DEPARTMENT OF CHEMISTRY

FACULTY OF NATURAL SCIENCES

JAMIA MILLIA ISLAMIA

(A Central University by an Act of Parliament)

M.Sc. CHEMISTRY
Syllabus w.e.f. 2010-2011

DEPARTMENT OF CHEMISTRY
JAMIA MILLIA ISLAMIA
NEW DELHI

COURSE OUTLINE OF M.Sc. CHEMISTRY w.e.f. 2010-11

M.Sc. CHEMISTRY (Ist SEMESTER) – 28 credits				
Theory papers of 4 credits each		4 x 5	= 20	
Paper No. (Code No.)	Title	Theory	Internal Assessment (IA)	Page
I (CH-101)	Inorganic Chemistry-I	75	25	1
II (CH-102)	Elements of Materials Chemistry	75	25	3
III (CH-103)	Stereochemistry and Role of Bonding in Organic Reactions	75	25	5
IV (CH-104)	Thermodynamics	75	25	7
V (CH-105)	Group Theory and Spectroscopy – I	75	25	9
Lab Course	Title	Lab.	IA	Page
2 credits	Inorganic Chemistry Lab-I	25	25	11
2 credits	Materials Chemistry Lab-I	25	25	12
2 credits	Organic Chemistry Lab-I	25	25	13
2 credits	Physical Chemistry Lab-I	25	25	14
TOTAL MARKS = 700				
M.Sc. CHEMISTRY (IInd SEMESTER) – 28 credits				
Theory papers of 4 credits each		4 x 5	= 20	
Paper No.	Title	Theory	IA	Page
VI (CH-201)	Inorganic Chemistry-II	75	25	15
VII (CH-202)	Defects, Deformation and Deterioration of Materials	75	25	16
VIII (CH-203)	Organic Reactive Intermediates, Mechanism and Pericyclic Reactions	75	25	17
IX (CH-204)	Surface Chemistry	75	25	19
X (CH-205)	Group Theory and Spectroscopy – II	75	25	21
Lab Course	Title	Lab.	IA	Page
2 credits	Inorganic Chemistry Lab-II	25	25	23
2 credits	Materials Chemistry Lab-II	25	25	24
2 credits	Organic Chemistry Lab-II	25	25	25
2 credits	Physical Chemistry Lab-II	25	25	26
TOTAL MARKS = 700				

M.Sc. CHEMISTRY (IIIrd SEMESTER) – 19 credits				
Theory papers of 4 credits each		4 x 4	= 16	
Inorganic Specialization:				
Paper No.	Title	Theory	IA	Page
XI(i) (CH-301)	Chemical Applications of Group Theory	75	25	27
XII(i) (CH-302)	Inorganic Reaction Mechanism	75	25	28
XIII(i) (CH-303)	Organometallic Chemistry-I	75	25	29
XIV(i) (CH-304)	Bio-inorganic Chemistry – I	75	25	31
Lab Course	Title	Lab.	IA	Page
3 Credits	Inorganic Chemistry Lab-III	38	37	32
Materials Specialization:				
Paper No.	Title	Theory	IA	Page
XI(ii) (CH-305)	Conventional Ceramics	75	25	33
XII(ii) (CH-306)	Basic Concepts of Crystallography and Crystal Structures	75	25	35
XIII(ii) (CH-307)	Polymer Chemistry and Technology	75	25	37
XIV(ii) (CH-308)	Chemistry of Advanced Materials	75	25	38
Lab Course	Title	Lab.	IA	Page
3 Credits	Materials Chemistry Lab-III	38	37	40
Organic Specialization:				
Paper No.	Title	Theory	IA	Page
XI(iii) (CH-309)	Medicinal Chemistry	75	25	41
XII(iii) (CH-310)	Chemistry of Natural Products – I	75	25	43
XIII(iii) (CH-311)	Methods in Organic Synthesis	75	25	44
XIV(iii) (CH-312)	Applications of Spectroscopy – I	75	25	46
Lab Course	Title	Lab.	IA	Page
3 Credits	Organic Chemistry Lab-III	38	37	47

Physical Specialization:				
Paper No.	Title	Theory	IA	Page
XI(iv) (CH-313)	Nuclear Chemistry	75	25	48
XII(iv) (CH-314)	Advanced Solid State Chemistry	75	25	50
XIII(iv)(CH-315)	Electrochemistry	75	25	52
XIV(iv)(CH-316)	Molecular Reaction Dynamics and Catalysis	75	25	53
Lab Course	Title	Lab.	IA	Page
3 Credits	Physical Chemistry Lab-III	38	37	55
TOTAL MARKS = 475				
M.Sc. CHEMISTRY (IVth SEMESTER) – 24 credits				
Theory papers of 4 credits each		4 x 4	= 16	
Research Project (7 Credits)		175		
Educational Tour (1 Credit)		25		
Inorganic Specialization:				
Paper No.	Title	Theory	IA	Page
XV(i) (CH-401)	NMR Spectroscopy and Lanthanide Shift Reagents	75	25	57
XVI(i) (CH-402)	Stereochemistry and Metal Ion Catalysis	75	25	58
XVII(i) (CH-403)	Organometallic Chemistry-II	75	25	59
XVIII(i) (CH-404)	Bio-inorganic Chemistry – II	75	25	61
Materials Specialization:				
Paper No.	Title	Theory	IA	Page
XV(ii) (CH-405)	Technical Ceramics	75	25	62
XVI(ii) (CH-406)	Processing and Characterization of Crystal Structures	75	25	64
XVII(ii)(CH-407)	Polymer Technology, Processing and Specialty Polymers	75	25	65
XVIII(ii)(CH-408)	Electronic, Electrical, Magnetic and Optical Properties of Materials	75	25	66

Organic Specialization:				
Paper No.	Title	Theory	IA	Page
XV(iii)(CH-409)	Advanced Medicinal Chemistry	75	25	67
XVI(iii)(CH-410)	Chemistry of Natural Products – II	75	25	69
XVII(iii)(CH-411)	Advanced Methods in Organic Synthesis and Photochemistry	75	25	70
XVIII(iii)(CH-412)	Applications of Spectroscopy – II	75	25	71
Physical Specialization:				
Paper No.	Title	Theory	IA	Page
XV(iv)(CH-413)	Quantum Chemistry	75	25	72
XVI(iv)(CH-414)	Nano Chemistry	75	25	73
XVII(iv) (CH-415)	Advance Electrochemistry and Micellar Phenomena	75	25	75
XVIII(iv)(CH-416)	Kinetics of Complex Reactions	75	25	76
TOTAL MARKS = 600				

M.Sc. CHEMISTRY – SEMESTER I
INORGANIC CHEMISTRY
PAPER – I

INORGANIC CHEMISTRY – I

12 hours

Unit I: Metal Ligand Equilibria in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate Effect and its thermodynamic origin, determination of binary formation constants by pH-metry and Spectrophotometry.

Unit II: Non–Aqueous Solvents

Role of Solvents in chemical reactions, physical properties of a solvent, types of solvent and their general characteristics, reactions in non-aqueous solvents with reference to liquid ammonia and liquid SO_2.

Unit III: Magnetic Properties of Transition Metal Complexes

Magnetic properties of transition metal complexes and lanthanides, 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, anamolous magnetic moments, magnetic exchange coupling and spin Crossover.

Unit IV: Inorganic Materials

Introduction to the solid state, metallic bond, band theory (zone model, brillouin zones, limitation of 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 super conductors.

Books Suggested:

1. Inczedy, J. *Analytical applications of complex equilibria* Halsted Press: New York, NY (1976).
2. Hartley, F. R., Burgess, C. & Alcock, R. M. *Solution Equilibria* Prentice-Hall: Europe (1980).
3. Ringbom, A. *Complexation in Analytical Chemistry* Wiley: New York (1963).
4. Non-aqueous Solution Chemistry by H.H. Sisler.
5. Magnetochemistry by R.L. Carlin.
6. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes* Chapman and Hall: U.K. (1973).

7. Elements of Chemistry by N. N. Greenwood and A. Earnshaw.
8. Keer, H.V. *Principles of the solid state* Wiley Eastern Ltd.: New Delhi (1993).
9. West, A.R. *Solid State Chemistry and its Applications* John Wiley & Sons (1987).
10. Cheetham, A. K. & Day, P., Eds. *Solid State Chemistry Techniques* Clarendon Press, Oxford (1087).

M.Sc. CHEMISTRY – SEMESTER I *(wef 2012-2013)*
MATERIALS CHEMISTRY
PAPER – II

ELEMENTS OF MATERIALS CHEMISTRY

Unit I: Multiphase Materials 12 Lectures

Introduction, solid solutions, interstitial and substitutional solid solutions, complex solid solutions intermetallic compounds, condensed phase rule, one component system Si and Fe. Binary isomorphous system: Cu-Ni, Au-Cu, Hume Rothery solid solubility rule, Liver Rule, Invarient phase Equilibrium Entetic formation (Pb-Sn) peritectic formation Fe-Ni, Fe-C phase diagram, phase transformation in Fe-C alloys, Ferrous and nonferrous alloys.

Unit II: Polymer Chemistry 14 Lectures

Classification of Polymers; Degree of Polymerization
General Characteristics of Chain Growth Polymerization; Alkene Polymerization by Free Radical, Cationic and Anionic Initiators;
General Characteristics of Step Growth Polymerization; Synthesis of Polymers by Step Growth Polymerization: Polyesters, Polyamides, Polycarbonates, Polysulphones, Polyphenyl Oxides and Polysiloxanes
Ring-opening Polymerization of Ethers and Lactones

Unit III: Glasses 8 Lectures

General features, Fabrication of glass, Factors that influence glass formation , Viscosity, Effect of electronegativity, and bond types on oxide glass, Zachariason's, Sun and Rawson criteria, Methods of glass formation, Silicate glasses, Pyrex glass, Phosphate glasses, Borate glasses, Thermodynamics of glass formation, Chalcogenide Glasses.

Unit IV: Nanomaterials 14 Lectures

Nanoscale Regime, Nano particle, Nanoporous materials, Gas phase Nanoparticles, Condensed Phase Nano Partcles, Inorganic Nano Particles, Semi conductors, Dielectric (insulator) Nano particles, Properties of nanoparticles (Physical, mechanical, chemical, magnetic, optical and electronic properties)Method of Preparation:- Bottom Dowuard Bottom approach, metal atom aggregation in inert gases and cold matrice (GEM, PCB, CFCB and SMAD process), Sonocative Decomposition of metal carbonyl, Borohydrated Reduction, Alkali metal reduction, Zeolite Method, Emulsion, inverse micelles , Sol-Gel Methods , Co-Precipitation Method.

Books Suggested:

1. Text Book of Polymer Science by F. W. Billmeyer
2. Materials Science and Engineering: An Introduction, W.D. Callister, Wiley

3. Principle of solid state, H. V. Keer, Wiley Eastern.
4. Chemistry of Advanced Materials by Leonard V.Interrante and M.J.Hampden-Smih

M.Sc. CHEMISTRY – SEMESTER I
ORGANIC CHEMISTRY
PAPER – III

STEREOCHEMISTRY AND ROLE OF BONDING IN ORGANIC REACTIONS

Unit I: Configurational Isomerism

Stereoisomerism: Classification, optical activity and chirality resolution of racemic mixture, molecules with one, two or more chiral centres; Fischer's projection formula, Relative and absolute configurations, D L, R S, and E Z system of naming. Stereochemistry due to the presence of perpendicular dissymmetric planes in allenes, spiranes, biphenyls and binaphthols. Chirality due to helical shape, Optical purity, % enantiomeric excess (ee), Enantiotopic and Diastereotopic atoms groups and faces, Stereospecific and stereoselective syntheses.

Unit II: Conformational Analysis

Conformation in open chain system (with reference to 1,2-disubstituted ethane). Baeyer's strain theory of cyclic compounds, conformations and stability of cyclohexanes (mono-, di- and tri-substituted). Confomation of rings containing sp^2 hybridized carbon atoms, conformation of sugars. Locking groups - t-butyl groups, decalins and steroids, Effect of conformation on reactivity.

Unit III: Nature of Bonding in Organic Molecules

Huckel's rule of aromaticity, annulenes, benzoid and non-benzoid aromatic systems; tropones, tropolones, azulene, pentalene and heptalene. Anti-aromaticity and Homo-aromaticity, PMO approach. Alternant and nonalternant hydrocarbons, Mesoionic compounds and squaric acid. Bonds weaker than covalent bonds, crown ether complexes and cryptands; inclusion compounds- Cyclodextrins, catananes and rotaxanes.

Unit IV: Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, Organozinc and Organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig Reaction.

Mechanism of condensation reactions involving enolates – Aldol addition/condensation, Knoevenagel condensation, Stobbe condensation, Claisen condensation, Mannich reaction, Benzoin condensation and Perkin reaction.

Hydrolysis of esters and amides, Ammonolysis of esters.

Books Suggested:

1. Advanced Organic Chemistry; Jerry March, Fourth edition, Wiley & Sons, (2005).
2. Mechanisms in Organic Chemistry; Peter Sykes, Sixth edition, Pearson, (2004).
3. Organic Chemistry; Solomons & Fryhle, Eighth edition, Wiley & Sons, (2007).
4. Organic Chemistry; Clayden, Greeves, Warren and Wothers; Oxford University Press, (2006).
5. Organic Chemistry; G. Marc Louden, Fourth edition, Oxford University Press, (2006).
6. Organic Chemistry; Paula Yurkanis Bruice, Third edition, Pearson, (2004).
7. Advanced Organic Chemistry; Francis A. Carey and Richard J. Sundberg, Part A & Part B Fourth edition, Kluwer Academics/Plenum Publishers, (2001).
8. Reaction Mechanisms in Organic Chemistry; S. M. Mukherji & S. P. Singh, Macmillan, (2004).
9. Organic Reactions, Stereochemistry and Mechanisms; P.S. Kalsi, Fourth edition, New Age International Publishers, (2006).
10. Eliel, E. L. Stereochemistry of Carbon Compounds Textbook Publishers (2003).
11. Bruckner, R. Advanced organic chemistry Elsevier(2002).
12. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981).

M.Sc. CHEMISTRY – SEMESTER I
PHYSICAL CHEMISTRY
PAPER – IV

THERMODYNAMICS

45 Lectures

Unit I: Basic Thermodynamics [10 L]

Brief description of the laws of thermodynamics, Concepts of Entropy and Residual Entropy, Free energy and its Temperature dependence, Thermodynamic Equilibria and Free Energy Functions, Physical Equilibria Involving Phase Transitions, Thermodynamic Maxwell Relations.

