UNIVERSITY OF DELHI

SCHEME OF EXAMINATION
AND
COURSES OF READING
FOR
M. Sc. CHEMISTRY EXAMINATION

I Semester Examination November 2006
II Semester Examination April 2007
III Semester Examination November 2007
IV Semester Examination April 2008

Syllabus applicable for the students seeking admission to the M.Sc. Chemistry Course in the academic year 2006-07

UNIVERSITY OF DELHI

Scheme of Examination for M. Sc. Course in Chemistry

Semester I

		Duration (Hours)	*Maximum Marks*
Paper I	Inorganic Chemistry	3	50
Paper II	Organic Chemistry	3	50
Paper III	Physical Chemistry	3	50

Semester II

		Duration (Hours)	*Maximum Marks*
Paper IV	Inorganic Chemistry	3	50
Paper V	Organic Chemistry	3	50
Paper VI	Physical Chemistry	3	50
Practical Test		18	200

Note: The Practical test shall consist of three papers, each of six hours duration, suitably spread over three days and shall be at the end of Semester II. One-fourth of the total marks for the Practical test shall be reserved for the Laboratory Record/ Sessional Work of the candidates and 30 marks for viva-voce.

12 marks in each theory paper are reserved for internal assessment, as per the University ordinance.

Semester III

		Duration (Hours)	*Maximum Marks*
Paper VII	Inorganic Chemistry	3	50
Paper VIII	Organic Chemistry	3	50
Paper IX	Physical Chemistry	3	50
Inorganic Group: Paper X(i)	Inorganic Chemistry (Special-I)	3	50
Organic Group: Paper X(ii)	Organic Chemistry (Special-I)	3	50
Physical Group: Paper X(iii)	Physical Chemistry (Special-I)	3	50

Semester IV

(1) *Inorganic Group:*

		Duration (Hours)	*Maximum Marks*
Paper XI(i)	Inorganic Chemistry (Special-II)	3	50
Paper XII(i)	Inorganic Chemistry (Special-III)	3	50
Paper XIII(i)	Inorganic Chemistry (Special-IV)	3	50
Paper XIV(i)	Inorganic Chemistry (Special-V)	3	50
Practical Test		18	200

(2) O*rganic Group:*

		Duration (Hours)	*Maximum Marks*
Paper XI(ii)	Organic Chemistry (Special-II)	3	50
Paper XII(ii)	Organic Chemistry (Special-III)	3	50
Paper XIII(ii)	Organic Chemistry (Special-IV)	3	50
Paper XIV(ii)	Organic Chemistry (Special-V)	3	50
Practical Test		18	200

(3) *Physical Group:* Only four of the following are to be opted:-

		Duration (Hours)	*Maximum Marks*
Paper XI(iii)	Physical Chemistry (Special)	3	50
Paper XII(iii)	Physical Chemistry (Special)	3	50
Paper XIII(iii)	Physical Chemistry (Special)	3	50
Paper XIV(iii)	Physical Chemistry (Special)	3	50
Paper XV(iii)	Physical Chemistry (Special)	3	50

Paper XVI(iii)	Physical Chemistry (Special)	3	50
Paper XVII(iii)	Physical Chemistry (Special)	3	50
Paper XVIII(iii)	Physical Chemistry (Special)	3	50
Paper XIX(iii)	Physical Chemistry (Special)	3	50
Paper XX(iii)	Physical Chemistry (Special)	3	50
Paper XXI(iii)	Physical Chemistry (Special)	3	50
Practical Test		18	200
		TOTAL	**1100**

Note:

(1) In the beginning of the Third Semester, the students will be required to choose their special subject, viz., Inorganic, Organic or Physical Chemistry. They will take one Special Paper in the Third Semester, four Papers of the specialization of their choice or, alternatively*, three special papers of the specialization of their choice and one paper out of the special papers offered in the other two specializations in the Fourth Semester. They will also have to take one Special Practical Test in Semester IV.

For Physical Chemistry (Special), the number of options available in a particular year will, however, depend on the availability of teachers, and it will be ensured that at least ten students take each course.

(2) Each of the Practical Tests shall consist of three papers of 18 hours duration, suitably spread over three days. One-fourth of the marks will be reserved for the Laboratory Record/ Sessional work of the candidates and 30 marks for presentation of a project report and viva-voce.

(3) 12 marks in each theory paper are reserved for internal assessment, as per the University ordinance.

* This arrangement will be implemented subject to the availability of logistic support.

DETAILED COURSES

M. Sc. (Previous)

Paper I- Inorganic Chemistry

Course A: *Stability constants of metal complexes and their applications*

Stoichiometric and thermodynamic equilibrium constants, stepwise formation of complexes, formation functions, ϕ, $\bar{n}$ and α_C and relationship between different functions. Calculation of stability constants. Graphical Methods: using sets of data $\{\phi,[A]\}$; $\{\alpha_C,[A]\}$ and $\{\bar{n},[A]\}$.

Curve fitting method, Elimination method, Numerical method, Potentiometric method, Method of corresponding solutions, Ion exchange method, Solvent extraction, Polarographic method, and Spectrophotometric methods which include Job's method of continuous variation, Logarithmic method, Bent and French mole ratio method. Turner and Anderson methods and Yatsimirskiis method.

Analytical applications of complex formation; gravimetric analysis, complexometric titrations (Conditional constants, titration curves, titration error, detection of end point using metal indicators and instrumental methods. Indicator errors, Indicator correction etc. Simultaneous titrations, stepwise titrations, back titrations). Use of masking and demasking agents in complexometric titrations.

Course B: *Supramolecular and Photoinorganic Chemistry*

Molecular recognition: Receptors, design and synthesis of co-receptors and Multiple recognition, Hydrogen bonds, strong, weak and very weak H-bonds, Utilisation of H-bonds to create supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.

Cation binding hosts, binding of anions, binding of neutral molecules, binding of organic molecules.

Supramolecular reactivity and catalysis.

Transport processes and carrier design.

Supramolecular devices, supramolecular photochemistry.

Redox reactions of metal complexes in excited states, excited electron transfer, examples using $[Ru(bpy)_3]^{2+}$ complex and $[Fe(bpy)_3]^{3+}$ complex. Role of spin-orbit coupling, life-times of excited states in these complexes.

Metal complex sensitizers: Electron relay, semiconductor supported metal oxide systems, water-photolysis, nitrogen fixation and CO_2 reduction.

Recommended Texts:

1. Inczedy, J. *Analytical applications of complex equilibria* Halsted Press: New York, NY (1976).
2. Martell, A. E. & Calvin, M. *Chemistry of the Metal Chelate Compounds*.Prentice-Hall: N. Y. (1952).
3. Ringbom, A. *Complexation in Analytical Chemistry* Wiley: New York (1963).
4. Hartley, F. R., Burgess, C. & Alcock, R. M. *Solution Equilibria* Prentice-Hall: Europe (1980).

5. Beck, M. T. *Chemistry of Complex Equilibria* van Nostrand Reinhold: New York (1970)
6. Rossotti, F. J. C. & Rossotti, H. *The Determination of Stability Constants* McGraw Hill: London (1961).
7. *Progress in Inorganic Chemistry*, Vol. 18, 3rd Ed.
8. Lehn, J. M. *Supramolecular Chemistry: Concepts & Perspectives* Wiley-VCH (1995).
9. Balzani, V. *Photochemistry of Coordination Compounds* Academic Press (1970).
10. Desiraju, G. R., Ed. *Perspectives in Supramolecular Chemistry*, Vol. 2: *Crystal Engineering and Molecular Recognition* Wiley: Chichester (1995).
11. Atwood, J. L. & Steed, J. W. *Supramolecular Chemistry: A Concise Introduction* John Wiley & Sons (2000).
12. Adamson, A. W. & Fleischauer, P. D. (Eds.) *Concepts of Inorganic Photochemistry,* Wiley: New York (1975).

Paper II- Organic Chemistry

Course A: *Organic Stereochemistry*

Molecular symmetry and chirality: Symmetry operations and symmetry elements, point group classification and symmetry number.

Stereoisomerism: Classification, racaemic modification, molecules with one, two or more chiral centres; Configuration nomenclature, D L, R S and E Z nomenclature. Axial and planer chirality and helicity (P & M); Stereochemistry and configurations of allenes, spiranes, alkylidine cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes.

Topicity and prostereoisomerism: Topicity of ligands and faces and their nomenclature; Stereogenicity, chirogenicity, and pseudoasymmetry, stereogenic centre.

Simple chemical correlation of configurations with examples, quasiracemates.

Cyclostereoisomerism: Configurations, conformations and stability of cyclohexanes (mono-, di-, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones.

Asymmetric induction: Cram's, Prelog's and Horeau's rules; Dynamic stereochemistry (acyclic and cyclic), Qualitative correlation between conformation and reactivity, Curtin-Hammett Principle.

Molecular dissymmetry and chiroptical properties: Linear and circularly polarised lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effect. The axial haloketone rule, octant diagrams, helicity, and Lowe's rule. Application of ORD and CD to structural and stereochemical problems.

Course B: *Study of Reactive Intermediates*

A review of reaction mechanisms including methods of determination.

Linear free energy relationships and their applications (Hammett equation and modifications).

Carbocations: Classical and non-classical, neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.

Carbanions: Generation, structure and stability, ambident ions and their general reactions; HSAB principle and its applications.

Radicals: Generation, structure, stability and reactions, cage effects; radical-cations & radical-anions.

Carbenes: Formation and structure, reactions involving carbenes and carbenoids.

Nitrenes: Generation, structure and reactions of nitrenes.

Nucleophilic aromatic substitution: Benzynes, S_NAr and $S_{RN}1$ mechanisms; Ipso effect.

Recommended Texts:

1. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
2. Eliel, E. L. *Stereochemistry of Carbon Compounds* Textbook Publishers (2003).
3. Finar, I. L. & Finar, A. L. *Organic Chemistry* Vol. 2, Addison-Wesley (1998).
4. Finar, I. L. *Organic Chemistry* Vol. 1, Longman (1998).
5. Lowry, T. H. & Richardson, K. S. *Mechanism and Theory in Organic Chemistry* Addison-Wesley Educational Publishers, Inc. (1981).
6. Nasipuri, D. N. *Stereochemistry of Organic Compounds: Principles & Applications* South Asia Books (1994).
7. March, J. *Advanced Organic Chemistry* John Wiley & Sons (1992).

Paper III- Physical Chemistry

Quantum Chemistry

Postulates of quantum mechanics. Linear and Hermitian operators. Commutation of operators and Uncertainty Principle.

Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigenvalue problem, orthonormal sets, Fourier and Laplace transforms.

Some exactly soluble problems: Particle in a box and ring. Concept of degeneracy and Jahn-Teller distortion.

Simple harmonic oscillator problem and its solution using series solution or factorization method. Calculation of various average values using ladder operators and recursion relations of Hermite polynomials.

Angular momentum operators. Eigenvalues and eigenfunctions. Ladder operators. Rigid rotator and hydrogen atom: Complete solution. Radial distributions. Virial theorem.

Approximate methods: First order time-independent perturbation theory for non-degenerate states. Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

Ground and excited state of helium atom. Pauli's Exclusion principle. Many-electron atoms. Concept of spin and determinantal wavefunctions. Qualitative treatment of Hartree theory and Hartree-Fock SCF procedure.

Chemical bonding: Born-Oppenheimer approximation. Variational treatment of hydrogen molecule ion. Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments and their equivalence limit. Configuration Interaction. Extension of MO theory to other systems- Homonuclear and heteronuclear diatomics, polyatomics, Walsh diagrams for dihydrides, linear and bent triatomics.

HMO method and its applications: π-Electron approximation, Hückel Molecular Orbital Theory of conjugated systems, Calculation of properties- Delocalization energy, electron density, bond order, alternant and nonalternant hydrocarbons. Pairing theorem. Electronic and ESR spectra. Effect of substituents on spectra. Reactivity and electrocyclic ring closures.

Recommended Texts:

1. Lowe, J. P. & Peterson, K. *Quantum Chemistry* Academic Press (2005).
2. McQuarrie, D. A. *Quantum Chemistry* Viva Books Pvt. Ltd.: New Delhi (2003).
3. Mortimer, R. G. *Mathematics for Physical Chemistry* 2nd Ed. Elsevier (2005).
4. Pilar, F. L. *Elementary Quantum Chemistry* 2nd Ed., Dover Publication Inc.: N.Y. (2001).
5. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
6. Levine, I. L *Quantum Chemistry* 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
7. Engel, T. & Reid, P. *Physical Chemistry* Benjamin-Cummings (2005).
8. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
9. Silbey, R. J., Alberty, R. A. & Bawendi, M. G. *Physical Chemistry* 4th Ed. Wiley (2004).

Paper IV-Inorganic Chemistry

Course A: *Group Theory and its Applications*

Molecular symmetry: Symmetry elements and symmetry operations, definition of group and its characteristics, subgroups, classes, similarity transformation.

Products of symmetry operations, equivalent atoms and equivalent symmetry elements, relations between symmetry elements and operations, classes of symmetry operations, point groups and classification.

Symmetry: Optical activity and dipole moment.

Representation of groups, reducible and irreducible representations. The Great Orthogonality theorem, character tables, position vector and base vector as basis for representation.

Wavefunctions as bases for irreducible representations (*p*- and *d*-orbitals). Direct product. Vanishing integral.

Russell-Saunders coupling for d^n states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules. Spectral transition probability, vibronic coupling, non-centrosymmetric complexes, polarization of allowed transitions.

Symmetry: Infrared and Raman Spectroscopy.

SALCs, projection operators, illustrative examples.

Hybridization and its applications, Hybrid orbitals as Linear Combinations of Atomic Orbitals. Selected examples. MOs using Group Theory principles.

Symmetry and chemical reactions.

Course B: *Chemistry of d-and f-block elements:*

Term-symbols, Russel-Saunders states, Crystal field theory and splitting in O_h, T_d, D_{4h} and C_{4v} systems, Orgel and Tanabe-Sugano diagrams, determination of *Dq* and Racah parameters, oxidation states and electronic absorption spectra of complex ions. Spectrochemical series and effects of covalency. nephelauxetic series, magnetic properties of transition metal complexes and lanthanides, metal-metal bonds, cluster compounds of *d*-block elements, poly-oxo metallates of Ru, Os, Mo. Structure and bonding in complexes containing π-acceptor ligands. Relativistic effects affecting the properties of heavier transition elements.

Recommended Texts:

1. Cotton, F. A. *Chemical Applications of Group Theory* Wiley Interscience: N.Y (1990).
2. Jaffe, H. H. & Orchin, M. *Symmetry in Chemistry* Dover Publications (2002).
3. Hatfield, W. F. & Palmer, R. A. *Problems in Structural Inorganic Chemistry* W. A. Benjamin, Inc.: N.Y (1971).
4. Hatfield, W. E. & Parker, W. E. *Symmetry in Chemical Bonding & Structure* C. E. Merrill Publishing Co.: USA (1974).
5. Bishop, D. M. *Group Theory and Chemistry*, Clarendon Press: Oxford, U.K. (1973).
6. Shriver, D. F., Atkins, P. W. & Langford, C. H. *Inorganic Chemistry*, 2nd Ed., Oxford Univ. Press (1998).
7. Purcell, K. F. & Kotz, J. C. *Inorganic Chemistry*, W. B. Saunders and Co.: N. Y. (1985).
8. Wulfsberg, G. *Inorganic Chemistry* Univ. Science books: USA (2000); Viva Books: New Delhi.
9. Sutton, D. *Electronic Spectra of Transition Metal Complexes* McGraw-Hill: New York (1968).
10. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes* Chapman and Hall: U.K. (1973).
11. Drago, R. S. *Physical Methods in Chemistry* W. B. Saunders Co.: U.K. (1977).

Paper V- Organic Chemistry

Course A*: Spectroscopy*

PMR: Natural abundance of ^{13}C, ^{19}F and ^{31}P nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, spin-spin coupling, splitting theory, magnitude of coupling constant; Simple, virtual and complex spin-spin coupling; Chemical and magnetic equivalence, proton exchange, factors affecting the coupling - First and non-first order spectra; Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents) and NOE. Applications of PMR in structural elucidation of simple and complex compounds.

CMR: Resolution and multiplicity of ^{13}C NMR, ^{1}H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR. DEPT; Introduction to 2D-NMR

ESR: Derivative curves, hyperfine splitting, g-values, ESR spectra of simple molecules

MASS: Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly and doubly charged ions, metastable peak, base peak, isotropic mass peaks, relative intensity, FTMS, etc.; Recognition of M^{+} ion peak; General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulphur, nitrogen and halogens; α-, β-, allylic and benzylic cleavage; McLafferty rearrangement.

Combined problems on UV, IR, NMR and MASS

Course B: *Methods in Organic Synthesis*

Organosilicon Compounds: Preparation and applications in organic synthesis; Applications of Pd(0) and Pd(II) complexes in organic synthesis- Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi Coupling.

Preparation and applications of lithium organocuparates.

Reductions: Stereochemistry, stereoselection and mechanism of the following reagents: Catalytic hydrogenation and metal-liquid ammonia reductions.

Hydride transfer reagents: Sodium borohydride, sodium cyanoborohydride, lithium aluminium hydride and alkoxy substituted LAH reducing agents, DIBAL; Applications of hydroboration (reductions, oxidations and cabonylations): diborane, diisoamylborane, thexylborane, 9-BBN, isopinocamphenyl and diisopinocamphenyl borane.

Homogeneous hydrogenations: Mechanisms and applications using Rh, Ru and other metal complexes.

Oxidations: Scope of the following oxidising reagents with relevant applications and mechanisms: DDQ, SeO_2, $Tl(NO_3)_3$, Sharpless epoxidation.

Recommended Texts:

1. Carruthers, W. *Modern Methods of Organic Synthesis* Cambridge University Press (1971).
2. Kemp, W. *Organic Spectroscopy* 3rd Ed., W. H. Freeman & Co. (1991).
3. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. *Spectroscopic Identification of Organic Compounds* John Wiley & Sons (1981).
4. March, J. *Advanced Organic Chemistry* John Wiley & Sons (1992).

Paper VI- Physical Chemistry

Statistical Mechanics, Thermodynamics, Kinetics and Macromolecules

Statistical mechanics and thermodynamics:

Fundamentals: Concept of distribution. Thermodynamic probability and most probable distribution. Canonical and other ensembles. Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Idea of microstates and macrostates. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function.

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures.

Einstein theory and Debye theory of heat capacities of monatomic solids.

Third law of thermodynamics, Residual entropy.

Electrochemistry: Solutions: Activity coefficients and ion-ion interactions. Physical significance of activity coefficients, mean activity coefficient of an electrolyte and its determination. Derivation of the Debye-Hückel theory of activity coefficients (both point ion size and finite ion size models). Excess functions.

Kinetics:

Theories of reaction rates: Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

Solution kinetics: Factors affecting reaction rates in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

Macromolecules: Concepts of number average and mass average molecular weights. Methods of determining molecular weights (osmometry, viscometry, sedimentation equilibrium methods). Theta state of polymers. Distribution of chain lengths. Average end-to-end distance.

Recommended Texts:

1. McQuarrie, D. A. *Statistical Mechanics* Viva Books Pvt. Ltd.: New Delhi (2003).
2. Nash, L. K. *Elements of Statistical Thermodynamics* 2nd Ed., Addison Wesley (1974).
3. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).
4. Billmeyer, F. W. *Textbook of Polymer Science* 3rd Ed. Wiley-Interscience: New York (1984).
5. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
6. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).

***Practical Test*- 200 Marks**

Inorganic Chemistry

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 some metal ions, such as iron, nickel, etc. by colourimetric method.

Organic Chemistry

I   i. Qualitative analysis of mono and bifunctional compounds

ii. Determination of specific rotation and resolution of racaemic mixtures

iii. Analytical and preparative TLC

II   Small scale organic synthesis using some of the following reactions:

i. Acetylation reaction

ii. Oxidations and reductions

iii. Coupling reactions

iv. Diels-Alder reaction

v. Nucleophilic aromatic/aliphatic substitution

vi. Bromination and bromine addition

vii. Condensations

viii. Diazotisation reactions

III   UV and IR spectra of simple compounds (for functional group identification)

Physical Chemistry

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_2SO_4)

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.

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.

Computational Methods

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

(Note. Any other experiment may be introduced during the year)

M.Sc. (Final)

Paper VII- Inorganic Chemistry

Course A: *Inorganic Reaction Mechanisms*

Mechanisms of substitution reactions of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes. Potential energy diagrams, transition states and intermediates, isotope effects, Berry's pseudo rotation mechanism, factors affecting the reactivity of square planar complexes, Swain-Scott equation, Trans effect and its application to synthesis of complexes.

