties; non Arrhenius behaviour of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in supercooled liquids

#### **Recommended Texts:**

1. An Introduction to Liquid State, P.A. Egelstaff, Academic Press
2. The Dynamic Liquid State A.F.M. Barton, Longman
3. Introduction to Statistical Thermodynamics, T.L. Hill Addison Wiley
4. The Liquid State, J.A. Pryce
5. Significant Liquid Structure, H Eyring and M. S. John

## **Physical Chemistry Special-IV (Physical Chemistry in Organic reactions)**

### **I. Concepts in Molecular Orbital (MO) and Valence Bond (VB) theories**

Introduction to Huckel Molecular Orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques and FMO theory. Molecular mechanics, semi empirical methods and ab initio and density functional methods. Scope and limitations of several computational programmes.

Quantitative MO theory – Huckel molecular orbital (HMO) method as applied to ethane, allyl and butadiene. Qualitative MO theory- ionization potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital

interaction diagrams. MO of simple organic systems such as ethane, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity.

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

## **II. Principles of Reactivity**

Mechanistic significance of entropy, enthalpy and Gibb's free energy, Arrhenius equation. Transition state theory. Use of activation parameters, Hammond's postulate. Bell-Evens-polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

## **III. Kinetic Isotope effect**

Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

## **IV. Structural Effects on Reactivity**

Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of  $\sigma$ -values. Reaction constant  $\rho$ . Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model.  $\sigma_1$ - and  $\sigma_R$ -scales.

## **V. Solvation and Solvent Effects**

Qualitative understanding of solvent-solute effects on reactivity. Thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibrium. Various empirical indexes of solvation based on physical properties, solvent-sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve crossing model.

## **VI. Acids, Bases, Electrophiles, Nucleophiles and Catalysis**

Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The  $\sigma$ -effect. Ambivalent nucleophiles. Acid-base catalysis-specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis. Catalysis by non-covalent binding-micellat catalyst.

## **VII. Steric and Conformational Properties**

Various types of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammet principle.

### **Recommended Texts:**

1. Molecular Mechanics, U. Burkert and N.L. Allinger Monograph 177, 1982
2. Organic Chemists' Book of Orbitals. L. sulern and W.L. Jorgensen, Academic Press.
3. Mechanism and Theory in Organic Chemistry, T.H. Lewry and K.C. Richardson, Harper and Row.
4. Introduction to theoretical Organic Chemistry and Molecular Modeling, W.B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman.
6. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

## **Physical Chemistry Special-V (Computational Chemistry)**

### **1. Fortran/C Programming and Numerical Methods**

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

#### **a. Solutions of Equations**

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

#### **b. Linear Simultaneous Equations**

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

**c. Eigenvalues and Matrix Diagonalization**

Jacobi and Householder methods, analysis of errors

**d. Interpolation**

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

**e. Numerical Differentiation**

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

**f. Numerical Integration**

Newton-Cotes formulae, Romberg integration, errors in integration formulae. The students should develop computer programs of the above numerical methods.

**2. Running of Advanced Scientific Packages**

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

**3. Introduction to Networking and Search using Internet**

**4. Project**

The students will develop utilities such as analysis of spectra, simulation programmes which will supplement laboratory or theory exercises in physical, organic, inorganic chemistry or biochemistry. This list is only indicative and a variety of small projects designed by the teacher based on the interest of the student and capabilities should be worked out.

### **Recommended Texts:**

1. Computational Chemistry, A.C. Norris, John Wiley.
2. Computer Based Numerical and Statistical Techniques, S.K. Pundir, Pragati Prakashan.
3. A Text Book of Fortran Programming, M. P. Thapliyal, M.M.S. Rauthan, Pragati Prakashan
4. Programming Computer with 'C', Chanchal Mittal, Unnati Publication
5. Numerical Analysis-A Practical Approach, M.J. Maron, John Wiley

### **Physical Chemistry Practicals:**

#### **Note:**

1. Duration of examination: Three days, six hours daily
2. One internal examiner from college and one external examiner from other university are to be appointed.
3. One experiment each from any three sections, total three experiments are to be conducted.