Unit II: Equilibrium Thermodynamics [10 L]

Chemical potential and Entropies, Partial molar quantities: Partial molar free energy, Partial molar volume and Partial molar heat content and their significances. Determinations of the partial molar quantities. Thermodynamic Functions of Mixing, Non-ideal systems: Excess functions for non-ideal solutions.

Unit III: Non Equilibrium Thermodynamics [10 L]

Thermodynamic criteria for non-equilibrium states, Basic Postulates and Methodology, Onsager's Theory, Phenomenological Laws and Equations, Transformations of the generalized fluxes and forces, Microscopic Reversibility and Onsager's Reciprocal Relations, Entropy Production and entropy flow, Theorem of Minimum Entropy Production, Chemical Reactions, Coupled Reactions and Electro-kinetic Phenomena.

Unit IV: Statistical Thermodynamics [15L]

Concept of distribution, Thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition function - Translational, Rotational, Vibrational and Electronic partition functions, calculation of thermodynamic properties in terms of partition function. Applications of partition functions. Heat capacity behaviour of solids - Chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics - distribution law and application to helium.

Books Suggested:

1. An Introduction to Chemical Thermodynamics, R. P. Rastogi and R. R. Mishra, Vikas Publishing House Pvt. Ltd.
2. Physical Chemistry, P. W. Atkins, ELBS.
3. Statistical Thermodynamics (Hardback) By (author) M.C. Gupta, Publisher: New Age International.
4. Thermodynamics, J. Rajaram and J.C. Kuriacose, Educational Publishers.
5. Thermodynamics, R. C. Srivastava, Subit K. Saha, Abhay K. Jain, Prentice Hall of India, Pvt. Ltd.
6. Statistical Physics (Part) Course of Theoretical Physics, Vol. 5, L. D. Landau and E. M. Lifshitz, Pergamon Press London.
7. Physical Chemistry, T. Engel and P. Reid, Pearson Education and Dorling Kindersley (India) 2006.
8. Statistical Mechanics, Donald A. McQuarrie, Viva Books Pvt. Ltd. New Delhi, 2003 (530.13 MCQ 270916).
9. Elements of Statistical Thermodynamics (2^{nd} Edition), Leonard K. Nash, Addison Wesley, 1974. (541.369 NAS X639)
10. Physical Chemistry, *Statistical Mechanics*, Horia Metiu, Taylor & Francis, 2006 (530.13 MET 276461)
11. Statistical Thermodynamics, B.J. McClelland, Chapman and Hall & Science Paperbacks, London, 1973 (536.7 MCC 37251)

M.Sc. CHEMISTRY – SEMESTER I

PAPER-V

GROUP THEORY AND SPECTROSCOPY - I

Unit I: Symmetry and Group Theory in Chemistry

Symmetry elements operation. Definition of a symmetry operation. Definition of a symmetry element. Symmetry planes and reflection. The inversion centre. Proper axes and proper rotations. Improper axes and improper rotations. Identity. Products and symmetry operations. Defining properties of a group. Abelian group. Symmetry operations as group elements (Multiplication table). Symmetry point group (schoenflies notations). Classes of symmetry operations. Equivalent symmetry elements and atoms.

Unit II: Rotation and Vibration of Diatomic Molecules

A. Infrared Spefctroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, Derivation of selection rules for diatomic molecules based on harmonic oscillator approximation. Dissociation energies from vibrational data.

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.

Vibrational-rotation spectroscopy, P, Q and R branches. Breakdown of Born-Oppenheimer approximation;

B. Raman Spectroscopy

Classical and quantum theories of Raman effect. Stokes and anti-Stokes lines. Polarizability ellipsoids. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules,

Unit III: Electronic Spectroscopy

Atomic Spectroscopy

The energies of atomic orbitals; Hydrogen atom spectrum; Orbital and spin angular momenta, total angular momentum; the fine structure of hydrogen atom spectrum; the spectra of alkali metal atoms.
The spectra of complex atoms: Singlet and triplet states; Spin-orbit coupling; Term Symbols and selection rules.

Unit IV: MAGNETIC RESONANCE SPECTROSCOPY

A. Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J', spin decoupling; Basic ideas about instrument, NMR studies of nuclei other than proton - ^{13}C, ^{19}F and ^{31}P. FTNMR, advantages of FTNMR.

B. Electron Paramagnetic Resonace Spectoscopv:

Intoduction-representation of the spectrum-hyperfine splitting in some simple system. Hyperfme splitting in various structures (methyl radical and bis(Salicylaldimine) copper(**II**)).

Factors affecting the magnitude of 'g' values. Zerofield Splitting and Kramers, degeneracy.

Books Suggested

1. Modern Spectroscopy, J.M. Hollas, John Wiley & Sons (2004).

2. Applied Electronic Spectroscopy for Chemical Analysis Ed. H Windawi and F. L. Ho, Wiley Interscience.

3. NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood.

4. Physical Methods in Chemistry, R.S. Drago, Saunders.

5. Chemical Applications of Group Theory, F.A. Cotton.

6. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (1962).

7. Basic Principles of Spectroscopy, R. Chang, McGraw Hill, N.Y. (1970)

8. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, and IBH-Oxford.

12. Fundamentals of Molecular Spectroscopy, Fourth Edition, C.N. Banwell and E.M. McCash, Tata McGraw-Hill Publishing Company Limited, New Delhi (1994).

M.Sc. CHEMISTRY – SEMESTER I
INORGANIC CHEMISTRY LAB-I

1. Synthesis and Characterization of Complexes

Preparation of the following inorganic compounds and their studies by IR, electronic spectra, Mossbauer and ESR spectra

(I) $VO(acac)_2$

(II) *Cis*-$K[Cr(C_2O_4)_2(H_2O)_2$

(III) $Na[Cr(NH_3)_2(SCN)_4]$

(IV) $K_3[Fe(C_2O_4)_3]$

2. Quantitative Analysis

(a) Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe, Ba-Cu etc. involving volumetric and gravimetric methods.

3. Spectrophotometric Determinations

1. Ni by extractive spectrophotometric method.
2. Fe by Job's method of continuous variations
3. Fe in vitamin tablets
4. Nitrite in water in colorimetric method.

Books Suggested.

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge.
2. Inorganic Synthesis, MC Graw Hill.
3. Handbook of Preparative Inorganic chemistry Vol. I and II, Academic press.
4. Standard methods of chemical analysis by W.W. Scaff, Technical Press.
5. Vogel's Qualitative Inorganic Analysis (revised), Orient Longman.
6. Vogel's textbook of quantitative Inorganic Analysis (revised). J. Besset, R.C. Denny, G.H. Jeffery and J. Mendhan, ELBS.

M.Sc. CHEMISTRY – SEMESTER I
MATERIALS CHEMISTRY LAB-I

1. To determine the percentage of manganese in the given sample of plain carbon steel
2. To determine the percentage of phosphorous in the given sample of plain carbon steel
3. To determine the percentage of sulphur in the given sample of plain carbon steel
4. To determine the percentage of silicon in the given sample of plain carbon steel
5. To determine the percentage of tin in the given sample of brass
6. To determine the percentage of lead in the given sample of brass
7. To determine the percentage of copper in the given sample of brass
8. To determine the percentage of zinc in the given sample of brass

M.Sc. CHEMISTRY – SEMESTER I
ORGANIC CHEMISTRY LAB–I

1. Determination of I_2 value of oils
2. Saponification value of oils
3. Acid value of oils
4. Determination of DO, COD & BOD of water sample
5. Determination of molecular weight of organic compounds
6. Separation, purification & identification of binary mixtures

M.Sc. CHEMISTRY – SEMESTER I
PHYSICAL CHEMISTRY LAB–I

1. Determine the percentage composition of a liquid mixture by viscosity method.
2. Determine the radius of sucrose molecule by viscosity method.
3. Determine molar surface energy of ethyl alcohol by surface tension.
4. To find out composition of a solution by surface tension measurement.
5. Find out molar surface area as a function of concentration for n– propyl alcohol and n-butyl alcohol over water.
6. Verify the law of refraction for mixtures, using glycerol and water.
7. Determine the formation of compounds between two liquids in the mixture.
8. Study the saponification of ethyl acetate by sodium hydroxide solution.
9. Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
10. Determine the specific reaction rate of the potassium persulphate iodide reaction by initial rate method.
11. Study of the kinetics of the iodination of acetone in the presence of acid by the initial rate method.
12. Study the adsorption of oxalic acid on charcoal.
13. Determine the heat of neutralization of hydrochloric acid and sodium hydroxide.
14. Determine the heats of reaction for the reactions:

    (i) $CO_3^{2-} + H_2O \rightarrow HCO^{3-} + OH^-$

    (ii) $HC_2O_4^- + H_2O \rightarrow H_2C_2O_4 + OH^-$

15. Find out the dimerization constant of benzoic acid in benzene by titration method.
16. Construct the phase diagram of water-ethanol-benzene system
17. Find out the molar mass of succinic acid by partition method.
18. Any other experiment(s) introduced during the year.

M.Sc. CHEMISTRY – SEMESTER II
INORGANIC CHEMISTRY
PAPER-VI

INORGANIC CHEMISTRY-II

Unit I: Electronic Spectra of Transition Metal Complexes

Spectroscopic ground states, correlation, crystal field theory and splitting in O_h, T_d, D_{4h} and C_{4v} systems, orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 –d^9),Calculation of Dq, B and β Parameters ,charge transfer spectra, spectroscopic method for assignment of absolute configuration inoptically active metal chelate and their stereochemical information.

Unit II: Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagram (tri- and penta atomic molecules), dπ-pπ bonds, Bent rule and energetic of hybridization, simple reactions of covalently bonded molecules.

Unit III: Isopoly and Heteropoly Acids and Salts

Isopolymolybdates, isopolytungstate, isopolyvanadates, heteropoly anions, organoheteropoly anions and Heteropoly blues

Unit IV: Metal Clusters

Higher boranes, carboranes and metalloboranes, compounds with metal –metal multiple bonds metal carbonyls and halide clusters

M.Sc. CHEMISTRY – SEMESTER II
MATERIALS CHEMISTRY
PAPER-VII

DEFECTS, DEFORMATION AND DETERIORATION OF MATERIALS

Unit I: Imperfection in Crystal Lattice **Lectures 12**

(a) Introduction: Types of Crystal Defects, Points Imperfection, Line Imperfection, Surface Imperfection and their classification vacancy (Interstitial and Substituted) Imperfection, Ionic Crystal Edge and Screw dislocation, Twining stacking fault and low and high angle sub grain boundary, estimation of point defects.

(b) Defect Clusters: Extended defects Split Interstitial or Doumble shaped Defects and Koch Cluster, Crystallograpic shear structure, slip motion of dislocation, Buerger's vector, effect of dislocation on mechanical properties of materials.

Unit II: Plastic and Elastic Deformations **Lectures 8**

Ring-opening Polymerization of Lactams, Ziegler-Natta Co-ordination Polymerization, Copolymerization; Types of Copolymers; The Copolymer Equation and its Application; Monomer Reactivity Ratios Polymers of Commercial Importance: PE, PP, PVC, PS and PU, Elastic Deformation, Modulus of Elasticity as a Parameter of Design; Resolved Shear stress, Relationship of slip and crystal structure of materials; Law of Critical Resolved Shear Stress

Unit III: Corrosion Deterioration **Lectures 16**

Introduction: Classification of corrosion, Electrochemical Corrosion, Relation Eight form of Corrosion :- uniform, Bimetallic crevice, intergranular , selective leaching pitting , stress and stress Corrosion, Hydrogen embrittlement, Inhibitor and Passivity, Cell Potential and EMF Series, Exchange Current Density, Activation and Concentration Polarization, Combined Polarization, Mixed Potential Theory, Mixed electrode, High temperature oxide, Thermodynamics of High Temperature Oxide. Continuous and porous scale Pilling Bed Worth ratio, linear, parabolic and lograthmic rate law of Oxidation.

Unit IV: Phase Transformation **Lectures 10**

Introduction: Time Scale for phase changes. Nucleation and Growth, The Nucleation Kinetics Homogeneous and Heterogeneous Nucleation, Growth and overall transformation Kinetics. Martenistic transformation, Buerger's classification: reconstructive and displacive transformation/ Transition

Books Suggested:

1. Sol Corrosion Engineering by Mars and Fontana
2. Material Science and Engineering by Raghavan
3. Solid state Chemistry by A.R.West

M.Sc. CHEMISTRY – SEMESTER II
ORGANIC CHEMISTRY
PAPER – VIII

ORGANIC REACTIVE INTERMEDIATES, MECHANISM AND PERICYCLIC REACTIONS

Unit I: Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity. Addition to cyclopropane rings. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction and Sharpless asymmetric epoxidation.

Unit II: Reactive intermediates In Organic Reactions

Carbocations: Stability and structure,generation and fate of carbocations.Nonclassical carbocations neighbouring group participation, ion-pairs, molecular rearrangements in acyclic, monocyclic and bicyclic systems, stability and reactivity of bridge-head carbocations.Bredts rule

Carbanions: Stability and structure, the structure of organomettalic compounds generation and fate, ambident ions and their general reactions; HSAB principle and its applications. Carbon freeradicals: Stability and structure,generation and fate of freeradicals, captodetive effects; radical-ions.

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

Nitrenes: Generation, structure and reactions of nitrenes.

Benzynes: Generation, structure and reactions of benzynes. Nucleophilic substitution at aryl carbon via Meseinheimer complex.

Unit III: Principles of Reactivity

Transition state theory, Hammond postulate, potential energy Surface model. Reactivity-Selectivity principle, Structural Effects on Reactivity: linear free energy relationship, Hammet principle.

Unit IV: 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.

Books Suggested:

1. Advanced Organic Chemistry; Jerry March, Fourth edition, Wiley & Sons, (2007).
2. Mechanisms in Organic Chemistry; Peter Sykes, Sixth edition, Pearson, (2004).
3. Organic Chemistry; Solomons & Fryhle, Eighth edition, Wiley & Sons, (2007).
4. Organic Chemistry; Clayden, Greeves, Warren and Wothers; Oxford University Press, (2006).
5. Organic Chemistry; G. Marc Louden, Fourth edition, Oxford University Press, (2006).
6. Organic Chemistry; Paula Yurkanis Bruice, Third edition, Pearson, (2004).
7. Advanced Organic Chemistry; Francis A. Carey and Richard J. Sundberg, Part A & Part B Fourth edition, Kluwer Academics/Plenum Publishers, (2004).
8. Reaction Mechanisms in Organic Chemistry; S. M. Mukherji & S. P. Singh, Macmillan, (2004).
9. Smith M.B & March,J. Advanced organic chemistry sixth edition, John Wiley & Sons (2007).
10. Fleming, I. Pericyclic reactions,Oxford science publication (1998).
11. Bruckner, R. Advanced organic chemistry Elsevier (2002).
12. Clayden, Greeves, Warren & Wothers. Organic chemistry Oxford university press(2001)
13. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981).
14. Carruthers, W. and Coldham,I. Modern methods of organic synthesis, Cambridge University Press(2004).