Molecular rearrangement processes: Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reluctant, chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

Course B: *Catalysis and Bio-inorganic Chemistry*

Transition metal ion catalysts for organic transformations and their application in hydrogenation (using symmetric and chiral organometallic catalysts), isomerization, olefin oxidation, carbonylation and polymerization reactions. Role of metal ions in biological systems. Toxic metal ions and their detoxification, chelation therapy/chelating agents in medicine. Recent advances in cancer chemotherapy using chelates. Biological nitrogen fixation. Natural and synthetic oxygen carriers. Na-K, ATPase or sodium pump. Futuristic aspects of organo transition metal complexes as catalysts and in bio-inorganic chemistry.

Recommended Texts:

1. Katakis, D. & Gordon, G. *Mechanism of Inorganic Reactions* John Wiley & Sons: N. Y (1987).
2. Langford, H. &.Gray, H. B. *Ligand Substitution Processes* W. A. Benjamin: N. Y. (1966).
3. Tobe, M. in *Inorganic Reaction Mechanisms* F. C. Wadington, Ed., Thomas Nelson: London (1973).
4. Hughes, M. N. *The Inorganic Chemistry of Biological Processes,* 2nd Ed., Wiley (1981).
5. Masters, C. *Homogeneous Transition Metal Catalysis* Chapman & Hall (1981).

Paper VIII-Organic Chemistry

Course A: *Photochemistry & Pericyclic Reactions*

Photophysical processes: Jablonskii diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effects, Stern-Volmer plot, delayed fluorescence, etc.

Photochemistry of alkenes: cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3-, 1,4- and 1,5-dienes; dimerizations.

Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic); α,β-unsaturated ketones; β,γ-unsaturated ketones; cyclohexenones (conjugated); cyclohexadienones (cross-conjugated & conjugated); Paterno–Buchi reactions; photoreductions.

Photochemistry of aromatic compounds: Isomerizations, skeletal isomerizations, Dewar and prismanes in isomerization. Singlet oxygen reactions; Photo Fries rearrangement of ethers and anilides; Barton reaction, Hoffman-Loefller-Freytag reaction.

Pericyclic reactions: Electrocyclic, cycloaddition, sigmatropic and chelotropic reactions; General Orbital Symmetry rules, Frontier Orbital approach, PMO approach, Correlation diagrams for different systems, Hückel–Mobius approach, General pericyclic selection rule and its applications, 1,3-dipolar additions, Ene reaction.

Course B: *Chemistry of Life Processes*

Introduction to metabolic processes: Catabolism and anabolism, ATP- currency of biological energy, energy rich and energy poor phosphates, role of NADH, NADPH, $FADH_2$, TPP, coenzyme A, lipoic acid and biotin.

Carbohydrate metabolism: Glycolysis, fate of pyruvate under anaerobic conditions, citric acid cycle, oxidative phosphorylation (electron transport system), gluconeogenesis, C4 pathway, pentose phosphate pathway and photosynthesis.

Fatty acid metabolism: Even chain and odd chain (saturated and unsaturated) fatty acids, ketone bodies, fatty acid anabolism, calorific values of food.

Protein metabolism and disorders: Degradation of amino acids (C3, C4, C5 family), urea cycle, uric acid and ammonia formation.

Proteins (structure and functions): Primary, secondary, tertiary and quaternary structure; Enzymes, active sites, allosteric sites and mechanisms of their actions, e.g., Chymotrypsin, carboxypeptidase, lipases, etc.

Nucleic acids: Chemical and enzymatic hydrolysis, structure and functions of DNA, RNA (m-RNA, t-RNA, r-RNA), an overview of gene expression (replication, transcription and translation), genetic code (origin, Wobble hypothesis and other important features), genetic errors, carcinogenesis and recombinant DNA technology.

Recommended Texts:

1. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
2. Horspool, W. M. *Aspects of Organic Photochemistry* Academic Press (1976).
3. Lowry, T. H. & Richardson, K. S. *Mechanism and Theory in Organic Chemistry* Addison-Wesley Educational Publishers, Inc. (1981).
4. March, J. *Advanced Organic Chemistry* John Wiley & Sons (1992).
5. Marchand, A. P. & Lehr, R. E. *Pericyclic Reactions* Academic Press (1977).
6. Stryer, L. *Biochemistry* 4th Ed., W. H. Freeman & Co. (1995).
7. Sykes, P. *A Guidebook to Mechanism in Organic Chemistry* 6th Ed., Prentice-Hall (1996).
8. Zubay, S. *Biochemistry* Addison-Wesley (1983).

Paper IX- Physical Chemistry

Molecular Structure: Spectroscopic and Diffraction Methods

Spectroscopic methods: Characterization of electromagnetic radiation. Born-Oppenheimer approximation. Heisenberg's Uncertainty Principle. Basic elements of spectroscopy. Time dependent perturbation. Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Transition dipole moments and general selection rules based on symmetry ideas.

Atomic spectra: Characterization of atomic states. Microstate and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Introduction to molecular spectroscopy: Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/ or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First order Stark effect.

Vibrational spectroscopy: Normal coordinate analysis of homonuclear and heteronuclear diatomic molecules. Extension to polyatomic linear molecules. Derivation of selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands.

Dissociation energies from vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimer approximation. Nuclear spin effect.

Symmetry of normal coordinates. Use of Group Theory in assignment of spectra and selection rules for simple molecules.

Raman spectroscopy: Stokes and anti-Stokes lines. Polarizability ellipsoids. Rotational and Vibrational Raman spectroscopy. Selection rules. Polarization of Raman lines.

Electronic spectroscopy: Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors. Dissociation energies. Photoelectron spectroscopy of diatomic (N_2) and simple polyatomic molecules (H_2O, formaldehyde). Adiabatic and vertical ionization energies. Koopmans' theorem.

Polyatomic molecules. Oscillator strengths. Use of Free Electron Model, HMO theory and Group theory for polyenes and carbonyl compounds (formaldehyde). Qualitative ideas of solvent effects- viscosity, polarity, hydrogen bonding.

Excited states: Deactivation. Jablonskii diagram. Fluorescence and phosphorescence and factors affecting these. Calculation of excited state life-times from absorption data. Quenching of fluorescence, Stern-Volmer equation.

NMR spectroscopy: Larmor precession. Mechanisms of spin-spin and spin-lattice relaxations and quantitative treatment of relaxation. Quantum mechanical treatment of the AB system. Selection rules and relative intensities of lines.

Principles of Mossbauer spectroscopy: Isomer shifts. Quadrupole and Nuclear Zeeman splittings. Applications in structure determination.

Diffraction Methods. Atomic scattering factors. Scattering by a small crystal. Direct and reciprocal lattice. Miller indices. Bragg's law and Laue's equations. Structure factors. Systematic absences for different types of unit cells (primitive, face-centred, body-centred, side-centred) and application to some common metal and metal salt structures (rock salt, zinc blende). Space groups. Glide planes and screw axes. Structure determination for organic crystals like naphthalene. Fourier series, Patterson's functions. Heavy atom method. Comparison of X-ray method with electron and neutron diffraction methods.

Recommended Texts:

1. Hollas. J. M. *Modern Spectroscopy* 4^{th} Ed., John Wiley & Sons (2004).
2. Barrow, G. M. *Introduction to Molecular Spectroscopy* McGraw-Hill (1962).
3. Brand, J. C. D. & Speakman, J. C. *Molecular Structure: The Physical Approach* 2^{nd} Ed., Edward Arnold: London (1975).
4. Chang, R. *Basic Principles of Spectroscopy* McGraw-Hill, New York, N.Y. (1970).
5. Moore, W. J. *Physical Chemistry* 4^{th} Ed. Prentice-Hall (1972).
6. Warren, B. E. *X-Ray Diffraction* Dover Publications (1990).
7. Bacon, G. E. *Fifty Years of Neutron Diffraction* Hilger (1987).

Paper X(i)-Inorganic Chemistry (Special-I)

Course A:

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.

Course B:

Introduction to the solution of multielectron 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.

The octahedral potential, contribution of spherical harmonics to the octahedral potential V_{xyz}. Single electron in a cubic field, quantitative basis (r,θ,ϕ) for the splitting of d orbital to e_g and t_{2g} in terms of D_q, 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.

Recommended Text:

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 Structural Chemistry* John Wiley & Sons
5. Azaroff, L. V. *Introduction to Solids* Tata McGraw Hill Publishing Co. Ltd.
6. Breck, D. W. *Zeolites Molecular Sieves- Structure, Chemistry and Use.* John Wiley & Sons.

Paper X(ii)- Organic Chemistry (Special-I)

Course A: *Newer Synthetic Reactions and Reagents*

Enolates, Thermodynamic versus Kinetic enolates, enonate equivalents and enamines: Applications in carbon-carbon bond formation and related reactions. Applications in chiral synthesis.

Phosphorus, Sulphur and nitrogen ylides: Preparation, applications in organic synthesis and mechanism.

Umpolung reactions (sulphur compounds, nitro compounds, lithiated ethers and related compounds).

Principles and applications of phase transfer catalysis, crown ethers and polymer-supported reagents in organic synthesis.

Principles of Green Chemistry and its applications: Biotransformations: Classification of enzymes, advantages and disadvantages, applications in organic synthesis; Principles of ultrasound and microwave assisted organic synthesis. Reactions in ionic liquids

Course B: *Heterocyclic Chemistry*

Introduction to heterocycles: Nomenclature, spectral characteristics, reactivity and aromaticity

Synthesis and reactions of three and four membered heterocycles, *e.g.,* aziridine, azirine, azetidine, oxiranes, thiarines, oxetenes and thietanes.

Five membered rings with two heteroatoms: pyrazole, imidazole, oxazole, thiazole, isothiazole and benzofused analogs;

Benzofused five membered heterocycles with one heteroatom, *e.g.*, indole, benzofuran, benzothiophene.

Chemistry of bicyclic compounds containing one or more heteroatoms.

Benzofused six membered rings with one, two and three heteroatoms: benzopyrans, quinolines, isoquinoline, quinoxazaline, acridine, phenoxazine, phenothiazine, benzotriazine, pteridines.

Seven and large membered heterocycles: azepines, oxepines, thiepines;

Chemistry of porphyrins and spiro heterocycles.

Recommended Texts:

1. Carey, F.A. & Sundberg, R. J. *Advanced Organic Chemistry*, Parts A & B, Plenum: U.S. (2004).
2. Carruthers, W. *Modern Methods of Organic Synthesis* Cambridge University Press (1971).
3. Acheson, R. M. *Introduction to the Chemistry of Heterocyclic Compounds* John Wiley & Sons (1976).