#### **4. Marks distribution**

Total marks	=100
Each experiment= 25 marks	=75 (3x25)
Viva	=15
Record	=10

**At least 10 experiments are to be performed in practice covering at least four sections.**

**A: Chemical Kinetics**

1. Determine the specific rate constant for the acid catalyzed hydrolysis of methyl acetate by the Initial Rate Method. Study the reaction at two different temperatures and calculate the thermodynamic parameters.
2. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
3. Study the saponification of ethyl acetate with sodium hydroxide volumetrically.
4. Determine the specific reaction rate of the potassium persulphate-iodide reaction by the Initial Rate Method.
5. Study the kinetics of the iodination of acetone in the presence of acid by the Initial Rate Method.
6. (a) Determine the specific rotation constant for sucrose.  
(b) Study the acid catalyzed inversion of cane sugar, and find out
  - (i) the order with respect to sucrose;
  - (ii) the rate constant;
  - (iii) Compare kinetically the strengths of two acids (HCl and H<sub>2</sub>SO<sub>4</sub>)

**B: Conductometry**

1. Determine the Cell Constant of the given conductivity cell at room temperature and study the equivalent conductance versus square root of concentration relationship of a strong electrolyte (KCl or NaCl) and weak electrolyte (acetic acid).
2. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.
3. Determine the equivalent conductance, degree of dissociation and

dissociation constant ( $K_a$ ) of acetic acid.

4. Study the conductometric titration of hydrochloric acid with sodium carbonate and determine the concentration of sodium carbonate in a commercial sample of soda ash.

5. Study the conductometric titration of

(i) Acetic acid vs. sodium hydroxide,

(ii) Acetic acid vs. ammonium hydroxide,

(iii) Sodium acetate vs. HCl,

Comment on the nature of the graphs.

6. Study the stepwise neutralization of a polybasic acid e.g. oxalic acid, citric acid, succinic acid by conductometric titration and explain the variation in the plots.

7. Study the conductometric titration of a mixture of a strong and weak acid.

8. Study the estimation of potassium sulphate solution by conductometric titration.

### **C: Potentiometry**

1. Prepare and test the Calomel Electrode.

2. Titrate hydrochloric acid and sodium hydroxide potentiometrically.

3. Determine the dissociation constant of acetic acid potentiometrically.

4. Titrate oxalic acid and sodium hydroxide potentiometrically.

5. Titrate a mixture of

(i) strong and weak acids (Hydrochloric and acetic acids)

(ii) weak acid (acetic acid) and dibasic acid (oxalic acid)

(iii) strong acid (hydrochloric acid) and dibasic acid (oxalic acid)

versus sodium hydroxide.

6. Titrate a solution of Mohr's salt against potassium permanganate potentiometrically.

7. Titrate a solution of Mohr's Salt and potassium dichromate

potentiometrically.

### **D: Computational Methods**

Familiarity with word processing, electronic spreadsheets, data processing, mathematical packages, chemical structure drawing and molecular modelling.

### **E: Thermodynamics**

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

### **F: Spectroscopy**

1. Determination of pK<sub>a</sub> of an indicator (e.g., methyl red) in (a) aqueous and (b) micellar media.
2. Determination of stoichiometry and stability constant of inorganic (e.g. ferric-salicylic acid) and organic (e.g amine-iodine) complexes.
3. Characterization of the complexes by electronic and IR spectral data.

### **Recommended Texts:**

1. Experimental Physical Chemistry, D.F. Shoemaker, C.W. Carland and J.W. Niber, McGraw Hill Interscience
2. Findlay's Practical Physical Chemistry, revised B.P. Lebiu, Longman
3. Experiments in Physical Chemistry, J.C. Ghosh, Bharti Bhavan
4. Experimental Physical Chemistry, Gurtu-Gurtu, Pragati Prakashan