M.Sc. CHEMISTRY – SEMESTER II
PHYSICAL CHEMISTRY
PAPER-IX

SURFACE CHEMISTRY

45 Lectures

Unit I: Adsorption [15L]

Surface tension, Capillary action, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET adsorption isotherm, Surface films (Electro-kinetic phenomenon), Catalytic activity at surfaces. Catalysis on metal surfaces, Metal oxide surfaces. Application of photoelectron spectroscopy, ESCA and Auger spectroscopy to the study of surfaces.

Unit II: Catalysis [8 L]

General characteristics of catalytic reactions, Acid-base catalysis, Enzyme catalysis, Mechanism and kinetics of enzyme-catalysed reactions, Michalis-Menten equation, Heterogeneous catalysis, Surface reactions, Autocatalysis and Oscillatory reactions.

Unit III: Micelles [10 L]

Surface active agents, Classification of Surface active agents, Co-surfactants, Micellization, Hydrophobic interaction, Critical Micellar Concentration (CMC), Surfactant packing parameter, Factors affecting the CMC of surfactants, Counter ion binding to micelles, Thermodynamics of micellization, Mass action models, Solubilization, Micro-emulsions, Aggregate structures of surfactants and Phase diagram of ternary microemulsion system..

Unit IV: Polymer Chemistry [12 L]

Definition, Classification of polymers, Chain configuration of macromolecules, Isotactic polymers, Atactic polymers, Syndiotactic polymers, Graft polymers, Electrically conducting polymers, Polymerizations reactions, Kinetics of polymerization, Mechanism of polymerization. Molecular mass of polymers, Number and Mass average molecular mass, Determinations of molar masses of polymers (Osmometry, Viscometry and Light scattering methods), Sedimentation, Calculation of average dimensions of various chain structures.

Books Suggested:

1. Physical Chemistry 8th Ed., P. W. Atkins and J. de Paula, Oxford University Press, 2006.
2. Physical Chemistry of Surfaces - A. W. Adamson - John Wiley Sons.
3. Catalytic Chemistry, Bruce C. Gates, John Wiley & Sons, Inc. 1992.(541.395 GAT)
4. Catalysis at Surfaces, I. M. Campbell, Chapman and Hall, New York, 1998.
5. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.
6. Introduction to Colloid and Surface Chemistry 2nd Ed., D. J. Shaw, Butterworths, 1970.
7. Principles of Physical Chemistry, Puri, Sharma, Pathania, Shoban Lal Nagin Chand & Co., Educational Publishers.
8. Micelles, Theoretical and Applied Aspects, Y. Moroi, Plenum Press, New York.
9. Introduction to Polymer Science, V. R. Gowarikar, N. V. Vishwanathan and J. Sridhar - Wiley Eastern.

M.Sc. CHEMISTRY – SEMESTER II

PAPER-X

GROUP THEORY AND SPECTROSCOPY - II

Unit I: Symmetry and Group Theory in Chemistry

Character tables for C_{2V} and C_{3V} point groups (Construction not required). Representation reducible and irreducible, analysis of reducible representation. Simple Applications of the character table.

Unit II: Rotation and Vibration of Polyatomic Molecules

A. Infrared Spefctroscopy

Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules. First order Stark effect.

Vibrational-rotation spectroscopy, P, Q and R branches. Breakdown of Born-Oppenheimer approximation; vibrations of polyatomic molecules, Selection rules, normal modes of vibration, group frequencies, overtones and combination bands, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations.

B. Raman Spectroscopy

Selection rules, mutual exclusion principle. Polarization of Raman lines.

Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

Unit III: Electronic Spectroscopy of Polyatomic Molecules

Energy levels of molecular orbitals, vibronic transitions, vibrational progressions and geometry of excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Electronic spectra of transition metals

Emission spectra: radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

Unit IV: Mass Spectroscopy

Principle of mass spectroscopy (instrument, operation and representation of spectra), mass spectrometer, interpretation of mass spectra, fragmentation pattern, mode of fragmentation, nitrogen rule, effect of isotopes, signals of doubly charged ion, applications viz; identification of substances, determination of molecular weight and molecular formula.

Books Suggested:

1. Modern Spectroscopy, J.M. Hollas, John Wiley & Sons (2004).

2. Applied Electronic Spectroscopy for Chemical Analysis Ed. H Windawi and F. L. Ho, Wiley Interscience.

3. NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood.

4. Physical Methods in Chemistry, R.S. Drago, Saunders.

5. Chemical Applications of Group Theory, F.A. Cotton.

6. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (1962).

7. Basic Principles of Spectroscopy, R. Chang, McGraw Hill, N.Y. (1970)

8. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, and IBH-Oxford.

9. Fundamentals of Molecular Spectroscopy, Fourth Edition, C.N. Banwell and E.M. McCash, Tata McGraw-Hill Publishing Company Limited, New Delhi (1994).

10. Molecular Spectra and Molecular Structure – I : Spectra of Diatomic Molecules, Gerhard Herzberg, D. Van Nostrand Company, Inc. Princeton, New Jersey, 1950 (539.12 HER 51323)

11. Modern Molecular Spectroscopy, HS Randhawa, MacMillan India Ltd., 2003 (539.74 RAN 229113)

M.Sc. CHEMISTRY – SEMESTER II
INORGANIC CHEMISTRY LAB-II

1. Qualitative Analysis

(a) less common metal ions- Tl, Mo, Ti, Zr, Th, V and U (Two metal ions in cationic/anionic forms).

(b) Insoluble- oxides, sulphates and halides.

2. Chromatography

Separation of cations and anions by

(i) Paper chromatography.

(ii) Column chromatography- ion exchange.

3. Synthesis and Characterization of Complexes

Synthesis of the following inorganic compounds and their studies by IR, electronic spectra, Mossbauer and ESR spectra

(I) $[Co(Py)_2Cl_2]$

(II) $[Ni(NH_3)_6]Cl_2$

(III) $[Cu(NH_3)_4]SO_4.H_2O$

(IV) Lanthanide complexes

4. Spectrophotometric Determination

(I) Cu in a brass sample by spectrophotometer

(II) Nitrate in water sample by colorimetric method

(III) Ca and Mg in milk and egg.

5. Sodium and potassium by flame photometric method

Books Suggested:

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge.
2. Inorganic Synthesis, MC Graw Hill.
3. Handbook of Preparative Inorganic chemistry Vol. I and II, Academic press.
4. Standard methods of chemical analysis by W.W. Scaff, Technical Press.
5. Vogel's Qualitative Inorganic Analysis (revised), Orient Longman.
6. Vogel's textbook of quantitative Inorganic Analysis (revised). J. Besset, R.C. Denny, G.H. Jeffery and J. Mendhan, ELBS.

M.Sc. CHEMISTRY – SEMESTER II
MATERIALS CHEMISTRY LAB-II

1. Preparation of polystyrene by bulk method and to determine its % yield and solubility.

2. To study the kinetics of aqueous corrosion of mild steel by weight loss method and to determine the GMD.

3. Synthesis of phenol formaldehyde resin.

4. Preparation of alumina by precipitation method and determination of its density.

5. To study the phase equilbria diagram of Pb-Sn system by direct cooling curve method (Eutectic formation).

6. To determine the acid value, saponification value and iodine value of a given polymer sample.

7. To determine the porosity and density of a given ceramic cube.

Books Suggested:

1. Experiments in Materials Science by E.C.Skubbarao (Tata McGraw Hill).
2. A laboratory manual of metals and alloys by S.M.Ashraf, Sharif Ahmad and Ufana Riaz.
3. A laboratory manual of Polymers by S.M.Ashraf, Sharif Ahmad and Ufana Riaz.
4. Practical course in Polymer Chemistry by Pinner.
5. Vogel's Textbook of quantitative inorganic analysis.

M.Sc. CHEMISTRY – SEMESTER II
ORGANIC CHEMISTRY LAB-II

1. Determination of percentage of hydroxyl group
   - i. by acetylation method
   - ii. by bromination method

2. Estimation of amino group
   - i. by acetylation method
   - ii. by bromination method

3. Organic synthesis using some of the following reactions
   - i. Acetylation reaction
   - ii. Coupling reaction
   - iii. Oxidations and reductions
   - iv. Grignards reaction
   - v. Aldol condensation

M.Sc. CHEMISTRY – SEMESTER II
PHYSICAL CHEMISTRY LAB-II

1. Determine the cell constant of the given conductivity cell at room temperature.
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 of acetic acid.
4. Find out strength of weak and strong acids in a given mixture by conductometric titration.
5. Find out solubility and solubility product of the given sparingly soluble salt in water.
6. Find cmc of a given surfactant and, hence, calculate ΔG_{mix} of the surfactant.
7. Verify Debye - Huckel equation for a strong electrolyte in water.
8. Determine the electrode potentials of zinc and copper electrodes in 0.1 M and 0.01 M Solutions and calculate E_O values for these electrodes.
9. Preparation of buffer solution of various pH and determine their pH values.
10. Determination of solubility and solubility product by e.m.f method.
11. Perform acid-base titration by pH metric method.
12. Find out the first and second ionization constant of H_3PO_4 by p^H metric method.
13. Verify Beer Lambert Law.
14. Any other experiment(s) introduced during the year.

Books Suggested:

1. Harris, D. C. Quantitative Chemical Analysis 6th Ed. W. H. Freeman & Co. (2002).
2. Experiments in Physical Chemistry, R.C. Das and B. Behra – Tata McGraw Hill.
3. Advanced Practical Physical Chemistry, J.B. Yadav - Goel Publishing House.
4. Advanced Experimental Chemistry, Vol. I - Physical, J.N. Gurtu and R. Kapoor – S. Chand & Co.
5. Selected Experiments in Physical Chemistry, N.G. Mukherjee – J.N. Ghose & Sons.
6. Experiments in Physical Chemistry, J.C. Ghosh - Bharti Bhavan.
7. Senior Practical Physical Chemistry, B.D.Khosla; V.C.Garg, Adarsh Khosla – R. Chand & Co.

M.Sc. CHEMISTRY – SEMESTER III
INORGANIC CHEMISTRY
PAPER-XI(i)

CHEMICAL APPLICATIONS OF GROUP THEORY

48 Lectures

Unit I: Symmetry Aspects of Molecular Vibrations

Introduction, the symmetry of normal vibrations. Determining the symmetry types of the normal modes (Normal mode analyses of water molecule, carbonate ion and N_2F_2). Contribution of particular Internal Coordinates to normal modes. Symmetry selection rules for fundamental vibrational transitions (Qualitative treatment). The symmetry of group vibrations (a discussion of molecule $Cl_3C\text{-}CH_2\text{-}CCl_3$ to demonstrate vibrational modes of CH_2 group). Use of symmetry considerations to determine the number of active infrared and Raman lines (example SF_4).

Unit II: Symmetry Aspects of Hybrid Orbitals

Transformations propertiesof atomic orbitals. Hybrid orbitals for sigma bonds in trigonal planar (BCl_3), tetrahedral (CH_4), square planar $[PtCl_4]^{2-}$ and trigonal bipyramidal (PF_5). Hybridization scheme for pi bonding in trigonal planar (AB_3) and tetrahedral (AB_4) systems.

Unit III: Hybrid Orbitals as Linear Combination of Atomic Orbitals

Mathematical form of equivalent and non-equivalent hybrid orbitals. Trigonal planar sp^2 equivalent hybrids in BCl_3; Tetrahedral sp^3 equivalent hybrid orbitals in CH_4 and trigonal bipyramidal dsp^3 non-equivalent hybrid orbitals in PF_5.

Unit IV: The Huckel Molecular Orbital Treatment and Symmetry Simplifications

The LCAO method and secular equation. The simple Hückel approach in constructing and solving secular determinants for conjugated systems (ethylene, allyl system and butadiene), delocalization energies. Symmetry simplifications of Hückel Molecular Orbital method (symmetry factoring of secular equation: 1,3- butadiene). Calculations of electron density, charge density, Bond order and free valence index.

Books Suggested:

1. Chemical Applications of Group Theory: by F.A. Cotton.
2. Group Theory and Symmetry in Chemistry: by Lowell H. Hall.
3. Symmetry, Orbitals and Spectra: by Milton Orchin and H.H. Jaffe.
4. Physical Methods in Chemistry: by R.S. Drago.
5. Molecular Spectroscopy: by G.M. Barrow, McGraw-Hill.

M.Sc. CHEMISTRY – SEMESTER III
INORGANIC CHEMISTRY
PAPER- XII(i)

INORGANIC REACTION MECHANISM

Unit I: Introduction to Inorganic Reaction Mechanism

Introduction to labile and inert octahedral complexes, interpretation of lability and inertness of transition metal complexes - Valence Bond and Crystal Field theories, factors affecting the lability of complex, transition state or activated complex, substrate, attacking reagents-electrophilic and nucleophilic, types of substitution reactions- nucleophilic or ligand substitution (SN) and electrophilic or Metal substitution (SE) reactions.

Unit II: Mechanism of Substitution Reactions in Octahedral Complexes

Mechanism of nucleophilic substitution reactions in octahedral complexes SN^1 or dissociation and SN^2 or association (or displacement) mechanisms, hydrolysis reactions-mechanisms of acid hydrolysis and base hydrolysis, reactions of octahedral Co(III) amine complexes.

Unit III: Mechanism of Substitution Reactions in Square Planar Complexes

Mechanism of substitution reactions in Pt(II) complexes, factors effecting the reactivity of square planar complexes, Trans-effect, theories of trans-effect-Grinberg's electrostatic polarization theory and Chatt and Orgel pi-bonding theory, application of trans-effect to synthesis of complexes.

Unit IV: Electron Transfer (or Oxidation -Reduction) Reaction

Electron transfer reactions, mechanism of one-electron transfer reactions-outer sphere and inner sphere mechanisms, two-electron transfer reactions-complimentary and non-complimentary reactions, mechanism of two-electron transfer reactions.