Paper X(iii)- Physical Chemistry (Special-I)

Irreversible thermodynamics: Meaning and scope of irreversible thermodynamics, Thermodynamic criteria for non-equilibrium states, Phenomenological laws- Linear laws, Gibbs equation, Onsager's reciprocal relations, Entropy production- specific examples of entropy production, Non-equilibrium stationary states, Prigogine's principle of maximum entropy production, Coupled phenomena. Some important applications.

Transport phenomena: Diffusion coefficients, Fick's first and second laws, relation between flux and viscosity, relation between diffusion coefficient and mean free path, relation between thermal conductivity/viscosity and mean free path of a perfect gas, Einstein relation, Nernst-Einstein equation, Stokes-Einstein equation, Einstein-Smoluchowski equation.

Surface phenomena: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micelle concentration (CMC), Krafft temperature, Factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization, solubilization, microemulsions, reverse micelles, surface films (eletrokinetic phenomena), catalytic activity at surfaces. Electrode/ electrolyte interface; electrical double layer, electrode kinetics, Nernst equation. Application of PES, ESCA and Auger spectroscopy to the study of surfaces.

Fast reactions: Luminescence and energy transfer processes, study of kinetics by stopped-flow technique, relaxation method, flash photolysis and magnetic resonance method. Kinetics of solid-state reactions.

Recommended Texts:

1. Katchalsky, A. & Curren, P. F. *Non Equilibrium Thermodynamics in Biophysics* Harvard University Press: Cambridge (1965).
2. Zwanzig, R. *Nonequilibrium Statistical Mechanics* Oxford University Press (2001)
3. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997).
4. Thomas, J. M. & Thomas, M. J. *Principles and Practice of Heterogeneous Catalysis* John Wiley & Sons (1996).
5. Campbell, I. M. *Catalysis at Surfaces* Chapman and Hall, New York/London (1988).
6. Chorkendorff, Ib. & Niemantsverdriet, J. W. *Concepts of Modern Catalysis and Kinetics* Wiley-VCH (2003).
7. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
8. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).
9. Shaw, D. J. *Introduction to Colloid and Surface Chemistry* 2nd Ed. Butterworths (1970).

10. Adamson, A. W. & Gast, A. P. *Physical Chemistry of Surfaces* 6^{th} Ed. Wiley Interscience.(1997)

Inorganic Chemistry Special Papers (II-V)

Paper XI(i)- Inorganic Chemistry (Special-II)

Spectral Techniques in Inorganic Chemistry

Course-*A:*

Vibrational spectroscopy: Vibrational motion and energies, number of vibrational modes, anharmonicity, absorption in infrared, FT spectrometers, cell systems, effects of phase on spectra, vibrational spectra and symmetry, selection rules, symmetry of an entire set of normal vibrations, F and G matrix. Raman spectra and selection rules, polarized and depolarized Raman lines, resonance Raman spectroscopy, use of symmetry to determine the number of active infrared and Raman lines, rotational fine structure in gas phase IR. Nonresonance overtones and difference bands. Application of Raman and Infrared selection rules to the determination of inorganic structures, bond strength frequency shift relations, changes in spectra of donor molecules on coordination, change in symmetry on coordination.

Mossbauer spectroscopy: Doppler shift and recoil energy, isomer shift and its interpretation, quadrupole interactions, effect of magnetic field on Mossbauer spectra, applications to metal complexes, metal carbonyls, Fe-S cluster and tin compounds, etc. Partial quadrupole splittings and geometry of the complexes.

Magnetism: Types of magnetic behaviour, magnetic susceptibilities, Pascal's constants, paramagnetism in experimental simple systems where S = ½, 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.

Mass spectroscopy: Experimental arrangements and presentation of spectra, molecular ions, appearance and ionization potential, fragmentation, ion reactions and their interpretation, effect of isotopes on the appearance of a mass spectrum, molecular weight determination, thermodynamic data. Application of mass spectroscopy to inorganic compounds.

Course-*B:*

Electronic spectroscopy: Vibrational and electronic energy levels in a diatomic molecule, potential energy level diagram. Symmetry requirements for n to π^* 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 β for Ni(II) O_h complexes, nephelauxetic effect, effect of σ and π 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*, *Ds* and *Dt* for tetragonal complexes, intervalence electronic transition, structural evidence from electronic spectra.

Nuclear magnetic resonance spectroscopy: Nuclear spin quantum number, I, and its calculation using the nuclear shell model, spin parity rules. Types of nuclei based on value of I, 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 ^{1}H, ^{11}B, ^{15}N, ^{19}F, ^{29}Bi, ^{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 $<S_z>$, contact shift, pseudo contact shift, factoring contact and pseudo contact shift for transition metal ions. Contact shift and spin density, π delocalization, simplified M.O. diagram for Co(II) and Ni(II). Application to planar tetrahedral equilibrium, Contrast agents.

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.

Nuclear Quadrupolar Resonance (NQR) Spectroscopy: Quadrupolar moment, energy lends of a quadrupolar nuclease and effect of asymmetry parameters and energy lends. 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).

Paper XII(i)- Inorganic Chemistry (Special-III)

Course A: *Organotransition metal chemistry*

General introduction, Structure and bonding, Survey of organometallic complexes according to ligands. π 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 π-allyl complexes and their characterization. Metallocycles, unsaturated nitrogen ligands including dinitrogen complexes.

Futuristic aspects of organotransition metal chemistry.

Course B: *Bio-inorganic chemistry*

Fundamentals of inorganic biochemistry, geo-chemical effects on life systems, essential and non-essential elements in bio-systems.

Role of alkali/alkaline earth metals in bio-systems. Role of 3*d* block elements and nonmetals in bio-systems. Role of metal ions in oxygen carriers and synthetic oxygen carriers. Designing of chelating agents and metal chelates as medicines. Fixation of dinitrogen biologically and abiologically, biotransformation of nonmetallic inorganic compounds. Environmental bioinorganic chemistry. Metal ions as probes for locating active sites. Anti-oxidants. Metal ions as antioxidants, metal ion enhancing catalytic activity of enzymes (Biocatalysts). Inhibitions as competitive and non-competitive, metals and metalloproteins.

Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA). Template temperature, stability of DNA.

Role of metal ions in replication and transcription process of nucleic acids.

Biochemistry of dioxygen, bioinorganic chips and biosensors.

Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land.

Metals in the regulation of biochemical events. Transport and storage of metal ions *in vivo*. Metal complexes as probes of structure and reactivity with metal substitution.

Fundamentals of Toxicity and Detoxification. Nuclear medicines.

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).

Paper XIII(i)- Inorganic Chemistry (Special-IV)

Analytical techniques (Instrumentation and Application)

Course A:

(i) *Electroanalytical methods:-* Polarography (DC, AC and pulse), cyclic voltammetry, coulometry and anode stripping voltammetry.

(ii) *Optical methods:-* UV/Visible, X-ray photoelectron spectroscopy (XPS), Auger Electron Spectroscopy (AES), ESCA, Atomic absorption and emission spectroscopy.

(iii) *Diffraction Methods:* Electron diffraction, X-ray diffraction

(iv) *Imaging Techniques:* Electron microscopy (SEM, TEM)

(v) Infrared Spectroscopy, Dispersive and Fourier Transformed Raman, Resonance Raman and Surface Enhanced Raman Spectroscopy-Dispersive and Fourier Transformed.

(vi) *Hifanated Techniques:* GC-IR, TG-IR Spectroscopy, GC-Mass Spectroscopy and any other.

Course B

(i) *Errors and Evaluation:* Definition of the terms- mean and median, precision –standard deviation, relative standard deviation, accuracy-absolute error. Types of errors in experimental data determination (systematic), indeterminate (random) and gross. Sources of errors and their effect upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data -indeterminate errors. The use of statistics.

(ii) *Separation Methods:* Theory and applications of separation methods in analytical chemistry: solvent extraction, ion exchangers including liquid ion exchangers and chromatographic methods for identification and estimation of multicomponent systems (such as TLC, GC, HPLC, etc.).

(iii) *Thermal Methods:* TG, DTA, DSC and thermometric titrations.

Recommeded Texts:

1. Cheetham, A. K. & Day, P., Eds. *Solid State Chemistry Techniques* Clarendon Press, Oxford (1987)
2. Christian, G. D., *Analytical Chemistry,* 6th Ed., John Wiley & Sons, Inc. (2004).
3. Skoog, D. A., West, D. M., Holler, R. J & Nieman, T. A. *Principles of Instrumental Analysis* Saunders Golden Sunburst Series (1997).
4. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) *Instrumental Methods of Analysis* - 7th Ed., Wadsworth Publishing (1988) ISBN 0534081428
5. Khopkar, S. M. *Concepts in Analytical Chemistry* Halsted (1984).

Paper XIV(i)- Inorganic Chemistry (Special-V)

Course A: *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. Principles of Electron Microscopy, Dynamic Light Scattering, Atomic Force Microscopy and characterization of nanomaterials.

Course B: *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. Harvey, B. C. ***Introduction to*** *Nuclear Chemistry* Prentice-Hall (1969).
2. Friedlander, G. Kennedy, J. W., Marcus, E. S. & Miller, J. M. *Nuclear & Radiochemistry*, John Wiley & Sons (1981).
3. Keer, H. V. *Principles of the Solid State* Wiley Eastern Ltd.: New Delhi (1993).
4. West, A. R. *Solid State Chemistry and its Applications* John Wiley & Sons (1987).
5. Hannay, N. *Treatise on Solid State Chemistry* Plenum (1976).
6. Cheetham, A. K. & Day, P., Eds. *Solid State Chemistry Techniques* Clarendon Press, Oxford (1987)
7. Timp, G., Ed. *Nanotechnology* Springer-Verlag: N. Y. (1999).

Organic Chemistry Special Papers (II-V)

Paper XI(ii)- Organic Chemistry (Special-II)

Course A: *Advanced Organic Synthesis*

Philosophy of organic synthesis: Disconnection approach, one group and two group disconnections, reversal of polarity, chemoselectivity, one group C-C disconnection, two group C-C disconnections, 1,3-difunctional and 1,5-difunctional compounds. Tandem reactions, Domino reactions and multi-component reactions.

Asymmetric synthesis: Development of methodologies for asymmetric synthesis, regioselectivity, stereoselectivity and stereospecificity.

Total synthesis of the following compounds using disconnection approaches: Vitamin B_{12}, prostaglandins E_2, F_{2a}, β-ecdysone, Menthol, Taxol and gandriol

Course B: *Supramolecular Chemistry and Carbocyclic Rings*

Principles of molecular associations and organizations: Non-covalent synthesis, Self assembly and self organization, Supramolecular reactivity and catalysis, Molecular devices, Ion channels, Novel liquid crystals, Gelators fibres and adhesives, Dendrimers, organic solids, organic conductors and organic superconductors, catenanes and rotaxanes

Chemistry of small, medium and large ring compounds

Chemistry of non-benzenoid aromatics: Tropones. tropolones, azulenes, metallocenes and annulenes

Bridged rings, caged molecules and adamantane.

Recommended Texts:

(1) Warren, S. *Organic Synthesis: The Disconnection Approach* John Wiley & Sons (1984).

(2) Lehn, J-M, *Supramolecular Chemistry*: *Concepts & Perspectives. A Personal Account* Vch Verlagsgesellschaft Mbh (1995).

(3) Vögtle, F. *Supramolecular Chemistry: An Introduction* John Wiley & Sons (1993).

Paper XII(ii)- Organic Chemistry (Special-III)

Course A: *Proteins and Lipids*

Peptides and proteins: Classification of naturally occurring peptides, depsipeptide and peptide alkaloids with examples, Sequence determination, chemical, enzymatic and mass spectral methods, Modern methods of peptide synthesis with protection and deprotection, Solid phase synthesis, combinatorial synthesis of peptides, Chemistry of oxytocin, valinomycin, enkephalins, self assembly and aggregation of peptides,

Lipids: Classification and biological importance of fatty acids and lipids, stereochemical notation in lipids, chemical synthesis of phospholipids and glycolipids, properties of lipid aggregates, micelles, bilayers, lyposomes and biological membranes.

Course B: *Nucleic Acids and Carbohydrates*

Nucleic acids: Secondary structure of DNA and RNA, stabilising forces, polymorphic nature of DNA, multistranded DNA structures, sequence determination by chemical and enzymatic methods, genome sequencing, chemical synthesis of DNA, solution phase and solid phase synthesis, phosphodiester-triester and phosphite methods, phosphoramide approach, PNA, LNA, automated DNA synthesizers, purification of oligonucleotides, HPLC and gel electrophoresis

Carbohydrates: Types of naturally occurring sugars, deoxy sugars, amino sugars, branched chain sugars, sugar methyl ethers and acid derivatives of sugars, polysaccharides of industrial and biological importance, dextran, chemistry of sialic acids, cell-cell recognition and blood group substances.

Recommended Texts:

1. Bodansky, M. *Peptide Chemistry: A Practical Textbook* Springer-Verlag (1988).
2. Dugas, H. & Penney, C. *Bioorganic Chemistry: A Chemical Approach to Enzyme Action* Springer-Verlag (1989).
3. Finar, I. L. & Finar, A. L. *Organic Chemistry* Vol. 2, Addison-Wesley (1998).
4. Finar, I. L. *Organic Chemistry* Vol. 1, Longman (1998).
5. Sinden, R. P. *DNA Structure and Function* Academic Press (1994).
6. Saenger, W. *Principles of Nucleic Acid Structure* Springer-Verlag (1984).
7. Gait, M. J., Ed. *Oligonucleotide Synthesis-A Practical Approach* IRL Press (1984).

Paper XIII(ii)- Organic Chemistry (Special-IV)

Course A: *Terpenes and Steroids*

Terpenes and steroids: Classification and biosynthesis of mono- sesqui-, di- and triterpenoids and steroids. Acetyl CoA, Mevalonic acid, acetoacetyl CoA, squalene to lanosterol, Cholesterol to estradiol, diosgenin and its utility in hormone synthesis.

General chemistry of the following compounds- Cholesterol, Artemisinin, Gibbereline A3, Azadirachtin.

Course B: *Alkaloids and Polyphenols*

Isolation and structure elucidation of alkaloids, Biosynthesis and biogenesis of alkaloids using thiokinase, mixed function oxygenases, methyl transferases, amino acid decarboxylases, oxidative phenol coupling of selected alkaloids.

Structure and synthesis of morphine, reserpine, ergotamine and acotinine

Biosynthesis of flavonoids and related polyphenols, Acetate and shikimic acid pathways, Structure and synthesis of apigenin, luteolin, quercetin, and Diadzen

Recommended Texts:

1. Finar, I. L. & Finar, A. L. *Organic Chemistry* Vol. 2, Addison-Wesley (1998).
2. Finar, I. L. *Organic Chemistry* Vol. 1, Longman (1998).

Paper XIV(ii)- Organic Chemistry (Special-V)

Course A: *Medicinal Chemistry*

Introduction to the history of medicinal chemistry

General mechanism of drug action on lipids, carbohydrates, proteins and nucleic acids, Drug metabolism and inactivation. Receptor structure and sites.

Drug discovery, development, design and delivery systems

General introduction to antibiotics, Mechanism of action of lactam antibiotics, non-lactam antibiotics and quinilones; antiviral and anti-AIDS

Neurotransmitters, classes of neurotransmitters, Drugs affecting collingeric and adrenergic mechanisms

Anti-histamines, anti-inflammatory, anti-analgesics, anticancer and anti-hypertensive drugs

New developments, e.g., gene therapy and drug resistance.

Course B: *Bioactive Compounds*

Vitamins: Classification, occurrence, chemistry of Vitamins A, C and E, structure elucidation and synthesis, deficiency syndromes, etc.

*Insect hormones**:*** Introduction to BH, JH and MH, chemistry of JH, structure elucidation and synthesis, structural analogs, biosynthesis; JH mimics– some structures; chemistry of Juvabione

*Precocenes**:*** Chemistry of Precocene I and II

*Antifeedants**:*** Different classes of antifeedants; role of azadirachtin in IPM.

Pyrethroids: Introduction; structure elucidation and synthesis of pyrethroids, namely pyrethrins, cinerins and Jasmoline; Synthetic pyrethroids: Structure–activity relationships; synthesis of various synthetic pyrethroids.

Insect pheromones: Semiochemicals, pheromones, primers and releasers, different classes of pheromones, synthesis of different pheromones; advantages of pheromones over conventional pesticides.

Hormones: General study of hormones including classification, mechanism of action of water soluble and fat soluble hormones, secondary messengers, negative feedback mechanism; Antifertility agents.

Recommended Texts:

1. Finar, I. L. & Finar, A. L. *Organic Chemistry* Vol. 2, Addison-Wesley (1998).
2. Finar, I. L. *Organic Chemistry* Vol. 1, Longman (1998).
3. Gringauz, A. *Introduction to Medicinal Chemistry: How Drugs Act and Why?* John Wiley & Sons (1997).
4. Patrick, G. L. *Introduction to Medicinal Chemistry* Oxford University Press (2001).

Physical Chemistry Special Papers

Paper XI(iii)- Physical Chemistry Special (Advanced Quantum Chemistry)

Perturbation theory for degenerate states. Many electron systems. Double perturbation theory. Determinantal wavefunctions. Orbital and spin angular momentum operators. Pauli matrices. Term symbols and term energies. Matrix elements for one and two electron operators. Introduction to second quantization in chemistry. Roothaan equations. Koopmans and Brillouin theorem. Basis sets (Slater, Gaussian and integral transform). Basis Set Superposition Error (BSSE). Electron correlation and CI theories.

A review of HMO, EHT and PPP methods. ZDO approximation and CNDO, INDO and other semiempirical theories.

Hohenberg-Kohn theorem. Nature of electron density distribution and Density Functional theories. Density functional interpretation of some concepts (electronegativity, electronegativity equalization, softness and hardness, etc.)

Computer experiments: Use of some packages to study molecular electronic structures (GAMESS, MOPAC, etc.). This project will carry 10 marks out of a total of 50 marks and shall replace the internal assessment test.

Recommended Texts:

1. Atkins, P. W. & Friedman, R. S. *Molecular Quantum Mechanics* 3rd Ed. Oxford University Press (1997).
2. Levine, I. N. *Quantum Chemistry* 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
3. Lowe, J. P. & Peterson, K. *Quantum Chemistry* Academic Press (2005).

Paper XII (iii) –Physical Chemistry Special (Advanced Statistical Mechanics)

Theory of Imperfect Gases and Condensation

Partition functions and cluster integrals, Pressure of gas expressed as a power series in activity, Irreducible cluster integrals, Virial expansion for a gas, Theory of condensation.

Theory of Liquids

Canonical Ensemble: Definition of distribution and correlation functions, Thermodynamic functions of a fluid and the radial distribution function, Potential of mean force and the superposition approximation, Kirkwood integral equation, Born-Green-Yvon (BGY) integral equation, HNC equation, PY equation, Fluid of hard spheres according to the superposition approximation, Fluid with modified Lennard-Jones molecular interaction potential according to the superposition approximation.

Grand Canonical Ensemble: Distribution functions in monatomic, one-component systems, Kirkwood-Salsburg integral equation, Distribution function at a phase transition.

Computational Techniques

Computer simulation: Motivation and applications, Intermolecular potentials

Molecular Dynamics and Monte Carlo Methods

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.

Methods for Structure Determination

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

Lattice Statistics

Nearest neighbour lattice statistics-Thermodynamics and interconnections, Exact and formal methods.

Recommended Texts:

1. Allen, M. P. & Tildesley, D. J. *Computer Simulations of Liquids* Oxford Science Publications: Oxford (1987).
2. Hill, T. L. *Statistical Mechanics: Principles and Selected Applications* Dover Publications Inc.: New York (1987).
3. Landau, L. D. & Lifshitz, I. M. *Statistical Physics* Vol. 5, Part 1, 3rd Ed., Pergamon Press (1980).
4. van Kampen, N. G. *Stochastic Processes in Physics & Chemistry* 2nd Ed., Elsevier Science (2001).

Paper XIII (iii) –Physical Chemistry Special (Advanced Electrochemistry)

Relaxation Methods-Theory and Techniques

Electrode kinetics: Overpotentials, Exchange current density, Derivation of Butler-Volmer equation and its implications, Tafel plot, Multistep electrode reactions, Determination of multistep electrode reactions, Mass transfer by diffusion.

Quantum aspects: Charge transfer at electrode-solution interfaces, Quantization of charge transfer, Tunnelling

Semiconductor interfaces: Structure of double layer at the semiconductor-solution interface, Effect of light at semiconductor-solution interface

Electrochemical methods: Controlled potential and current techniques, Hydrodynamic techniques, Electrochemical instrumentations, Scanning probe techniques.