Books Suggested

1. Inorganic Reaction Mechanism - F. Basolo & G. Pearson.
2. Inorganic Reaction Mechanism - J. O. Edwards.
3. Selected Topics in Inorganic Chemistry- Malik, Madan & Tuli.
4. Katakis, D. & Gordon, G. *Mechanism of Inorganic Reactions* John Wiley & Sons: N.Y. (1987).
5. Langford, H. & Gray, H.B. *Ligand Substitution Processes* W.A. Benjamin

M.Sc. CHEMISTRY – SEMESTER III
INORGANIC CHEMISTRY
PAPER – XIII(i)

ORGANOMETALLIC CHEMISTRY - I

Unit I: Organometallics- Main Group and Transition Elements

ntroduction, general classification- main group,transition and inner transition elements organometallics, Nomenclature of organometallic compounds, Synthesis of organometallic compounds- viz: direct synthesis, redistribution method, metal exchange, ligand exchange, addition reaction, cyclization, sigma-pi -rearrangements and substitution methods.

Unit II: Metal Carbonyls, Nitrosyls, Dinitroge and Oxygen Complexes.

Metal carbonyls, structure and bonding, Vibrational spectra of metal carbonyls for bonding and structural elucidation. Important reactions of metal carbonyls; preparation; bonding, structure and important reactions of transition metal nitrosyls; dinitrogen and oxygen complexes; Tertiary phosphine as ligand.

Unit III: Metal-Alkyls, Aryls, Allyls and Cyclopentadienyl Complexes

Structure and bonding in metal alkyls, allyls and cyclopentadienyl,aryl derivatives with special reference to Ziese's salt and metalocenes.Reactions of cyclopentadienyl, arene pi- complexes – alkylation, acylation ,arylation, Sulphonation ,formylation , Condensation reactions, Addition reactions, Oxidation reactions.

Unit IV: Isomerism in Organometallic

Isomerism in organometallic complexes – Geometrical, Structural, Conformationals and Optical isomerism, Structure elucidation of metal pi-complexes – special reference to Zieses Salt and metalocenes

Books suggested:

1. Metallo-organic Chemistry- Anthony J Pearson, John Wiley & Sons Inc, (1985)

2. Inorganic Chemistry – Principles of Structure & Reactivity, J E Huheey, Elllen A Keiter & Richard L Keiter, IV Edition (2005)

3. Introduction to metal pi-complex chemistry- M. Tsutsui, M.N. Levy, A. Nakamura, M. Ichikawa and K. Mori, Plenum Press, New York I Heme (1970).

4. Organometallic Chemistry - R. C. Mehrotra & A. Singh, Wiley Eastern Ltd. (2000)

5. Advanced Inorganic Chemistry - F. Albert Cotton, Geoffrey Wilkinson, Carlos A Murillo & Manfred Bochmann, VI Edition, John Wiley & Sons Inc (1999)

6. Principles and application of organotransition metal chemistry, J.P.Collman, L.S.Hegsdus, J.R.Norton and R.G.Finke, University Science Book.

7. The Organometallic Chemistry of the transition metals, R.H.Crabtree, John Wiley,(1988).

M.Sc. CHEMISTRY – SEMESTER III
INORGANIC CHEMISTRY
PAPER- XIV(i)

BIO-INORGANIC CHEMISTRY–I

Unit I: Metal Ions in Biological System

Occurrence and availability of Inorganic elements in organisms, transport and storage of Inorganic elements, Dose response of an element, biological function of inorganic elements, beneficial and toxic elements, essential and trace metals.

Unit II: Metal Storage, Transport and Biomineralization

Sidrophore, phytosidrophores, ferretin, fransferrin, hemosiderine, biomineralization, assembly of advanced materials e.g. calcium phosphate, calcium carbonate, iron biominerals.

Unit III: Uptake, Transport and Storage of Inorganic Molecule

Oxygen transport and storage through hemoglobin and myglobin, Alternative oxygen transport in lower organisms.
Photosynthesis: Photochemistry, absorption spectra of photosynthetic pigments, photophosphorylation - energy conversion process.

Unit IV: Transport and Function of Alkali and Alkaline Earth Metals

Roll of Alkali and alkaline earth metals in neuro sensation. Ion Channels, ion pumps, magnesium catalysis of phosphate, ubiquitous regulatory role of calcium.

Books Suggested:

1. Principles of Bioinorganic Chemistry S.J. Lippard and J. M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J. S. Valentine, University Science Books.
3. Inorganic Biochemistry, Vols. I and II, Ed. G. L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols. 18 and 38, Ed. J.J. Lippard, Wiley.
5. Inorganic Chemistry, James E. Huheey, Harper International, Sixth Edition (1983).

M.Sc. CHEMISTRY – SEMESTER III
INORGANIC CHEMISTRY LAB-III

1. Preparations

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

a. Synthesis and thermal analysis of group 2 metal oxalate hydrate.
b. Synthesis of metal acetylacetonate; magnetic, IR, NMR studies.
c. Magnetic moment of $Cu(acac)_2.H_2O$.
d. *Cis*- and *Trans*-$[Co(en)_2Cl_2$

2. Spectrophotometric Determination

a. Mn/Cr/V in steel sample
b. Mo/W/V/U/ by extractive spectrophotometric method
c. $F^-/NO_2^-/PO_4^{3-}$
d. Iron-phenanthroline complex: Jobs method of continous variations.
e. Zr-Alizarin Red-S complex: Mole ratio method.
f. Cu-Ethylenediamine complex:Slope-Ratio Method**.**

3. Chromatographic Separations

(a) Cd and Zn

M.Sc. CHEMISTRY – SEMESTER III
MATERIALS CHEMISTRY
PAPER XI-(ii)

CONVENTIONAL CERAMICS

Unit I: A Functional Ceramics

General concepts, oxide and non-oxide ceramics- functions and applications; microstructure of ceramics; grain boundaries in ceramics, significance and their types, fabrication of polycrystalline ceramics- general aspect, brief treatment of synthesis of powders, forming processes, hot pressing, hot isostatic pressing.

B <u>Structural Ceramics and their Properties</u>

oxide ceramics- classification and general characteristics, non-oxide ceramics- classification and general characteristics, general aspects and characteristics of alumina, zircona, silicon nitride, silicon carbide, electronic configuration of atoms, bonding, Polymorphic forms and transformations, Physical , thermal, electrical, magnetic properties of ceramics.

Unit II: Ceramic Insulators

Introduction, general aspects of linear dielectrics; glass- different types of glasses and their characteristics, selection criteria for glass insulators, important glass compositions and their thermal mechanical and electrical characteristics and applications, glass insulating films, thin and thick films- composition and application, sealing glass- composition and applications.Procelain: triaxial porcelain- composition and application, non feldspathic porclains- compositions and applications.

Unit III: A. Ceramic Capacitors

Significance of capacitors, history of development, ferroelectricity and capacitors,. Basic capacitor materials- porcelain and steatite, rutile, barium titanate, solid solutions, fine grained materials, additives, relaxor dielectrics; classification of ceramic capacitors,- thick film capacitors, single layer discrete capacitors, multi-layer capacitors.

B. Basic multi-layer fabrication methods- lamination, stacking,spray deposition, build up process, electrode alloys; Barrier layer capacitors- composition, fabrication, characteristic, applications; capacitor performance parameters.

Unit IV: Aerogel

Introduction, Production of Aerogels, silica aerogels, organic aerogels, drying, structural investigations- aerogel structure, thermal and infrared optical properties and mechanical properties, applications.

Books Suggested:

1. Introduction to Fine ceramics by Noburu Ichinose (ed.) John Wiley and Sons., New York (1987)
2. Ceramic Materials for Electronics – R.C. Buchanan (ed.) Marcel Deller, New York (1991)
3. Chemical Processing of Ceramics by Burtrand I. Lee, Edward J. A. Pope (ed) Marcel Deller, New York
4. Modern Ceramic Engineering, Properties, Processing and Use in design, By David W. Richerson, Marcel Deller, New York.

M.Sc. CHEMISTRY – SEMESTER III
MATERIALS CHEMISTRY
PAPER-XII (ii)

BASIC CONCEPTS OF CRYSTALLOGRAPHY AND CRYSTAL STRUCTURES

Unit I: Crystal Lattice and Unit Cell **Lecturers: 10**

Unit cell and Crystal lattices, brief concept of molecular symmetry, concept of Symmetry in crystal systems, ,Herman Mauguin notation for symmetry elements in crystal systems, representation of screw axis and glide planes ,restriction of symmetry elements in crystals systems, representation of lattice planes and directions , Bravias lattices, concept of Miller indices and Weiss indices ,hexagonal crystal system, Determination of miller indices in hexagonal systems, planes of form in crystals, zone rule ,possible combination of rotational symmetries, determination of d spacing in crystals.

Unit II: Point Groups and Space Groups in Crystal Systems **Lecturers :10**

Point groups in crystals systems, Herman maugiun notation of point groups in crystal systems, centrosymmetric and non centrosymmetric point groups, representation of point groups in crystallography, Concept of space groups , structural elucidation of the following space groups: P1,C2,C2/m,$P222_1$, $I4_1$,determination of atomic coordinates and special positions of space groups ,systematic absent reflections, space group and crystal structure of perovskite (ABO_3)

Unit III: Packing in Crystals Structures **Lecturers :15**

Cubic close packing, hexagonal close packing ,packing of ions ,alloys and molecular structures atomic coordinates and nomenclature ,structural relationships ,polyhedral representation of crystal systems ,packing of structures in terms of the distribution of tetrahedral sites ,octahedral sites and packing ions .Structural elucidation and distribution of interstitial sites in hcp structures : AX type - wurtzite (ZnS), nickel arsenide (NiAs);AX_2 type -rutile (TiO_2) cadmium Iodide (CdI_2),Structural elucidation and distribution of interstitial sites in ccp structures : AX type - rock salt (NaCl), sphalerite (ZnS), AX_2 type - cadmium chloride ($CdCl_2$), antifluorite(Na_2O), fluorite(CaF_2), classification and structures of silicates and spinels.

Unit IV: Preparation of Single Crystals **Lecturers :10**

Czochralski method, Bridgman and stock Barger method, zone melting, flux method, Verneuli method ,vapor phase transport ,hydrothermal methods, high pressure hydrothermal methods vapour phase transport comparison of the different methods ,dry high pressure methods, preparation of nanophase single materials by hydrothermal, microwave- and microwave-solvothermal methods, concept of epitaxial growth factors effecting growth of single crystal structures

Books Suggested:

1. Solid state Chemistry by A.R.West (Wiley).
2. Introduction to crystallography by D.P Sands And W.A. Benjamin.
3. Understanding solids :The science of materials by Richard Tilley (Wiley).

M.Sc. CHEMISTRY – SEMESTER III
MATERIALS CHEMISTRY
Paper XIII (ii)

POLYMER CHEMISTRY AND TECHNOLOGY

Unit I: Polymer Physics

Polymer Molecules, Conformation and Molecular Dimensions of Polymer Molecules, Properties of Isolated Polymer Molecules, Elasticity and Swelling of Polymer Gels, Molecular Motion of Polymers in Dilute Solutions, Amorphous Polymers, Structure of Amorphous Phase in Bulk Polymers, Mobility in Polymers, Glass Transition- Measurement of T_g, Effect of Various Parameters on T_g, Theoretical Interpretations, Crystallinity in Polymers, Determination of Degree of Crystallinity, Two Phase Structure of Semi-Crystalline Polymers and its Characterization and Correlation with Properties, Crystal Morphologies: Extended Chain Crystals, Chain Folding, Lamellae, Spherulite, Melting: Determination of Polymer Melting Point, The Effect of Various Parameters on Melting, Mechanical Properties: Stress-Strain Properties, Yield Behavior, Breaking Phenomena

Unit II: Polymer Characterization

Thermodynamics of Polymer Solutions, Flory-Huggins and Lattice Theory of Polymer Solution, Entropy and Enthalpy of Mixing, Theta Temperature, Molecular Weight and Molecular Dimensions by Osmometry, Light Scattering, Viscometry and Gel Permeation Chromatography, Thermal Analysis of Polymers: Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA) and Differential Thermal Analysis (DTA), Polymer Degradation and Stabilization

Unit III: Polymer Rheology

Definition of Rheology, Geometry of Deformation, Newtonian and Non-Newtonian Behaviors, Measurement of Rheological Properties, Power Law, Free Volume Theory of Polymer Fluidity, Dynamic Flow Behavior, Time-Dependent Fluid Responses, Viscoelastic Properties, Mechanical Models of a Viscoelastic Material, Stress Relaxation, Creep and Relaxation behavior of Plastics

Unit IV: Polymer Technology 1

Polymers of Commercial Importance, Mass Polymerization: Solution, Emulsion and Suspension Polymerizations, Ziegler Natta Coordination Polymerization, Methathesis Polymerization

Books Suggested:

1. Text Book of Polymer Science By F. W. Billmeyer
2. Introduction to Polymers by R. J. Young and P. A. Lovell
3. Polymer Chemistry by G. Challa
4. Polymers: Chemistry and Physics of Modern Materials by JMG Cowie
5. Principles of Polymerization by George Odian

M.Sc. CHEMISTRY – SEMESTER III
MATERIALS CHEMISTRY
PAPER-XIV(ii)

CHEMISTRY OF ADVANCED MATERIALS

Unit I: Composite Materials **Lectures 12**

Definition, General characteristics and classification, Matrix, Fillers, Types of matrix and fillers, Division of composites based on filler reinforcement pattern, Dispersion strengthed composites, Al-based (SAP) and Ni-based fibrous composites, Critical length of fibers ,Effect of reinforcement pattern of fillers on mechanical properties of fibrous composites, types of fillers, Non-metallic and metallic composites:- Epoxy, Phenol, formaldehyde, Polyurethane based composites, Al, Mg, Ti, Ni- based fibrous composites, Applications of Composites.

Unit II: Organic Conductors, Magnets & Super Conductors **Lectures 8**

Introduction: Electrically conducting organic solids, Conjugate system: Polyacetylene, Polyaniline, Polypyrole, Polythiophene etc. Historical background general(Electron transfer salt based conductors, superconductors and Magnets) One dimensional conductors: Salts of partially oxidized Tetra cyano complexes, Quasi one and two dimensional conductors (TMTSF, BEDT-TTF, salts) tree dimensional conductors and superconductors fullerides and alkali metal doped fullerides. Para and Ferromagnetic conductors and superconductors.

Unit III: Mesoprphic Materials (Liquid Crystal) **Lectures 12**

Mesomorphic behaviour, thermotropic liquid crystal, positional rdr, bond orientational order, nematic and smectic mesophases, mectic-nematic transition and clearing temperature, homotropic, planer and schlieren textures, twisted nematics, chiral nematics, moleculararrangement in smectic. A and C smectic phases, optical properties of liquid crystals, dielectric susceptibility and dielectric constant. Optical storage memory switches and sensors.