Adsorption and Electric Double Layer

Thermodynamics of the double layer, Electrocapillary phenomena; Adsorption – Ionic and organic molecules, Adsorption isotherms - Langmuir, Frumkin, Temkin; Experimental evaluation of surface excesses and electrical parameters, Structure of electrified interfaces - Gouy-Chapman, Stern, Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan models

Electrocrystallization

Electrogrowth of metals on electrode- Nucleation, Growth, Surface Diffusion, Underpotential deposition, Variety of shapes formed in electrodeposition.

Bioelectrochemistry

Membrane potentials, Nernst-Planck equation, Hodgkin-Huxley equations, Core Conductor model, Electrocardiography

Applied Electrochemistry

Corrosion: Introduction to corrosion, forms of corrosion, Corrosion monitoring and prevention methods

Conversion and storage of electrochemical energy: Fuel cells and batteries.

Electrocatalysis: Influence of various parameters, Hydrogen electrode

Recommended Texts:

1. Bard, A. J. Faulkner, L. R. *Electrochemical Methods: Fundamentals and Applications,* 2nd Ed., John Wiley & Sons: New York, 2002.
2. Bockris, J. O' M. & Reddy, A. K. N. *Modern Electrochemistry 1: Ionics* 2nd Ed., Springer (1998).
3. Bockris, J. O' M. & Reddy, A. K. N. *Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science* 2nd Ed., Springer (2001).
4. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. *Modern Electrochemistry 2A: Fundamentals of Electrodics* 2nd Ed., Springer (2001).
5. Brett, C. M. A. & Brett, A. M. O. *Electrochemistry* Oxford University Press (1993).
6. Koryta, J., Dvorak, J. & Kavan, L. *Principles of Electrochemistry* John Wiley & Sons: NY (1993).

Paper XIV(iii) –Physical Chemistry Special (Advanced Chemical Kinetics)

Statistical theories of kinetics: Collision theory. Activated Complex theory. Potential energy surfaces- attractive and repulsive forces. Lindemann's theory of unimolecular reactions- energy transfer, fall-off region and its limitations. Rice-Ramsperger and Kassel (RRK) model, and Marcus refinement of RRK model (RRKM) for the calculation of rate constants of simple unimolecular (isomerization) reactions.

Complex reactions: Chain reactions and oscillatory reactions, Photochemical reactions, Homogeneous catalysis.

Enzyme kinetics: Michaelis-Menten mechanism - single and double intermediates. King-Altman method for working out the kinetics of complex enzyme reactions.

Enzyme inhibition- reversibility and products inhibition. Computer simulation (analog computer) in chemical kinetics.

Reaction Dynamics: Molecular beams, principle of crossed-molecular beams. Molecular encounters and principal parameters, e.g. Impact parameter, Collision cross-section, Reaction cross-section and relation between reaction cross-section and reaction rate (single velocity). Dependence of collisional cross-section on translational energy.

Probing the transition state, Dynamics of barrierless chemical kinetics in solution, dynamics of unimolecular reactions.

Recommended Texts:

1. Pilling, M. J. & Seakins, P. W. *Reaction Kinetics* Oxford Press (1997).
2. Laidler, K. J. *Chemical Kinetics* 3rd Ed., Benjamin Cummings (1997). .

Paper XV(iii) –Physical Chemistry Special (Advanced Molecular Spectra)

Vibrational spectroscopy: Group theory and symmetry classification of normal modes of vibration. Normal coordinate analysis in Cartesian and internal coordinates of small molecules: BF_3, NH_3. Square planar, trigonal bipyramid, framework and cage molecules. Jahn-Teller distortions.

Electronic spectroscopy: Electronic spectroscopy of transition metal complexes. Octahedral and tetrahedral complexes, Correlation diagrams for octahedral fields and fields of lower symmetry.

Electronic spectroscopy of organic molecules - benzene, effect of substitution-pyridine, pyrimidine, pyrazine, methyl substitution. Vibronic analysis.

Electron Spin Resonance spectroscopy: Basic principles. Relaxation and Line Widths. Zero-field splitting and Kramer’s degeneracy. *g*-factor for paramagnetic ions. *g*-factor for organic radicals. Factors affecting the *g*-factor.

Isotropic and anisotropic hyperfine coupling constants. Spin Hamiltonian, Spin densities and McConnell relationship. Fine splitting in triplet spectra.

Applications of ESR spectroscopy - Structure determination, Interpretation of ESR spectra of simple organic radicals like benzene radical anion, naphthalene radical anion, toluene and *o*-, *m*- and *p*-xylene radical ions from HMO theory. Study of unstable paramagnetic species, Kinetic studies of electron transfer reactions, Spin-labelling studies of biomolecules.

Recommended Texts:

1. Harris, D. C. & Bertolucci, M. D. *Symmetry and Spectroscopy*: *An Introduction to Vibrational and Electronic Spectroscopy* Dover Publications: New York (1990).
2. Bishop, D. M. *Group Theory and Chemistry*, Clarendon Press: Oxford, U.K. (1973).

Paper XVI(iii) –Physical Chemistry Special (Crystal Structure)

Crystal Structures and Basic Symmetry

Overview: Description of a crystal structure in terms of atom positions, unit cells, and crystal symmetry; Relation of the crystal symmetry to the symmetry observed in a diffraction experiment for primitive, orthorhombic,.tetragonal, trigonal, hexagonal, and cubic crystal systems. Concept of Reciprocal space.

Scattering and Diffraction Theory

X-ray Diffraction: Interaction of radiation with condensed matter and how this can be used in generalized crystallography. Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, Structure factor and its relation to intensity and electron density, Fourier synthesis. Phase problem, Patterson synthesis. Heavy atom method. Direct method. Refinement, R factor. Fourier refinement. Least squares refinement. Determination of absolute configurations (Bijvoet method). Chemical interpretation of results. Estimation of errors. Effects of thermal motion, limitations. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

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 Frenkel defect formation, colour centres, non-stoichiometry and defects.

Protein Crystallography

Basics of modern protein crystallography using Web-based material; different levels of structure exhibited by proteins; instrumentation, steps, and methods used in protein crystallography with appropriate case studies; concept of non-crystallographic symmetry to protein crystallography, Ramachandran diagram.

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, super conductors.

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

Organic solids: Electrically conducting solids, organic charge transfer complexes, organic metals, new superconductors.

Electron Microscopy

Fundamentals of electron microscopy as a useful subsidiary technique for crystallographers; Examples of its application in materials science and macromolecular structural biology.

Electron diffraction: Scattering intensity *versus* scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

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

Recommended Texts:

1. Moore, E. & Smart, L. *Solid State Chemistry: An Introduction* 2nd Ed. Chapman & Hall (1996)
2. Rhodes, G. *Crystallography Made Crystal Clear: A Guide for Users of Macromolecular Models* 3rd Ed. Elsevier (2006)

3. Massa, W. *Crystal Structure Determination* 2nd Ed. Springer (2004).
4. Warren, B. E., *X-Ray Diffraction* 1st Ed. Dover Publications (1990).
5. Sands, D. E. *Introduction to Crystallography* Reprint Dover Publications (1994).

Paper XVII(iii) –Physical Chemistry Special (Advanced Photochemistry and Radiation Chemistry)

Photochemistry

Molecular photochemistry: An overview: Transitions between states (Chemical, classical and quantum dynamics, vibronic states). Potential energy surfaces; transitions between potential energy surfaces, The Franck-Condon Principle and radiative transitions. A classical model of radiative transitions. The absorption and emission of light - state mixing, spin-orbit coupling and spin forbidden radiative transitions, absorption complexes, delayed fluorescence and phosphorescence.

Photophysical radiationless transitions: Wave mechanical interpretation of radiationless transitions between state factors that influence the rate of vibrational relaxation. Energy transfer: Theory of radiationless energy transfer, energy transfer by electron exchange: An overlap or collision mechanism. The role of energetics in energy transfer mechanism. Diffusion controlled quenching. The Perrin formulation. Triplet-triplet, triplet-singlet, singlet-triplet energy transfer. Multiphoton energy transfer processes, reversible energy transfer.

Radiation Chemistry

An overview, G-value. The mechanism of interaction of high energy radiation with matter, Photoelectric effect, Compton effect, Pair production, total absorption co-efficient, excitation and ionization, Stopping power and linear energy transfer.

Radiation dosimetry: Radiation dose and its measurement, standard free air chamber method, chemical dosimeter (Frick's Dosimeter). Short lived intermediates (ions, excited molecules, free radicals: Various mechanisms of their formation and energy transfer processes).

Flash photolysis: Principle and its applications. Radiolysis of water and aqueous solutions. Radiolysis of molecules of biological interest (carbohydrates, amino acids, peptides, and nucleic acids).

Recommended Texts:

1. Turro, N. J. *Modern Molecular Photochemistry* Univ. Science Books (1991).
2. Gilbert, A. & Baggot, J. *Essentials of Molecular Photochemistry* Blackwell Scientific (1990)
3. Atkins, P. W. & Paula, J. de *Atkin's Physical Chemistry* 8th Ed., Oxford University Press (2006).
4. McQuarrie, D. A. & Simon, J. D. *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books (2001).

Paper XVIII(iii) –Physical Chemistry Special (Macromolecules)

Recapitulation: Polymers and their classification and nomenclature. Types of polymerization. Molecular weight and size, degree of polymerization, polydispersity. Practical significance of polymer molecular weight.

Kinetics of polymerization: Kinetics and statistics of step growth polymerization, size distribution in linear polymers, nonlinear polymerization and prediction of gel point. Kinetics of free radical chain polymerization, cationic polymerization, anionic polymerization and polycondensation.

Structure of macromolecules: Polymer crystals: crystallization in polymers, factors determining crystal structure. Morphology of solution grown single crystal and bulk grown crystal. Semi-crystalline polymers: spherulites, degree of crystallinity, crystallization and melting. Kinetics of crystallization. Molecular mechanism of crystallization, factors affecting melting.

Amorphous polymers: Structure in amorphous polymers.

Polymer microstructure: Microstructure based on chemical structure and geometrical structure.

Meaning of glass transition temperature (T_g), factors influencing the glass transition temperature, importance of glass transition temperature T_g and molecular weight, T_g and melting point

Polymer solutions: Process of polymer dissolution, Thermodynamics of polymer dissolution. The Flory-Higgins Theory of polymer solutions, nature of polymer molecules in solution. Viscosity of polymer solutions. Colligative properties. Conformations and configurations of polymers in solutions.

Electrically conducting polymers: Discovery of electrically conducting polymers, Factors affecting the conductivity of conducting polymers. Electrochemical polymerization. Doping of conducting polymers. Important structural features. Nature of charge carriers in conducting polymers: solitons, polarons and bipolarons. Mechanism of conduction in polymers.

Electronic structure of polymers: Band theory of polymers. Methods for determining band structure of polymers: An introduction.

Designing of conducting polymers: Substitution, copolymerization. Donor-acceptor polymerization; ladder polymerization, topological routes. Applications of conducting polymers.

*Stimuli-sensitive (smart) polymers: p*H- and temperature-sensitive smart polymers and their applications in biotechnology and medicine.

Degradable polymers: Types of degradable polymers, Chemical and biodegradation. Applications of degradable polymers.

Recommended Texts:

1. DeGennes, P. G. *Scaling Concepts in Polymer Physics* Cornell University Press (1979).
2. Young, R. J. & Lovell, P. A. *Introduction to Polymers* 2nd Ed. Chapman & Hall (1991).

Paper XIX(iii) –Physical Chemistry Special (Biophysical Chemistry)

Fundamentals of biological macromolecules: Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; Structures of nucleic acids. Protein structure and function. Properties of nucleosides and nucleotides; composition of nucleic acids.

Molecular modelling and conformational analysis: Complexities in modelling macromolecular structure; polypeptide chain geometries and internal rotational angles; Ramachandran plots; Molecular mechanics; Stabilizing interactions in biomolecules; simulating macromolecular structure; energy minimization; Molecular Dynamics.

Methods for the separation of biomolecules: General principles, including Chromatography; Sedimentation, Moving Boundary Sedimentation, Zonal Sedimentation, Electrophoresis, Isoelectric focusing, Capillary electrophoresis, MALDI-TOF.

Structural determinations: Physical methods: Ultracentrifugation and other hydrodynamic techniques; Light scattering, fundamental concepts, scattering from a number of small particles: Rayleigh scattering, scattering from particles that are not small compared to the wavelength of radiation; Dynamic light scattering; Low angle X-Ray scattering; Neutron scattering; Raman scattering

Optical methods and applications: Optical techniques in biological systems: Absorption spectroscopy, Fluorescence spectroscopy, Linear and Circular Dichroism, Single and multidimensional NMR spectroscopy.

Recommended Texts:

1. Cantor, C. R. & Schimmel *Biophysical Chemistry* Vols. 1-3, W. H. Freeman (1980).
2. Lehninger, A. L., Nelson, D. L. & Cox, M. M. *Lehninger Principles of Biochemistry* 4th Ed., W. H. Freeman (2004).

Paper XX(iii) –Physical Chemistry Special (Computational Methods in Chemistry)

Programming: BASIC and FORTRAN/C languages. Introduction to LINUX/UNIX and shell scripts. Some illustrative numerical methods in chemistry: Least squares fit, root finding, numerical differentiation, integration and solution of ODE, matrix inversion and diagonalization, interpolation. Pattern recognition techniques and molecular graphics.

Basics of electronic structure calculations, Molecular Mechanics, Monte Carlo and Molecular Dynamics simulations.

Computer experiments: Use of some packages to study molecular electronic structures and molecular modelling (GAMESS, MOPAC, molecular dynamics packages, etc.) Use of electronic spreadsheets in chemistry. Basic ideas on structure-activity relationships, drug and catalysis design, etc. Development of some simulation programs and use of the internet for chemical information retrieval. Chemoinformatics.

The course should be coupled with practical training in the laboratory, and, out of a total of 50 marks, 10 marks should be reserved for internal assessment based on project work, which will replace the mid-semester internal assessment test. Each student should complete at least one project.

Recommended Texts:

1. Hinchliffe, A. *Modelling Molecular Structures* 2nd Ed., John Wiley & Sons (2003).

2. Höltje, H-D., Sippl, W., Rognan, D. & Folkers, G. *Molecular Modeling: Basic Principles and Applications* 2nd Ed. Wiley-VCH (2003).

3. Leach, A. R. *Molecular Modelling: Principles and Applications*.2nd Ed. Pearson Education: England (2001).

4. Press, W. H., Tenkolsky, S. A., Vetterling, W. T. & Flannery, B. P. *Numerical Recipes in Fortran/C* 2nd Ed., Cambridge University Press (1996).

Paper XXI(iii) –Physical Chemistry Special (Physical Chemistry of Materials)

Glasses, ceramics, composites and nanomaterials. Glassy state, glass formers and glass modifiers, Applications. Ceramic structures, mechanical properties, clay products. Refractories, characterization, properties and applications.

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

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.

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

Colloids: Types of colloids, forces between colloidal particles, characterization of colloids, charge stabilization, steric stabilization, effect of polymer on colloid stability, kinetic properties, sols, gels, clays, foams, emulsions, food colloids, concentrated colloidal dispersions.

Polymer: Polymer melts- The tube model, viscoelastic behaviour, experimental observations of single chain dynamics- Rouse and Zimm models, polymer blends, copolymers, incompatibility and segregation.

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

High T_c materials: Defect perovskites, high T_c 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-paying and multigap structure in high T_c materials, applications of high T_c materials.

Materials for solid-state devices: Rectifiers, transistors, capacitors IV-V compounds, low-dimensional quantum structures; optical properties.

Organic solids, fullerenes, molecular devices: Conducting organics, organic superconductors, magnetism in organic materials.

Fullerenes - doped fullerenes as superconductors.

Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches- sensors.

Nonlinear optical materials: nonlinear optical effects, second and third order-molecular hyperpolarizability and second order electric susceptibility- materials for second and third harmonic generation.

Recommended Texts:

1. Ashcroft, N. W. & Mermin, N. D. *Solid State Physics* Holt-Saunders (1976)
2. Callister, W. D., Jr. *Materials Science & Engineering: An Introduction* John Wiley & Sons: New York.
3. Keer, H. V. *Principles of the Solid State* Wiley Eastern Ltd.: New Delhi (1993).
4. Gray, G. W., Ed. *Thermotropic Liquid Crystals* John Wiley & Sons: New York (1987).
5. Serpone, N. & Pelizzetti, E. *Photocatalysis: Fundamentals and Applications* John Wiley & Sons (1989).
6. Cowie, J. M. G. *Polymers: Chemistry and Physics of Modern Materials* 2nd Ed. CRC Press (1991)
3. Hamley, I. W. *Introduction to Soft Matter: Polymers, Colloids, Amphiphiles and Liquid Crystals* John Wiley & Sons (2000).

Practical Test- 200 Marks

Inorganic Chemistry

I. Synthesis of inorganic complexes/compounds and their characterization by various physicochemical methods, viz. IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other from the existed literature.

(i) Metal acetylacetonates

Inorg. Synth. 1957, **5**, 130; 1963, **1**, 183.

(ii) *Cis* and *trans* isomers of $[Co(en)_2Cl_2]Cl$

J. Chem. Soc., 1960, 4369.

(iii) Ion-exchange separation of oxidation states of vanadium.

J. Chem., Educ., 1980, **57**, 316; 1978, **55**, 55.

(iv) Preparation of Ferrocene.

J. Chem. Educ. 1966, **43**, 73; 1976, **53**, 730.

(v) Preparation of triphenyl phosphene Ph_3P, and its transition metal complexes.

(vi) Determination of Cr(III) complexes.

$[Cr(H_2O)_6]NO_3.3H_2O$; $[Cr(H_2O)_4Cl_2]Cl.2H_2O$; $[Cr(en)_3]Cl_3$; $Cr(acac)_3$.

(vii) Tin(IV) iodide, Tin(IV) chloride, Tin(II) iodide.

Inorg. Synth. 1953, **4** 119.

(viii) (*N,N*)-bis(salicyldehyde)ethylenediamine Salen H_2; and its cobalt complex [Co(Salen)].

J. Chem. Educ. 1977, **54**, 443, 1973, **50**, 670.

(ix) Reaction of Cr(III) with multidentate ligands, a kinetics experiment.

J. Am. Chem. Soc., 1953, **75**, 5670.

(x) Vanadyl acetylacetonate.

(xi) Mixed valence dinuclear complex of Mangenese(III,IV).

(x) Other new novel synthesis reported in literature from time to time

II(a) Analysis of ores, alloys and inorganic substances by various chemical methods.

II(b) Instrumental methods of analysis utilising flame photometer, atomic absorption spectrophotometer, pH-meter, potentiometer, turbidimeter, electrochemical methods, separation of mixtures of metal ions by ion exchange chromatography.

III. Synthesis and thermal analysis of group II metal oxalate hydrates.

IV. Any other experiments done in the class during the current academic year.

Organic Chemistry

1. Semi-micro qualitative analysis of single/poly functional compounds (including use of spectral data).
2. Separation of mixtures by chemical and chromatographic methods
3. Isolation of natural products
   - i. Isolation of caffeine from tea leaves
   - ii. Isolation of piperine from black pepper
   - iii. Isolation of β-carotene from carrots
   - iv. Isolation of lycopene from tomatoes
   - v. Isolation of cholesterol from bile stones
   - vi. Isolation of limonene from lemon peel
   - vii. Isolation of euginol from cloves

I. *Quantitative analysis*

- i. Estimation of glucose by chemical methods
- ii. Estimation of amino acids by chemical methods
- iii. Estimation of nitro group in organic compounds
- iv. Estimation of iodine by Vij's solution
- v. Estimation of carbohydrates, amino acids, proteins and caffeine by UV/VIS spectra
- vi. Estimation of a given mixture by NMR spectra
- vii. Estimation of ascorbic acid by chemical/UV method
- viii. Any other estimations

II. *Advanced organic synthesis*

(i) Multistage synthesis including photochemical and enzymatic methods (some examples are given below)

Benzophenone $\rightarrow$benzopinacol $\rightarrow$ benzopinacolone

Benzoin $\rightarrow$benzil $\rightarrow$ benzilic acid

Benzaldehyde $\rightarrow$ chalcone $\rightarrow$ chalcone epoxide, chalcone $\rightarrow$ chalcone dibromide $\rightarrow\alpha$-bromochalcone

Cyclohexanone $\rightarrow$cyclohexanone oxime $\rightarrow$ caprolactone

(ii) Enzymatic reaction: reduction of ethyl acetoacetate with Baker's yeast; PPL catalysed deacetylation of 2,4-diacetoxyacetophenone.