Unit IV: High Tc Materials **Lectures 14**

Defect pervoskites, high Tc 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, Superconductivity state, heat capacity, coherence length, elastic constants,position life times, microwave absorption pairing and multigap structure in high Tc materials, application of high Tc materials.

Books Suggested

1. Principle of solid state, H. V. Keer, Wiley Eastern.
2. Handbook of Liquid Crystals, Kelkar and Hatz
3. Thermotropic Liquid Crystals, Ed., G. W. Groy, Chemie Verlog, John Wiley.
4. Materials Science by Azimasov (Mir Publications)

5. Chemistry of Advanced Materials by Leonard V.Interrante and M.J.Hampden-Smith

M.Sc. CHEMISTRY – SEMESTER III
MATERIALS CHEMISTRY LAB-III

1. Prepare PMMA by suspension polymerization method and determine its molecular weight by viscometry.

2. Prepare polystyrene by emulsion polymerization method and determine its viscosity average molecular weight.

3. Prepare polyvinyl acetate by solution polymerization and synthesize polyvinyl alcohol from the prepared polymer by hydrolysis.

4. Prepare a copolymer of styrene and methylmethacrylate by solution method.

5. Grow single crystals from the aqueous solutions of: (a) potash alum and (b) Rochelle salt.

6. Determine the bulk density, porosity and specific gravity of the sintered clay piece.

7. Determine the band gap energy of Ge and Si crystals.

8. Study the kinetics of high temperature oxidation of mild steel.

9. Synthesize cobalt ferrite ($CoFe_2O_4$) inverse spinel by chemical route.

10. Measure the dielectric constant of Barium titanate, $BaTiO_3$.

Books Suggested:

1. Crystal and crystal growing by Alam Holden and Phylis Singer
2. A laboratory manual of Polymers by S.M.Ashraf, Sharif Ahmad and Ufana Riaz
3. Practical course in Polymer Chemistry by Pinner
4. Experiments in Polymer Chemistry by Billmeyer

M.Sc. CHEMISTRY – SEMESTER III
ORGANIC CHEMISTRY
PAPER – XI(iii)

MEDICINAL CHEMISTRY

Unit I: Drug Design

Development of new drugs, procedures followed in drug design, concept of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship (QSAR). History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).

Unit II: Antineoplastic Agents

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors.
Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil mustards and 6-mercaptopurine.
Recent development in cancer chemotherapy. Hormone and Natural products.

Unit III: Local Antiinfective Drugs

Introduction and general mode of action.
Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econozole, griseofulvin, chloroquin and primaquin.

Unit IV: Antibiotics

Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis.
Synthesis of Penicillin G, Penicillin V, Ampicillin, Amoxicillin, Chloramphenicol, Cephalosporin, Tetracycline and Streptomycin.

Books Suggested:

1. Introduction to Medicinal Chemistry, A. Gringauge, Wiley-VCH.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Edited by J.N. Delgado and W. A. Remers, J.B. Lipincott Company.
3. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
4. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley & Sons Ltd.
5. A Text Book of Medicinal Chemistry, Vol-I and Vol-II, Surendra N. Pandeya, SG Publishers.

6. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International Publishers.
7. Medicinal Chemistry, Ashutosh Kar, New Age International Publishers.
8. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
9. Burger's Medicinal Chemistry and Drug Discovery, Vol. I-V, Edited by M.E. Wolff, John Wiley & Sons Ltd.

M.Sc. CHEMISTRY – SEMESTER III
ORGANIC CHEMISTRY
PAPER-XII(iii)

CHEMISTRY OF NATURAL PRODUCTS - I

Unit I: Alkaloids

Introduction, occurrence, nomenclature, physiological actions, isolation, methods of structural determination.
Structure determination and synthesis of the following alkaloids:
Atropine, Coniine. Ephedrine, Morphine, Nicotine and Quinine.

Unit II: Terpenoids and Carotenoids

Introduction, occurrence, classification, nomenclature, isolation, isoprene rule, methods of structural determination.
Structure determination and synthesis of the following molecules:
β-Carotene, Citral, Phytol, Terpeneol and Zingiberene.

Unit III: Plants Pigments

Introduction, occurrence, nomenclature, isolation, methods of structural determination, synthesis of Apigenin, Cyanidine, Cyaniding-7-Arabinoside, Diadzein, Luteolin, Myrcetin, Quercetin, Quercetin-3-Glucoside and vitexin.

Unit IV: Steroids

Introduction, occurrence, nomenclature, isolation, basic skeleton, Dicl's hydrocarbon and stereochemistry, methods of structural determination.
Structure determination and synthesis of the following steroids:
Aldosterone, Androsterone, Cholesterol, Estrone, Progesterone and Testosterone.

Books Suggested:

1. I.L. Finar, Organic chemistry, Vol. II, ELBS Publications, UK.
2. J. Mann, R.S. Devison, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Natural products chemistry and biological significance, Longman Publisher, Essex, UK.
3. B.A. Bohm, Introduction to flavonoids, Harwood Acad. Publishers, USA.

M.Sc. CHEMISTRY – SEMESTER III
ORGANIC CHEMISTRY
PAPER-XIII(iii)

METHODS IN ORGANIC SYNTHESIS

Unit I: Formation of new C-C single bonds

Generation of thermodynamic and kinetic enolates Alkylation of enolates and enamines,. Silyl enol ethers, Conjugate addition reactions of enolates and enamines,Michael Addition, Aldol reactions, Mukaiyama aldol reactions and stereoselective aldol reactions, Preparation and application of Gillman's reagent(lithium organocuprate).

Unit II: Rearrangements

General mechanistic considerations- nature of migration, migratory aptitude, memory effects, Cationotropic and Anionotropic rearrangements, A detailed study of the following rearrangements: Pinacol-Pinacolone, Wagner-Meerwein, Demjanov, Dienone-Phenol, Benzilic acid,Favorskii, Arndt-Eistert, Neber, Hoffmann, Losson, Curtius, Schmidt,Beckmann, Baeyer-Villiger rearrangements.

Unit III: Oxidations

Oxidation of hydrocarbons (Alkanes,alkenes,and aromatic hydrocarbons) : Selenium dioxide, DDQ,Etard's and related reaction, epoxidation,Sharpless asymmetric epoxidation, kinetic resolution of chiral allylic alcohol,Prevost and Woodward dihydroxilation, Sharpless asymmetric dihydroxilation, Asymmetric amino-hydroxilation.Palladium catalyzed oxidation of alkenes.

Oxidation of alcohols: Chromium reagents,oxidation via alkoxysulfonium salts (DCC & Swern oxidation), manganese reagents(MnO_2,PCC,Jones reagent,Collins reagent) other metal based oxidants(Ag_2CO_3, RuO_4 and $Tl(NO_3)_3$) oxidative cleavage of C-C bonds.Oxidation of alpha,beta-unsaturated ketones.

Unit IV: Reductions

Catalytic hydrogenation: Of Alkenes, alkynes, aromatic compounds,nitrile,oximes and nitro compounds.

Heterogeneous and homogeneous catalysis, stereochemistry and mechanism, Induced asymmetry via homogeneous hydrogenation. Reduction by desolving metals: Of carbonyl compounds,aromatic compounds(Birch reduction), Alkynes and conjugated dienes.

Hydride transfer reagents:Aluminium alkoxides(Meerwein-Pondorff-Verly reduction), Lithium aluminium hydride,sodium borohydride,sodium cyano borohydrideand Diisobutyl aluminium hydride(DIBAL-H) Wolff-Kishner's reduction, reductions with diimides and trialkyl tin hydrides.

Enzymetic reductions

Books Suggested:

1. Smith M.B & March,J. Advanced organic chemistry sixth edition, John Wiley & Sons (2007).

2. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).

3. Carruthers,W. and Coldham,I. Modern methods of organic synthesis, Cambridge University Press(2004).

4. Eliel, E. L. Stereochemistry of Carbon Compounds Textbook Publishers (2003).

5. Bruckner,R. Advanced organic chemistry Elsevier(2002)

6. Clayden, Greeves, Warren & Wothers. Organic chemistry Oxford university press(2001)

7. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981).

M.Sc. CHEMISTRY – SEMESTER III
ORGANIC CHEMISTRY
PAPER-XIV(iii)

APPLICATIONS OF SPECTROSCOPY - I

Unit I: Ultraviolet and Visible Spectroscopy

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

Unit II: Infra red Spectroscopy

Instrumentation and sample handling.

Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effects of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

Unit III: Nuclear Magnetic Resonance Spectroscopy

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nulei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra- nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-F, P.

Books Suggested:

1. Carruthers, W, *Modern Methods of Organic Synthesis* Cambridge University Press.

2. Kemp, W, *Organic Spectroscopy* , W.H. Freeman & Co.

3. R. M. Silverstein, G. C. Bassler and T. C. Morrill, *Spectroscopic Identification of Organic Compounds*, John Wiley & Sons.

M.Sc. CHEMISTRY – SEMESTER III
ORGANIC CHEMISTRY LAB - III

1. Isolation of Natural Products

i. Isolation of caffeine from tea leaves
ii. Isolation of piperine from black pepper
iii. Isolation of beta-carotene from carrots
iv. Isolation of lycopene from tomato

2. Small scale organic synthesis using some of the following reactions.

i. Sandmeyer reaction
ii. Friedel Crafts reaction
iii. Diazotisation reactions
iv. Diels-Alder reaction
v. Aromativ electrophilc substitution reaction

3. UV and IR spectra of simple compounds

M.Sc. CHEMISTRY – SEMESTER III
PHYSICAL CHEMISTRY
PAPER-XI(iv)

NUCLEAR CHEMISTRY

45 Lectures

Unit I:

Natural radioactivity, half life, mean life. Units of radioactivity, the natural radioactive series, secular and transient equilibrium.

The nuclear atom, neutron-proton model of the atom, isotopes and their separation, neutron decay, β-spectrum, the neutrino, electron capture and internal conversion; nuclear stability, stability lines, exotic nuclei.

Standard α, β, γ and neutron laboratory sources.

Nuclear sizes, binding energy per nucleon, nuclear saturation, liquid drop model leading to Weizsacker formula.

Regions of fission and fusion.

For short study only: Magic numbers, shell model, ground state nuclear spins. Qualitative idea of collective models.

Nuclear scattering and reactions, cross-sections, units, phase shifts, Resonance, Breit-Wigner formula. Qualitative idea of Bohr's picture of a nuclear reaction.

Qualitative idea of the nucleon-nucleon and the complex nucleon-nucleon potential (the optical model). Different types of reactions, notation. Nuclear reaction cycles in stars, the p-p chain and the C-N cycle. **[11L]**

Unit II:

Artificial radioactivity, radioactive isotopes of the elements. The Szilard-Chalmers process. Preparation of suitable compounds containing ^{35}S and ^{131}I.

Slow neutron absorption in nuclei. Discovery of induced fission its important features. Discovery of spontaneous fission.

Broad ideas of research reactors, power reactors. Recovery of unused fuel and waste disposal. Broad idea of Breeder reactors. Broad sketch of a fusion reactor.

Metallurgy of U and Th. Enrichment of Uranium, separation of heavy water from ordinary water.

Production of the Trans-Uranic elements. A somewhat detailed study of Pu.

[12L]

Unit III:

Energy loss suffered by charged particles in traversing matter-excitation, ionisation, Bremsshtrahlung and Cerenkov radiation.

Attenuation of γ-rays in traversing matter-photoelectric effect, Compton effect and pair production.

Instruments for detection and measurement of charged particles and neutrons-G.M. counter, solid state detectors and neutron counters. Cloud chamber.

Instruments for γ-rays-scintillation counters.

A broad idea of counting and scaling circuits.

Shielding of charged particles, γ-rays and neutrons.

Van de Graaff and heavy ion beam accelerators. Cyclotron. Very broad idea of Synchrotron principle leading to the era of super-energy machines. Electron Synchrotron and Synchrotron radiation.

Damage caused by nuclear radiations to inorganic crystals and plastics. Effect of nuclear radiations on living systems; damage and the preventive measures.

Applications of nuclear chemistry to biology, medicine, agriculture, industry etc. Radio-dating of wood and Pb-containing minerals. **[12L]**

Unit IV: **Some Applications to Chemistry**

Finding the elements in a mixture by activation analysis, extraction of radionuclides and transuranic elements by use of carriers. Study of reaction mechanisms like esterification, hydrolysis, oxidation of CO in the presence of MnO, study of PCl_5 with respect to the presence of the last two chlorine atoms and structure of the thiosulphate ion.

Radiometric titration including radiometric indicators.

Brief introduction to radio-chromatography. Direct isotope dilution analysis and inverse isotope dilution analysis.

Short Study of:

Selection rules for γ-emission (or absorption), Nuclear isomerism, PIXE, Pair production chemistry, Muon chemistry, Mössbauer effect, Cow and Milk system.

[10L]

Books Recommended

1. G. Friedlander, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry, John Wiley (1981).
2. G. Choppin, J. O. Liljenzin and J. Rydberg, Radiochemistry and nuclear chemistry, Butterworth (1996).
3. H. J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern Ltd. (1995).
4. B. K. Sharma, Nuclear and Radiation Chemistry, Krishna Publication.
5. D. D. Sood, A.V.R. Reddy and N. Ramamoorthy, Fundamentals of Radiochemitry, Indian Association of Nuclear Chemistry & Allied Scientists (2004).

M.Sc. CHEMISTRY – SEMESTER III
PHYSICAL CHEMISTRY
PAPER-XII(iv)

ADVANCED SOLID STATE CHEMISTRY

45 Lectures

Unit I: Concepts of Solids [12L]

Crystalline and Amorphous Solid, Unit cell, Summary of crystal lattices, Reciprocal lattice, Bonding & packing in crystals, Lattice planes, Symmetry elements, Space lattice, Glide planes, Screw Axis, Point groups and notations of 222, mm2 and mmm point groups, space groups and elucidations of representing point groups; viz. Monoclinic C2, Orthorhombic $p222_1$ and Tetragonal $I4_1$.

Unit II: Crystal Defects and Non-Stoichiometry [10L]

Perfect and imperfect crystals, Intrinsic and extrinsic defects- point defects, line defects and plane defects, Schottky and Frenkel defects, Thermodynamics of Schottky and Frenkel defect formation, Colour centers, Non-stoichiometry and calculations.

Unit III: Structures of Solids [8L]

Perovskite structure (e.g. $CaTiO_3$ and $BaTiO_3$), Spinel structure (e.g. $MgAl_2O_4$), Rutile TiO_2 structure, Rock salt NaCl structure, Sphalerite and Wurtzite structures of ZnS, K_2NiF_4 (e.g. Sr_2TiO_4) and β-K_2SO_4 (e.g. Ba_2TiO_4) structures.

Unit IV: Properties of Solids [Total = 15L]

(a) Magnetic Properties: Classification of materials, Line of forces, Effect of temperature, Magnetic moment calculations, Ferro- and antiferromagnetic ordering, Dependence of magnetic properties on size, Magnetic domains and Hysteresis. **[5L]**

(b) Electrical Properties: Dielectric materials, Dielectric properties (dielectric constant and dielectric loss), Dependence of dielectric properties on size, Polarizability, Concepts of ferroelectricity, Pyroelectricity and Piezoelectricity. **[5L]**

(c) Electronic Properties: Metals, Insulators, Semiconductors and Superconductors, Density of states, Origin of bands, E-k diagrams, Bonding in solids, Band theory, Intrinsic and extrinsic semiconductors p-n junction. **[5L]**

Books Suggested:

1. Solid State Chemistry and its applications, Anthony R. West, John Wiley & Sons.
2. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.
3. Solid State Chemistry, Lesley Smart and Elaine Moore, Chapman & Hall.
4. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalakrishnan, Cambridge University Press.
5. Principles of the Solid State, H. V. Keer, New Age International Publishers.
6. Solid State Chemistry, D. K. Chakrabarty, New Age International Publishers.
7. Solid State Chemistry Techniques, A. K. Cheetham and Peter Day, Oxford Science Publications.

M.Sc. CHEMISTRY – SEMESTER III
PHYSICAL CHEMISTRY
PAPER-XIII (iv)

ELECTROCHEMISTRY

45 Lectures

Unit I: Electrolyte Solution : [14L]

Structure of water, effect of an ion on the structure of water, solvation number, activity, activity coefficients and ion – ion interactions, physical significance of activity coefficient of an electrolyte, determination of mean ionic activity coefficient by freezing point depression and e.m.f. measurement methods, derivation of Debye – Hückel – Onsager equation, limiting law, electro – chemical potential.

Unit II: Transport Phenomena: [12L]

Diffusion coefficients, Fick's first law of steady – state diffusion, Fick's second law of non – steady state diffusion, relation between diffusion coefficient and mean free path, relation between thermal conductivity / viscosity and mean free path of a perfect gas, Einstein's relation between diffusion coefficient and absolute mobility of ions, Stokes – Einstein equation, Nernst – Einstein equation, Nernst – Planck flux equation.

Unit III: Adsorption and Electrical Double Layer: [10L]

Electrical double layer, thermodynamics of electrified interfaces, derivation of electrocapillary equation, determination of charge density on electrode, electrical capacitance of the interface.

Unit IV: Electrical Double Layer Models: [9L]

Structure of electrified interfaces (Electrical double layer models), Helmholtz – Perrin, Gouy – Chapman, stern, Graham – Devanathan – Mottwatts, Tobin, Bockris, Devanathan models.

Book Suggested:

1. J. O. M. Blockris and A. K. N. Reddy : Modern Electrochemistry, Vol. 1 : Ionics, 2nd Ed., Plenum Press, New York, 1998.

2. J. O. M. Blockris and A. K. N. Reddy and M. Gamboa – Aldeco : Modern Electrochemistry, Vol. 2A, Fundamentals of Electrodics, 2nd Ed. Plenum Press, New York, 2000.

3. A. J. Bard and L. R. Faulkner, Electrochemical Methods : Fundamentals and Applications, 2nd Ed., John Wiley & Sons : New York, 2002.

M.Sc. CHEMISTRY – SEMESTER III *(wef 2012-2013)*
PHYSICAL CHEMISTRY
PAPER – XIV (iv)

MOLECULAR REACTION DYNAMICS AND CATALYSIS

45 Lectures

Unit I: THEORIES OF REACTION RATES [15L]

Collision theory, Potential energy surfaces (basic idea), generalized kinetic theory, rate theories based on thermodynamics, conventional transition state theory (CTST) - equilibrium hypothesis, statistical mechanics and chemical equilibrium, derivations of the rate equations, applications of CTST - reaction between atoms, thermodynamic formulation of conventional transition state theory.

Unit II: ELEMENTARY REACTIONS IN SOLUTION [11L]

Factors determining reaction rates in solution, collision in solution, encounter, Franck - Rabinowitch effect, reaction between ions, single-sphere and double-sphere model for activated complex, influence of ionic strength (primary salt effects),

Unit III: ACID-BASE CATALYSIS [10L]

General catalytic mechanisms, fast pre-equilibrium: Arrhenius intermediates, Steady-state conditions: van't Hoff intermediates, activation energies of catalyzed reactions, acid-base catalysis, General and Specific acid-base catalysis, mechanisms of acid-base catalysis - reaction between acetone and iodine, catalytic activity and acid - base strength, salt effects, acidity functions.

Unit IV: ENZYME CATALYSIS [9L]

Enzyme catalysis, Simple enzyme mechanisms, single-intermediate mechanism, influence of substrate concentration, Michaelis-Menten equation- single and double intermediates, Lineweaver - Burk plot, Eadie-Hofstee plots, Complex enzyme mechanism, King-Altman algorithm (Edward L. King and Carl Altman, *J. Phys. Chem.* **60(10)**, 1375-1378, 1956) for working out the kinetics of complex enzyme reactions, Enzyme inhibition-reversibility and products inhibition, influence of pH and temperature.

BOOKS RECOMMEDED:

1. Chemical kinetics by K.J. Laidler, Third Edition, 1987.

2. Chemical Kinetics by L. Wilkinson.

3. Pilling, M.J. & Seakins, P.W., Reaction Kinetics, Oxford University Press (1995).

4. Chemical kinetics and Reaction Mechanism by James H. Espenson, 2nd Ed., McGraw-Hill, 1995.

5. Physical Chemistry (Kinetics) by Horia Metiu, Taylor and Francis, New York (2006).

6. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).

7. Physical Chemistry by Gordon M. Barrow, McGraw-Hill.

8. Chemical Kinetics and Reaction Dynamics by Santosh K. Upadhyay, Anamaya Publishers, New Delhi, 2006.

9. Enzyme Kinetics by D.V. Roberts, Cambridge University Press, 1977.

10. Chemical Kinetics and Dynamics, J.I. Steinfeld, J.S. Francisco and W.L. Hase, 2nd Edition, Prentice Hall International, Inc., 1999.

11. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, by L. Arnaut, Sebastiao Formosinho, Hugh Burrows, Elsevier, 2007.

12. An Introduction to Chemical Kinetics, Margaret Robson Wright, John Wiley & Sons, Ltd., 2004.

13. Concepts of Modern Catalysis and Kinetics, I. Chorkendorff, J.W. Niemantsverdriet, Wiley-VCH, 2003.

M.Sc. CHEMISTRY – SEMESTER III
PHYSICAL CHEMISTRY LAB-III

1. Determine the molecular weight of the given polymer sample by viscosity method.

2. Determine the ionization constant of acetic acid by conductivity method.

3. Titrate using conductometer a moderately strong acid (salicylic/mandelic acid) by the
   (a) salt-line method
   (b) double alkali method.

4. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid against sodium hydroxide conductometrically.

5. Titrate a tribasic acid (phosphoric acid) against NaOH and $Ba(OH)_2$ conductometrically.

6. Carry out the following titrations conductometrically:
   (a) Magnesium sulphate against $BaCl_2$ and its reverse titration
   (b) HCl versus NH_4OH
   (c) Sodium oxalate against HCl.

7. Determine the rate constant of saponification of ethyl acetate at different temperatures and calculate the energy of activation of the reacton by conductivity method.

8. Find out the rate constant of acid-catalysed hydrolysis of sucrose by polarimeter.

9. Study the rate equation for mutarotation of D-glucose in water using polarimeter.

10. To determine the partial molar volumes of sodium chloride in water by density measurements. (Page 30 - Das & Behra).

11. To find the formula of the copper - ammine complex ion in aqueous solutions by partition method. (Page 108 - Das & Behra)

12. To determine the hydrolysis constant of aniline hydrochloride by partition method. (Page 113 - Das & Behra)

13. Titrate phosphoric acid potentiometrically against sodium hydroxide.

14. Titrate potentiometrically solutions of
   (a) KCl/ KBr/ KI;
   (b) mixture of KCl + KBr + KI and determine the composition of each component in the mixture.

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

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

17. Determine the hydrolysis constant of aniline hydrochloride by pH meter.

18. Determine potentiometrically the heat of reaction equilibrium constant and other thermodynamic functions for a given reaction such as:
    $Zn + Pb^{++} \Leftrightarrow Zn^{++} + Pb$

19. Determine the mean ionic activity coefficients of hydrochloric acid solutions at different concentrations by potentiometer.

20. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.

21. Determine the transport numbers of cations and anions in a solution of its salt by moving boundary method.

22. To determine the degree of ionization of sodium chloride at different concentrations of its aqueous solutions from the depression of freezing point measurements. (Page 45 - Das & Behra)

23. Estimation of Pb^{2+} and Cd^{2+}/Zn^{2+} and Ni^{2+} ions in a mixture of these ions by polarography.

24. Determination of dissolved oxygen in aqueons solution of organic solvents by polarography.

25. Determine the formula and overall stability constant of lead oxalate complex at 25° C by polarographic method.

26. To determine the rate constant of the acid hydrolysis of acetal by dilatometry at 298.15k. (Das & Behra)

27. Any other experiment(s) introduced during the year.

M.Sc. CHEMISTRY – SEMESTER IV
INORGANIC CHEMISTRY
PAPER- XV(i)

NMR SPECTROSCOPY AND LANTHANIDE SHIFT REAGENTS

48 Lectures

Unit I: Lanthanide Complexes of β-Diketones

Introduction, Overview of β-diketone ligands and types of complexes. Synthesis, Structural, Physical and Chemical properties. Volatile β-diketone complexes.

Unit II: Applications of Nuclear Magnetic Resonance Spectroscopy

1. Applications of spin-spin coupling to structure determination.
   (a) $Rh(\phi_3P)_3CI_3$
   (b) Diphosphate anion ($HP_2O_5^{3-}$)
   (c) SbF_5

2. Measurement of magnetic susceptibility by NMR.

3. NMR of paramagnetic transition metal ion complexes- Contact and Pseudo contact shifts. Contact shift andCovalency, Contact shifts in coordinated pyridine.

Unit III: Lanthanide Shift Reagents

Historical development and general principles. NMR of paramagnetic lanthanide complexes – Nature of the shift. The lanthanide shift reagents. Relative shifting and broadening abilities of the lanthanides. Hinckley's shift reagent. Effect of increasing coordination number of the lanthanide on the NMR spectra of added substrate.

Unit IV: NMR of Lanthanide Complexes

NMR of dia and paramagnetic lanthanide(III) complexes.

(a) Complexes containing N-donor ligands.
(b) Complexes of O-donors.
(c) Mixed-ligand complexes
(d) Complexes with varying coordinates.
(e) Study of NMR spectra of eight and ten-coordinated paramagnetic lanthanide complexes.
(f) Shift reagents as structural probes.
(g) Effect of aromatic solvents on the spectra of lanthanide complexes.

Books Suggested:

1. Physical Methods in Chemistry: by R.S. Drago.

2. NMR of Paramagnetic molecules-Principles and Applications, Edited by LaMar, Horrocks and Holm, Academic Press (N.Y.).

M.Sc. CHEMISTRY – SEMESTER IV
INORGANIC CHEMISTRY
PAPER-XVI(i)

STEREOCHEMISTRY AND METAL ION CATALYSIS

Unit I: Stereochemical Changes in Octahedral Complexes-I

Outer sphere orientations, reactions of geometrical and optical isomers SN^1 dissociation or SN^2 displacement mechanisms, stereochemistry of the acid and base hydrolysis of Co(III) complexes, optical inversion reactions of some Co(III) complexes.

Unit II: Stereochemical Changes in Octahedral Complexes-II

Isomerization reactions of octahedral complexes, recimerization of octahedral co(iii) complexes, salt, salt and solvent effects, photorecimization.

Unit III: Photochemical Reactions

Introduction, types of excitation, fate of excited molecules, quantum yield, types of photochemical reactions

Unit IV: Metal Ion Catalysis

Metal ion catalysis in acid-base reactions-hydrolysis, aldol condensation, carboxylation and decarboxylation, Metal ion catalysis in redox reactions autoxidation of organic substances.

Books Suggested:
Fundamental of photochemistry.

M.Sc. CHEMISTRY – SEMESTER IV
INORGANIC CHEMISTRY
PAPER- XVII(i)

ORGANOMETALLIC CHEMISTRY-II

Unit I: Fluxionality and Dynamic Equilibria

Fluxionality and dynamic equilibria, Fluxionality in tricarbonyl (Diene) Iron Complexes, Fluxionality in pi-Olefin complexes, Pi-allyl complexes, Tricarbonyl cyclooctatetraene (COT) metal complexes

Unit II: Distinctive organometallic Reactions

Distinctive organometallic Reactions - Nucleophilic and Electrophilic attack of co-ordinated ligands and elimination reactions, Oxidative – Addition reactions, Insertion reaction – at M-C bond & M-H bond, Transmetallation reaction and Cyclization reaction, , Ring Expansion reaction, Condensation reaction , Sigma-pi rearrangement reaction , Ligand & Metal exchange reactions.

Unit III: Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structure characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit IV: Homogeneous Catalysis

Catalytic applications of organometallic complexes - Alkene hydrogenation, Synthesis gas (H_2/CO), Hydroformylation, Mosanto-acetic acid process, Wacker- Schmidt process and Ziegler-Natta catalysis. Bioorganometallic chemistry and surface organometallic chemistry.

Books Suggested:

1. Metallo-organic Chemistry- Anthony J Pearson, John Wiley & Sons Inc, (1985).
2. Inorganic Chemistry – Principles of Structure & Reactivity, J E Huheey, Elllen A Keiter & Richard L Keiter, IV Edition (2005).
3. Introduction tom metal n-complex chemistry- M. Tsutsui, M.N. Levy, A. Nakamura, M.Ichikawa and K. Mori, Plenum Press, New York | Heme (1970).
4. Organometallic Chemistry - R. C. Mehrotra & A. Singh, Wiley Eastern Ltd. (2000).
5. Advanced Inorganic Chemistry - F.Albert Cotton, Geoffrey Wilkinson, Carlos A Murillo & Manfred Bochmann, VI Edition, John Wiley & Sons Inc (1999).