(iii) Use of ultrasound and microwaves in organic synthesis

(iv) Application of phase transfer catalysis in organic synthesis

Physical Chemistry

<u>List of Experiments</u> (Sets **A - F**)

<u>Set **A**</u>

CONDUCTOMETRY

1. Titrate a moderately strong acid (salicylic/mandelic acid) by the

(a) salt-line method

(b) double alkali method.

2. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid with sodium hydroxide.
3. Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.
4. Titrate
   (i) Magnesium sulphate against $BaCl_2$ and its reverse titration
   (ii) HCl versus NH_4OH
   (iii) Sodium oxalate against HCl.
5. Estimate the concentration of each component of a mixture of $AgNO_3$ and HNO_3 by conductometric titration against NaOH.
6. Determine the degree of hydrolysis of aniline hydrochloride.
7. Determine the critical micelle concentration of a surfactant (sodium lauryl sulphate) by the conductivity method.
8. Study the effect of dielectric constant (ε) on the nature of the conductometric titration between maleic acid and sodium methoxide using different mixtures of benzene and methanol as solvents.
9. Determine the velocity constant for the saponification of ethyl acetate conductometrically.

Set **B**

SPECTROPHOTOMETRY

1. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture by the MLRA method
2. Determine the dissociation constant of an indicator spectrophotometrically.
3. Record the U.V. spectrum of a given compound (acetone) in cyclohexane

   (a) Plot transmittance *versus* wavelength.

   (b) Plot absorbance *versus* wavelength.

   (c) Assign the transitions by recording spectra in solvents of different polarities (H_2O, CH_3OH, $CHCl_3$, CH_3CN and 1,4-dioxane). Comment on the energy of hydrogen bonding.

   (d) Calculate the energy involved in the electronic transition in different units, i.e. cm^{-1}, Joules/mol, cal/mol. & eV.

   (e) Calculate the oscillator strength/ transition probability.

4. Study the spectra of mesityl oxide in different solvents (as in 3(c)), and classify the observed transitions in terms of $n\rightarrow\pi^*$ and $\pi\rightarrow\pi^*$ transitions. Discuss the shift in transitions relative to those in acetone by means of a qualitative MO diagram.

5. Record the UV spectra of *p*-nitrophenol (in 1:4 ethanol:water mixture). Repeat after adding a small crystal of NaOH. Comment on the difference, if any.

6. Record the UV spectra of benzene, pyridine and pyrimidine in methanol. Compare and discuss the various transitions involved in terms of MO theory.

7. Find the stoichiometry of the charge transfer (CT) complex formed between thiocyanate ions and iron(III) by Job's method of continuous variation. Determine the concentration equilibrium constant and extinction coefficient for the charge transfer complex by applying the Benesi-Hildebrand equation.

8. Study the vibrational-rotational spectrum of HCl in the gas phase, and

   (a) Explain the intensities of the rotational lines

   (b) Calculate

      (i) the force constant of the H-Cl bond,

      (ii) the moment of inertia of the molecule, and

      (iii) the internuclear distance.

   (c) Calculate the rotational partition function, and the rotational contribution to the molar heat capacity of the HCl molecule.

9. Record the fluorescence spectrum of phenolphthalein in the aqueous phase at pH 3 and 10 and compare the two spectra. Comment on the difference, if any.

10. Find the dissociation constant of a weak acid (β-naphthol or 4-methyl-7-hydroxy coumarin) in its ground state (by absorptiometry), and in its excited state (by fluorimetry). Comment on the difference, if any.

Set **C**

POTENTIOMETRY

1. Set up a calomel electrode (saturated) and measure its potential using the quinhydrone electrode as the reference.

2. Set up the following electrodes and measure their potentials. Obtain values for their standard electric potentials:

(a) Zn | $ZnSO_4$ (0.1 M and 0.01 M);

(b) Cu | $CuSO_4$ (0.1 M and 0.01 M).

3. Determine the solubility and solubility product of an insoluble salt, AgX (X=Cl, Br or I) potentiometrically.

4. Determine the mean activity coefficient ($\gamma_{\pm}$) of 0.01 M hydrochloric acid solution.

5. Titrate phosphoric acid potentiometrically against sodium hydroxide.

6. Find the composition of the zinc ferrocyanide complex by potentiometric titration.

7. Titrate potentiometrically solutions of

(a) KCl/ KBr/ KI;

(b) mixture of KCl + KBr + KI and determine the composition of each component in the mixture.

8. Titrate potentiometrically a solution of ferrous ions against $KMnO_4$/ $K_2Cr_2O_7$. Carry out the titration in the reverse order.

9. Determine the dissociation constant (pK$_a$) of a weak acid using a *p*H-meter.

Set **D**

COMPUTATIONAL TECHNIQUES

I. BASIC programming

(a) Elements of the BASIC language including string manipulation and graphics

(b) Numerical methods and their applications in chemistry

(c) Some typical exercises based on the above

i. Decimal-binary conversion
ii. Numerical differentiation, quadrature and finding roots
iii. Titration curves and end-point location
iv. H and S from C_p data
v. *p*H of a weak acid
vi. Roots of cubic equations (e.g. van der Waals' equation)
vii. Chemical kinetics simulations
viii. Least-squares fit including graphics
ix. Density Functional modelling of atoms
x. Numerical solution of differential equations (e.g. in kinetics)
xi. Intrapolation & interpolation of data

xii. Gauss-Siedel method and its use in solving simultaneous equations (e.g. Lambert-Beer's law)

II. Molecular modelling and its applications to problems from chemistry, biochemistry and solid-state chemistry, particularly for interpretation of UV/Vis and IR data from Set B (Spectoscopy).

III. Use of spreadsheets and mathematical packages in data analysis and solving problems in chemistry (e.g. potentiometric titrations, kinetics, regression, and solving simultaneous equations).

Set **E**

PHOTOCHEMISTRY & COLOURIMETRY

1. Determine the intensity of light from a UV source using the reaction between Fe^{3+} and oxalate ions.
2. Study the kinetics of the photosensitized decomposition of oxalic acid by uranyl ions.
3. Prepare the transition metal complex cyano acid of potassium ferrocyanide (or ferricyanide) by the ion-exchange method.
   (a) Determine the nature of this acid by the conductometric method.
   (b) Study the titration curves of the photolyzed acid (UV radiation), and suggest a possible mechanism for its decomposition.

4. Verify Lambert-Beer's law, and determine the concentration of $CuSO_4$/ $KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration *colourimetrically*.

5. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.

6. Determine the dissociation constant of an indicator *colourimetrically*.

7. Study the kinetics of iodination of acetone *colourimetrically* in acidic and basic media and comment on the difference, if any.

7. Find the order and the energy of activation of the decomposition of the violet coloured Ce(IV) oxidation product of *N*-phenylanthranilic acid using a *colourimeter*. (*J. Chem. Ed.*, 327 (1976))
8. Study the kinetics of oxidation of ethanol by potassium dichromate. Determine the order, rate constant, energy of activation and possible mechanism for the reaction.
9. Find the stoichiometry of the complex formed between a metal ion (Fe^{3+}) and a ligand (salicylate) by Job's continuous variation method and determine the stability constant of the complex formed.

Set **F**

POLAROGRAPHY

1. Record polarograms of a solution of KCl (0.1M) in the absence and presence of 0.005% gelatin in the solution. Explain the nature of the polarograms. Repeat the experiment after expelling the dissolved oxygen with a stream of nitrogen gas (5-10 mins.). What do you conclude from the experiment?

2. Determine the diffusion current and the half-wave potentials of Cd^{2+} and Zn^{2+} ions:

(a) Cd^{2+} (0.001 M) in KCl (0.1 M);

(b) Zn^{2+} (0.001 M) in KCl (0.1M) containing 0.005% gelatin;

(c) Cd^{2+} (0.001 M) + Zn^{2+} (0.001 M) + KCl (0.1 M) + gelatin(0.005%).

How can you identify the ion from the polarogram? Estimate the concentrations of the ions in separate and mixed solutions.

3. Titrate amperometrically lead nitrate (0.001 M) in KNO_3 (0.1M) + gelatin (0.005%) against standard potassium dichromate (0.01 M). Repeat the experiment in the reverse order.

4. Determine the stability constant of the lead oxalate complex by the polarographic method.

VISCOMETRY

5. Determine the molecular weight of a given macromolecule (PVP) by the viscosity method.

NEPHELOMETRY

6. Estimate the concentration of sulphate ions in solution and in a sample of tap water by precipitation with barium chloride.

7. Estimate chloride ions in a given solution/ water from various sources.

(Note: Any other experiment may be introduced during the year.)

Recommended Practical Chemistry Manuals and Books:

1. Vogel, A. I. *Vogel's Qualitative Inorganic Analysis* - 7th ed. (revised by G. Svehla) Longmans (1996) ISBN 058-221866-7
2. Vogel, A. I. *Vogel's Textbook of Quantitative Chemical Analysis* - 6th Ed. (revised by Mendham *et al*) Longman
3. Addison Ault *Techniques and Experiments for Organic Chemistry* 6th Ed. University Science Books (1998).
4. Mann, F. G. & Saunders, B. C. *Practical Organic Chemistry* 4th Ed. Orient Longmans (1990).
5. Vogel, A. I. *Vogel's Textbook of Practical Organic Chemistry* 5th Ed. (revised by A.R. Tatchell *et al*.) Wiley (1989) ISBN 0582-46236-3
9. Daniels, F., Williams, J. W., Bender, P., Alberty, R. A., Cornwell, C. D. & Harriman, J. E. *Experimental Physical Chemistry*, McGraw-Hill (1962).
10. Das & R. C. & Behera, B., *Experimental Physical Chemistry*, Tata McGraw-Hill Publishing Co. Pvt. Ltd. (1993).
11. Shoemaker, D. P., Garland, C. W. & Nibler, J. W. *Experiments in Physical Chemistry*, McGraw-Hill: New York (1996).
12. Day, R. A., Jr. & Underwood, A. L. *Quantitative Analysis* 3rd Ed. Prentice-Hall India Pvt. Ltd.: New Delhi (1977).
13. Burns, D. T. & Rattenbury, E. M. *Introductory Practical Physical Chemistry* Pergamon Press (1966)
14. Harris, D. C. *Quantitative Chemical Analysis* 6th Ed. W. H. Freeman & Co. (2002).
15. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) *Instrumental Methods of Analysis* - 7th Ed., Wadsworth Publishing (February 1988) ISBN 0534081428