6. Infrared and Raman spectra of Inorganic & Coordination Compounds; Kazuo Nakamoto, IV Edition, John Wiley & Sons Inc (1986).

7. Chemistry of the elements, N.N. Greenwood and A. Earnshaw, Pergamon.

8. Comphrensive coordination chemistry Eds.: G. Wilkinson, R.D.Gillards and J.A. McCleverty, Pergamon.

M.Sc. CHEMISTRY – SEMESTER IV
INORGANIC CHEMISTRY
PAPER- XVIII(i)

BIO-INORGANIC CHEMISTRY – II

Unit I: Metallo-Proteins

Biological ligands for metal ions: Macrocycle, nucleobase, nucleotides and nucleic acids, coordination of metals by protein.
Heme and nonheme protein, oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanin, hemotherine.

Unit II: Metalloenzyme

Principle involved and role of various metals viz. Zn, Fe, Cu and Co; carboxy peptidase, carbonic anhydrase, Alcohol dehydrogenase, Zinc Fingures, other gene regulatory Zinc proteins, cobalomine, mutase activities of coenzyme B_{12}.

Unit III: Iron-Sulfur and other Non-Heme Proteins

Rubredoxine Structure and function of iron sulphur protein, cytochromes, cytochrpm P-450, oxygen transfer long distance electron transfer.

Unit IV: Application of Bioinorganic Chemistry

Medicinal and therapic; metal deficiency and disease, toxic effect of metals, metals used for diagnosis and chemotherapy, gold compound as Anti-Rheumatic agent.
Nitrogen cycle; biological nitrogen fixation, metalloenzyme in biological nitrogen cycle, molybdenum nitrogenase, other nitrogenase model.

Books Suggested:

1. Principles of Bioinorganic Chemistry S.J. Lippard and J. M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J. S. Valentine, University Science Books.
3. Inorganic Biochemistry, Vols. I and II, Ed. G. L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols. 18 and 38, Ed. J.J. Lippard, Wiley.
5. Inorganic Chemistry, James E. Huheey, Harper International, Sixth Edition (1983).

M.Sc. CHEMISTRY – SEMESTER IV
MATERIALS CHEMISTRY
PAPER-XV(ii)

TECHNICAL CERAMICS

Unit I: Piezoelectric and Optoelectric Ceramics

History of development, centrosymmetric and noncentrosymmetric (n.c.s.) crystals, polarization in n.c.s. crystals, piezoelectric ceramics, piezoelectric equations, definition of piezoelectric terms and their characteristics, poling of piezoelectric ceramics, dimensional changes, ferroelectric ceramics general features and applications.

Electroptic ceramics (e.o.c): general aspects, birefringence in e.o.c. Optical phase retardation, generation of various colours, Electroptic coefficients r and R, mode of application of e.o.c., characteristics required in e.o.c., composition systems- role of donars, acceptors and isovalent additives, processing and fabrication; loop in e.o.c. special features, intermediate polarization state, different types of hyteresis loop; electrochemical properties, piezoelectric deformation (extended treatment); applications.

Unit II: Ferrite Ceramics

Magnetic ferrite- general aspects, ferromagnetic, anti-ferromagnetic ordering in spinels, site preference in spinels, Garnet, magnetic moments and accupancy of A&B sites, various ferrite compositions and their magnetic properties. Processing of ferrites – extended treatment. Nonmicrowave ferrite compositions, their B/H other characteristics, applications; microwave ferrites – characteristics and applications.

Unit III: Ceramic Sensors

General aspects, intrinsic and extrinsic conductors,.NTC thermistors- History of development; NTC device construction principle, device types and dimensions, electrical properties, resistivity temperature behaviour, stability and sensitivity of thermal sensors, time constant and dissipation constant. Device chemistry - - dependence of B and resistivity upon composition.Factors affecting sensor performance, stability and life resistance shift r on aging, thermophysical properties of thermistor materials. NTC sensor applications, PTC thermistors, History of development, general applications, PTC thermistors – electrical behaviour, resistivity-temperature relationship, other electrical parameters, V-1 curve- important features. Device chemistry – role of dopant, isovalent, altervalent and barrier layer modifiers, sintering aids, curie temperature control.

Gas sensors- general aspects, self generating galvanic type oxygen sensors, construction, special features; modulating type gas sensors - general aspects, material requirements , temperature dependence of resistivity, its control.

Unit IV: Bioceramics

Bioceramics, Bioinert versus Biocompatible Materials, Partially stabilized Zirconia, Carbons and Carbon-composite ceramics, Mica glass ceramics, Bioactive ceramics-Bioactive glass:bone bonding, Conventional Bioactive glasses, Sol- GEL routes to

Bioactive glass, Problems of Longevity of implant use, Bioceramic composites, Composites based on HAP, Bone graft materials and applications.

Books Suggested:

1. Introduction to Fine ceramics by Noburu Ichinose (ed.) John Wiley and Sons., New York (1987)
2. Ceramic Materials for Electronics – R.C. Buchanan (ed.) Marcel Deller, New York (1991)
3. Chemical Processing of Ceramics by Burtrand I. Lee, Edward J. A. Pope (ed) Marcel Deller, New York
4. Chemistry of Advanced Materials, an overview (ed) By Leonard V. Interrante, Mark J .Hampden –Smith, John Wiley and Sons., New York

M.Sc. CHEMISTRY – SEMESTER IV
MATERIALS CHEMISTRY
PAPER-XVI (ii)

PROCESSING AND CHARACTERIZATION OF CRYSTAL STRUCTURES

Unit I: Preparation Of Thin Films Of Crystals **Lectures: 12**

Electrochemical methods**:** anodic oxidation, cathodic deposition, electro-less deposition**.** Chemical method: chemical vapour deposition, sol gel method, Langmuir Blodgett, photolithography Physical methods: cathode sputtering, magnetron sputtering, vacuum evaporation, molecular beam epitaxy, Application techniques: spin coating, flow coating dip coating and printing (screen printing, gravure printing, flexo printing and ink jet printing

Unit II: Preparation Of Solid Solutions **Lectures: 10**

General concepts on the requirement solid solution formation, substitution solid solutions, interstitial solid solution, Mechanism of complex solid solutions, Creation of cation , anion vacancies creation of interstitial of cations and anions, double substitution ,experimental techniques for studying solid solutions

Unit III: Chracterization Of Crystals Strucutres **Lectures: 10**

X-ray techniques: X-ray diffraction and Bragg Law, Diffraction under ideal and non-ideal condition, X-ray scattering and structure factor, X-ray diffractometer, X-ray data file analysis, Chemical analysis by emission (x-ray fluorescence), X-ray absorption techniques (AEFS,EXAFS)Single crystal X-ray diffraction ,different cameras and their special features Electron spectroscopic techniques; principles, instrumentation, data analysis and applications of UPS.XPS, AES , Electron loss energy spectroscopy, neutron diffraction

Unit IV: Elecron Microscopic and Thermal Chracterization of Crystals Strucutres
Lectures:15

Scanning Electron Microscopy – basic principle, instrumentation, electron specimen interaction, topographical and atomic number contrast, Transmission Electron Microscopy; practical aspect of microscopy, amplitude and phase contrast imaging, kinematical theory of image contrast, electron diffraction. Atomic Force Microscopy-basic principles, Atomic Force Microscopy modes, phase imaging, face curve, application of Atomic Force Microscopy; Thermal techniques: principles, instrumentation, data analysis and applications of DSC,TGA ,DTA and their special features

Books Suggested:

1. Introduction to Materials Chemistry by H.R. Allcock Wiley.
2. Elements of X-Ray Diffraction (3rd Edition) by B. D. Cullity and S.R. Stock.
3. Introduction to X-Ray Powder Diffractometry by Ron Jenkins and Robert Snyder.
4. Scanning and Transmission Electron Microscopy: An Introduction by Stanley L. Flegler, John W. Heckman Jr., and Karen L. Klomparens.

M.Sc. CHEMISTRY – SEMESTER IV
MATERIALS CHEMISTRY
PAPER-XVII (ii)

POLYMER TECHNOLOGY, PROCESSING AND SPECIALITY POLYMERS

.

Unit I: Polymer Technology - II

Additives for Plastics: Fillers, Plasticizers, Stabilizers, Lubricants, Flame Retardants, Foaming Agents, Crosslinking Agents,Manufacture, Properties and Applications of Major Thermoplastics and Thermosetting Polymers: PE, PP, PVC, PS, Polyamides, Polyesters, Phenolic Resins, Amino Resins and Epoxy Resins,Polymeric Coatings

Unit II: Polymer Processing

Classification of Polymer Processing, Simple Model Flows for Analyzing Processing Operations with Examples,Extrusion and Extruders, Calendaring, Film Blowing, Injection Molding, Blow Molding, Rotational, Transfer and Compression Molding, Vacuum Forming, Reaction Injection Molding

Unit III: Biopolymers

Structure, Functions and Properties of Naturally Occurring Polymers such as Proteins, Polysaccharides and DNA, Polymer Chemistry of Biological Processes, Synthetic Biopolymers, their Fabrication and Applications

Unit IV: Speciality Polymers

Conductive Polymers: Theory of Conduction, Synthesis and Applications of Conductive Polymers, Biodegradable Polymers, Biomaterials, Polymers in Medicine, Drug Delivery Systems, Recycling of Polymers

Books Suggested:

1. Text Book of Polymer Science By F. W. Billmeyer
2. Introduction to Polymers by R. J. Young and P. A. Lovell
3. Polymer Chemistry by G. Challa
4. Polymers: Chemistry and Physics of Modern Materials by JMG Cowie
5. Principles of Polymerization by George Odian.

M.Sc. CHEMISTRY – SEMESTER IV
MATERIALS CHEMISTRY
PAPER –XVIII (ii)

ELECTRONIC, ELECTRICAL, MAGNETIC AND OPTICAL PROPERTIES OF MATERIALS

Unit I: Electronic State in Solids **Lectures 12**

Free electron theory of standing and running waves, density of state, band theory, K. space and Brillionzones, band structures of metals, insulator and semi conductors, the concept of hole, extrinsic (impurity) semiconductors, Fermi energy, position of Fermi level, free carrier concentration in intrinsic and extrinsic semiconductors, application of semiconductors, application of semiconductors, I-VI compounds,II -IV compounds,III-V compounds

Unit II: Electrical Properties **Lectures 14**

Introduction, electron drift in an electrical field, relaxation time and mean free path, electrical conductivity of non degenerate and degenerate gases , specific conductance of conductor,Widemann-Franz-Lorentz law,electrical conductivity of metals and alloys., piezoelectric materials temperature dependence carrier mobility ,electrical conductivity of pure metal ,electrical conductivity of alloys

Unit III: Magnetic Poperties **Lectures 10**

Introduction: Classification of magnetic materials, diamagnetism, paragmagnetism, ferromagnetic anisotropy, ferromagnetic domains, origin of domain wall anti-ferromagnetism,antiferromagnetic, domains, ferrimagnetism, normal spinel's inverse spinels, ferromagnetic domain.

Unit IV: Optical Propeties **Lectures 10**

Introduction: Refractive index, dispersion, absorption birefringence, photoluminescence laser, nonlinear optical materials- non linear optical effect, second and third order molecular hyper polarisability and second order electric susceptibility materials for second and third order harmonic generation.

BOOKS RECOMMENDED

1. Solid state physics by Epifanov.
2. Materials Science by Anderson and lever.
3. Physical properties of materials by M.C.Lovel,A.J.Avery and M..W.Verjooon.

M.Sc. CHEMISTRY – SEMESTER IV
ORGANIC CHEMISTRY
PAPER – XV(iii)

ADVANCE MEDICINAL CHEMISTRY

Unit I: Pharmacokinetics and Pharmacodynamics

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry,

Unit II: Cardiovascular Drugs

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators.

Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapmil, methyldopa, atenolol, oxyprenolol.

Unit III: Psychoactive Drugs - The Chemotherapy of Mind

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs – the neuroleptics, antidepressants, butyrophenones, sernndipity and drug development, stereochemical aspects of psychotropic drugs.

Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide.

Unit IV: Antimicrobial Drugs

Quinolone, Mechanism of action, Non-benzoid nitro compounds, nitrofurans, parasitic diseases, Chemotherapy of maleria, 8 & 4-aminoquinolines, other antiprotozoal drugs, antifungal drugs, Imidazole compounds, mechanism of action of imidazoles, antihelmintics, antiviral chemotherapy.

Books Suggested:

1. Introduction to Medicinal Chemistry, A. Gringauge, Wiley-VCH.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Edited by J.N. Delgado and W. A. Remers, J.B. Lipincott Company.
3. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
4. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley & Sons Ltd.
5. A Text Book of Medicinal Chemistry, Vol-I and Vol-II, Surendra N. Pandeya, SG Publishers.
6. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International Publishers.
7. Medicinal Chemistry, Ashutosh Kar, New Age International Publishers.

8. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
9. Burger's Medicinal Chemistry and Drug Discovery, Vol. I-V, Edited by M.E. Wolff, John Wiley & Sons Ltd.

M.Sc. CHEMISTRY – SEMESTER IV
ORGANIC CHEMISTRY
PAPER-XVI(iii)

CHEMISTRY OF NATURAL PRODUCTS - II

Unit I: Proteins and Enzymes

Introduction, primary, secondary, tertiary and quaternary structures of proteins, degradation of amino acids, urea cycle, uric acid and ammonia formation.

Introduction of enzymes, structure and mechanisms of chymotrypsin, carboxypeptidase and lipases.

Unit II: Nucleic Acids

Introduction, structures and functions of DNA and RNAs (m-RNA, t-RNA, r-RNA), Chemical and enzymatic hydrolysis of DNA and RNAs, an overview of gene expression (replication, transcription and translation), genetic code (origin, Wobble hypothesis), genetic errors, mutation and carcinogenesis and recombinant DNA technology.

Unit III: Carbohydrates

Introduction, ADP, ATP, $FADH_2$, NADH, NADPH, TPP, coenzyme A, lipoic acid and biotin, glycolysis, citric acid cycle, oxidative phosphorylation (electron transport system), gluconeogenesis, C_4 pathway and pentose phosphate pathway.

Unit IV: Porphyrins

Introduction, types of chlorophylls, functions of hemoglobin and chlorophyll, structure and synthesis of hemoglobin and chlorophyll a.

Books Suggested:

1. L. Stryer, Biochemistry 4th Ed., W. H. Freeman & Co., USA.
2. Z. Zubay, Biochemistry, Addison-Wesley, USA.
3. A.L. Lehninger, Principles of biochemistry, W. H. Freeman & Co., USA.

M.Sc. CHEMISTRY – SEMESTER IV
ORGANIC CHEMISTRY
PAPER-XVII(iii)

ADVANCED METHODS IN ORGANIC SYNTHESIS AND PHOTOCHEMISTRY

Unit I: Advanced Organic synthesis

Phosphorous ylides (Wittig and related reactions.), Preparation and application of sulpher ylides, Comparison of action and reactivity of phosphorous and sulpher ylides, Preparation and uses of 1,3-dithiane in organic synthesis(.Umpolung), Formation of alkene by fragmentation reactions, Shapiro and bamford-Stevens reaction, Preparation and application of organosilicon reagents in organic synthesis, Organopalledium chemistry- Heck reaction, Stille,Suzuki and Negishi coupling, Schrock's molybdenum catalyst and Grubb's Ru catalyst for Alkene metathesis.

Unit II: Basic Principles of Photochemistry

Excited states and ground state, Singlet and triplet states. Forbidden transitions, Fate of the excited molecules: Jablonski Diagram, Fluorescence and phosphorescence, The determination of Photochemical mechanism and quantum yield.

Unit III: Photochemistry of Alkenes and Carbonyl Compounds

Cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3-, 1,4- and 1,5-dienes: Di-pie-methane rearrangement, Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic), α,β-unsaturated ketones; β,γ-unsaturated ketones; cyclohexenones (conjugated), Paterno–Buchi reactions.

Unit IV: Photochemistry of Aromatic Compounds

Isomerizations, skeletal isomerizations, and. Singlet oxygen reactions. Photo Fries rearrangement of ethers and anilides. Synthetic applications of Barton and Hoffman-Loeflller-Freytag reaction.

Books Suggested:

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. Smith M.B & March,J. Advanced organic chemistry sixth edition, John Wiley & Sons (2007).
5. Carruthers,W. and Coldham,I. Modern methods of organic synthesis, Cambridge University Press(2004).
6. Cox,A. and Camp,T. Introduction to Photochemistry, McGraw-Hill.
7. Turro,N.J. and Benjamin,W.A. Molecular Photochemistry.

M.Sc. CHEMISTRY – SEMESTER IV
ORGANIC CHEMISTRY
PAPER - XVIII(III)

APPLICATIONS OF SPECTROSCOPY - II

Unit I: Carbon-13 NMR Spectroscopy

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants.

Two dimention NMR spectroscopy- COSY, DEPT, and INADEQUATE techniques.

Unit II: Mass Spectrometry

Introduction, ion production-El, Cl, FD and FAB, factors effecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Unit III: ESR

Derivative curves, hyperfine splitting, g-value, ESR spectra of simple molecule.

Unit IV: Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)

Definition, deduction of absolute configuration, octant rule for ketones.

Books Suggested:

1. M. L. Martin, J. J. Delpeuch and G. J. Martin, Heyden.,*Practical NMR Spectroscopy*, *Spectrometric Identification of Organic Compounds*, John Wiley.
2. R. J. Abraham, J. Fisher and P. Loftus, *Introduction to NMR spectroscopy*, Wiley.
3. J. R. Dyer, *Application of Spectroscopy of Organic Compounds*, Prentice Hall.
4. D. H. Williams, I. Fleming, *Spectroscopic Methods in Organic Chemistry*, Tata McGraw-Hill.

M.Sc. CHEMISTRY – SEMESTER IV
PHYSICAL CHEMISTRY
PAPER-XV(iv)

QUANTUM CHEMISTRY

45 Lectures

Unit I: Some Exactly Solvable Problems [11L]

Postulates of Quantum Mechanics. Discussion of the solution of the Schrödinger equation to some model systems viz. free particle, the rigid rotor, the harmonic oscillator and the hydrogen atom (derivation only of eigenvalue in last two problems. The method to find the wave function is only sketched and result is given). Simple discussion of potential barrier (short study).

Unit II: Approximate Methods [12L]

The Variation theorem, linear variation principle. Time independent Perturbation theory (first order and non-degenerate), second order change of energy non-degenerate (without proof). Applications of variation method and perturbation theory to Helium atom. Only a brief sketch of time dependent perturbation theory. Formula of the Golden rule written down (without proof). Some simple applications indicated (without proof).

Unit III: Angular Momentum, Spin and Electronic Structure [12L]

Angular momentum operators, Eigen values and eigen functions, addition of angular momenta, 6j and 9j symbols (without proofs), spin, Antisymmetry and Pauli Exclusion Principle. Electronic configuration, atomic state, Russell-Saunders coupling schemes, term separation energies of the p^n configuration, magnetic effects; spin orbit coupling and Zeeman splitting, introduction to the method of self-consistent field.

Unit IV: Molecular Orbital Theory [10L]

Hybridization & valence MO's of H_2O, NH_3 and CH_4. Huckel Molecular Orbital Theory of conjugated systems. Delocalization energy, electron density, bond order. Application of HMO to ethylene, butadiene, cyclopropenyl radical & benzene (only qualitative discussion for benzene).

Books Suggested:

1. I. L. Levine, Quantum Chemistry 5th Ed. Prentice Hall Inc. New Jersy (2000).
2. T. Engel and P. Reid, Physical Chemistry, Published by Pearson Education and Dorling Kindersley (India) (2006).
3. Donald A. McQuarrie, Quantum Chemistry, Oxford University Press, 1983 (541.28 MCQ).
4. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill Publishing Company New Delhi.
5. Eyring, Walter & Kimball, Quantum Chemistry, John Wiley & Sons, Inc., Chapman & Hall Ltd, 1946.

M.Sc. CHEMISTRY – SEMESTER IV *(wef 2012-2013)*
PHYSICAL CHEMISTRY
PAPER-XVI(iv)

NANO CHEMISTRY

Unit I: Fundamentals of Nanoscience and Nanotechnology [7L]

Solid materials and their strength, Perspective of length, Nanomaterials, Nanoscience and Nanotechnology, Nanostructures in nature, Prime materials, Carbon nanostructures viz. Carbon nanotube (Single-walled and multi-walled), Fullerenes, Surface effects of Nanomaterials, Surface plasmon resonance, Quantum size effects.

Unit II: Applications of Nanomaterials [5L]

Importance of Nanomaterials (Gold, Silver, Dielectric and Magnetic Oxide Nanoparticles), Some selected applications like, Nanomaterials in medicine, Nanomaterials for energy sector, Kinetic energy (KE) penetrators with enhanced lethality, High energy density batteries, Nanomaterials in Next-Generation Computer, Nanomaterials in catalysis and sensors, Nanomaterials for water purification, Nanomaterials in communication sector, Nanomaterials in food, Nanomaterials for the environment, Nanomaterials in automobiles, Nanomaterials in ceramics industry.

Unit III: Synthesis of Nanomaterials [12L]

Introduction, Nanomaterials synthesis, Top-Down and Bottom-Up Approaches, Solvothermal synthesis, Hydrothermal synthesis, Reverse micellar/Micro-emulsion method, Reverse micelles works as nano reactor, Mechanism for nanoparticle synthesis inside the reverse micelles, Co-precipitation, Sol-Gel Method, Polymeric Precursor Method and Sono-chemical Methods. Theory, Experimental conditions, Kinetics of solid state reactions and molten–salt routes.

Unit IV: Characterization of Nanomaterials [16L]

(a) X-Ray DiffractionTechnique: Structure of nanomaterials, X-ray diffraction (XRD), The Laue method, The Rotating crystal method, The Powder method, Determination of grain size/crystallite size using X-ray line broadening studies (Scherrer's formula), Determination of crystallite size distribution using X-ray line shape analysis.

(b) Electron Microscopic Techniques: Principles of electron microscopy, Scanning Electron Microscopy (SEM), Strengths and limitations of Scanning electron microscopy, Energy dispersive X-ray analysis (EDX), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM) and Scanning Tunneling microscopy (STM).

(c) Dynamic Light Scattering (DLS) Studies: Principle, Theory and Methodology.

(d) BET Surface Area Studies: Principle, Theory and Methodology.

Books Suggested:

1. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.
2. Nano Materials, B. Viswanathan, Narosa Publications, 2009.
3. Nano: The Essentials, T. Pradeep, Tata Mcgraw Hill, 2009.
4. Chemistry of Nanomaterials: Synthesis, Properties and Applications by C.N.R. Rao, A. Muller and A. K. Cheetham (eds.), Wiley-VCH, Weinheim, 2004.
5. Nanoscale Materials by Luis M. Liz-Marzan and Prashant V.Kamat, Kluwer Academic Publishers (Boston), 2003.
6. "Nanomaterials Chemistry: Recent Developments and New Directions", ed. by C.N.R. Rao, A. Muller & A.K. Cheetham (Eds.), Wiley-VCH, 2007.
7. Solid State Chemistry and its applications, Anthony R. West, John Wiley & Sons.
8. Physical Principles of Electron Microscopy: An introduction to TEM, SEM and AFM by R.F. Eqerton, Springer, 2008.
9. Introduction to Atomic Force Microscopy, Paul E. West, Pacific Nanotechnology, USA.
10. Solid State Chemistry Techniques, A. K. Cheetham and Peter Day, Oxford Science Publications.
11. Scanning Probe Microscopy and Spectroscopy, Ronald Weisendanger, Cambridge University Press.

M.Sc. CHEMISTRY – SEMESTER IV *(wef 2012-2013)*
PHYSICAL CHEMISTRY
PAPER-XVII(iv)

ADVANCE ELECTROCHEMISTRY AND MICELLAR PHENOMENA

45 Lectures

Unit I: Electrode Kinetics [12L]

Charge transfer under zero – field, charge – transfer under the influence of an electric field, two – way electron transfer, equilibrium exchange current – density, interface out of equilibrium, derivation of Butler – Volmer equation, Tafel plots, multistep electrode reactions.

Unit II: Electrochemical Techniques [6L]

Polarography – Theory, diffusion current, identification of cations, half – wave potential, its significance, voltametry and amperometry.

Unit III: Electrochemical Cells: [5L]

Conversion and storage of electrochemical energy, introduction, types of fuel cells and batteries.

Unit IV: Micellar Systems (Advance Treatment): [14L]

Thermodynamic causes of micelle formation, mass – action model, major problem with it, pseudo – phase separation model and its weaknesses, change in shape of micelle and structure with surfactant concentration, krafft point determination of aggregation number by conductance and fluorescence methods, enthalpy – entropy compensation phenomenon for micellization.

Unit V: Solubilization [8L]

Phase rule of solubilisation, distribution of solubilizate molecules among micelles, factors influencing solubilisation, location of solubilizates in micelles.

Book Suggested :

1. J. O. M. Bockris, A. K. N. Reddy and M. Gamboa – Aldeco: Modern Electrochemistry, Vol. 2A, Fundamentals of Electrodics, 2nd Ed. Plenum Press, New York, 2000.

2. Y. Moroi, Micelle – Theoretical and applied Aspects, Plenum Press, New York, 1992.

M.Sc. CHEMISTRY – SEMESTER IV *(wef 2012-2013)*
PHYSICAL CHEMISTRY
PAPER – XVIII(iv)

KINETICS OF COMPLEX REACTONS

45 Lectures

Unit I: Effect of Ions on Reaction Rates [10L]

Theory of unimolecular reactions, Lindemann mechanism and Hinshelwood treatment. ion-dipole and dipole-dipole reactions, pressure effects and volume of activation - van't Hoff's equation, substitution and correlation effects on reactivity, Linear Free Energy Relationships(LFER) - Hammett equation, uses and limitation.

Unit II: Chain Reactions [12L]

Linear chain reactions, Autocatalysis, Reaction between hydrogen and halogen, Calculation of Energy Barriers for Elementary Steps and comparison of the Mechanisms of the Hydrogen–Halogen Reactions, pyrolysis of acetaldehyde and ethane, general considerations of free radical chain mechanism,, Explosive Reactions - Combustion between hydrogen and oxygen, kinetic aspect of polymerization reactions, molecular mechanisms, Kinetic Chain Length, free radical mechanisms, cationic and anionic polymerization.

Unit III: Photochemical Reactions [11L]

General principals, Einstein's Law of photochemical equivalence, primary photochemical processes of atoms and diatomic molecules, reactions of electronically excited species, Quantum efficiency, Photochemical reactions of hydrogen-bromine and hydrogen-chlorine systems, Negative feedback and Oscillatory reactions - Lotka-Volterra, Brusselator, Oregonator (Belausov-Zhabotinsky Reaction) mechanisms.

Unit IV: Reactions on Surfaces [12L]

Adsorption, Adsorption Isotherms - Langmuir isotherm, Adsorption with dissociation, Competitive adsorption, Kinetics on Surfaces : Unimolecular surface reactions, Activation energies of unimolecular surface reactions, Reaction between two adsorbed molecules, Reaction between a molecule in the gas phase and an adsorbed molecule, Unimolecular surface reactions, Bimolecular reactions - Langmuir–Hinshelwood mechanism, Eley–Rideal mechanism.

Books Suggested:

1. Chemical kinetics by K.J. Laidler, Third Edition, 1987.
2. Chemical Kinetics by L. Wilkinson.
3. Pilling, M.J. & Seakins, P.W., Reaction Kinetics, Oxford University Press (1995).

4. Chemical kinetics and Reaction Mechanism by James H. Espenson, 2nd Ed., McGraw-Hill, 1995

5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).

6. Chemical Kinetics and Reaction Dynamics by Santosh K. Upadhyay, Anamaya Publishers, New Delhi, 2006.

7. Chemical Kinetic Methods: Principles of Relaxation Techniques and Applications by C. Kalidas, New Age International (P) limited, Publishers, 1996

8. Chemical Kinetics and Dynamics, J.I. Steinfeld, J.S. Francisco and W.L. Hase, 2nd Edition, Prentice Hall International, Inc., 1999.

9. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, by L. Arnaut, Sebastiao Formosinho, Hugh Burrows, Elsevier, 2007.

M.Sc. CHEMISTRY – SEMESTER IV

Max. Marks

PROJECT **175**

The student is required to carry out research based project work under the supervision of the concerned faculty member in the discipline. They shall submit a project report towards the semester end, which shall be evaluated by an external expert and internal examiners followed by the presentation/Viva Voce.

EDUCATIONAL TOUR **25**

A visit to different laboratories of premier research/academic institutes and/or industries is arranged by the department. A brief tour report is submitted by the students which is evaluated by faculty members.