DEPARTMENT OF CHEMISTRY

M. Sc. CHEMISTRY
COURSE CONTENT– 2015 Batch

PCH 1524 M – ORGANIC REACTION MECHANISM

SEMESTER I (THEORY)

5 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit

I Identify and describe the different types of reaction mechanisms.

II Recognize the relationship between structure and reactivity.

III Compare the mechanistic details of substitution and elimination reactions.

IV Analyze them mechanistic details of electrophilic substitution and addition reactions.

V Employ the name reactions for carrying out organic conversions.

COURSE OUTLINE:

UNIT I : INTRODUCTION TO REACTION MECHANISM **15 hrs**

Structure and stability of carbocations, carbanions, free radicals, carbenes, nitrenes **– types of reaction mechanisms** - Hammond postulate – microscopic reversibility **- Methods of determining mechanism** – isotopic labeling – kinetic evidence – isotope effect – cross over experiments

REFERENCE BOOKS:

Edwin S. Gould , **Mechanism and Structure in Organic Chemistry**, Holt Rinehart and Winston, Inc. 1959.

Jerry March, **Advanced Organic Chemistry**, Wiley eastern limited, Fourth Edition, New Delhi, 1999.

Lowry T.H. & Richardson K.S., **Mechanism and Theory in Organic Chemistry**, Harper and Row, 1976.

Moody C. J. and Whitham G. H., **Reactive intermediates**, Oxford chemistry Primers, 1992.

Reinhard Bruckner**, Advanced Organic Chemistry - Reaction Mechanisms**, Academic Press, 2003

UNIT II : STRUCTURE AND REACTIVITY **15 hrs**

Effect of structure and Reactivity – Resonance and field effects – steric effects -**quantitative treatments of the effect of structure and reactivity** – LFER – Hammett and Taft equation – importance of σ and ρ values in aromatic electrophilic substitutuions -Labelling and kinetic isotopic effects.

Aromaticity: Huckel's rule – **aromaticity in** 5,6,7 and 8 membered rings (recall). Aromatic systems with electron numbers other than six – systems of two electrons, four electrons (anti aromaticity), eight electrons, ten electrons and more than ten electrons – annulenes and hetero annulenes.

REFERENCE BOOKS:

Carey F.A., **Organic Chemistry**, Second Edition, McGraw-Hill, Inc., 1992.

Edwin S. Gould, **Mechanism and Structure in Organic Chemistry**, Holt Rinehart and Winston, Inc. 1959.

Jerry March, **Advanced Organic Chemistry**, Wiley eastern limited, Fourth Edition, New Delhi, 1999.

Raj. K. Bansal, **Organic Reaction Mechanism**, Tata McGraw Hill, New Delhi, 1990.

Solomons T.W.G., **Organic Chemistry**, John Wiley & Sons, Inc., U.S.A., 1976.

Sykes P., **A Guidebook to Mechanism in Organic Chemistry**, 6th edition, Orient Longman Private limited, New Delhi, 1988.

UNIT III: NUCLEOPHILIC SUBSTITUTION AND ELIMINATION REACTIONS 15 hrs

Aliphatic nucleophilic substitution – Mechanisms – S_N2, S_N1, mixed S_N1 & S_N2, S_Ni, SET, **Neighbouring group mechanism** – NGP by π and σ bonds (non classical carbocations) – **Reactivity** – effect of substrate, attacking nucleophile, leaving group and reaction medium – **substitutuion at** vinylic, trigonal and allylic carbons.

Elimination - mechanisms of β eliminations – (E2, E1, E1CB) – E1 – E2 – E1CB spectrum, orientation of double bonds – **reactivity**- effect of substrate, attacking base, leaving group and medium.

REFERENCE BOOKS:

Carey F.A., **Organic Chemistry**, Second Edition, McGraw-Hill, Inc., 1992.

Edwin S. Gould , **Mechanism and Structure in Organic Chemistry**, Holt Rinehart and Winston, Inc. 1959.

Jerry March, **Advanced Organic Chemistry**, Wiley eastern limited, Fourth Edition, New Delhi, 1999.

Raj. K. Bansal, **Organic Reaction Mechanism**, Tata McGraw Hill, New Delhi, 1990.

Solomons T.W.G., **Organic Chemistry**, John Wiley & Sons, Inc., U.S.A., 1976.

UNIT IV: ADDITION REACTIONS AND AROMATIC SUBSTITUTION 15 hrs

Addition to C – C multiple bonds – mechanisms- electrophilic, nucleophilic, free radical – **orientation and reactivity** – addition of conjugated systems, cyclopropane rings, carbon – hetero multiple bonds.

Electrophilic additions – mechanism of addition of halogens and hydrogen halides on carbon – carbon double bond system.

Aromatic Electrophilic Substitution- Arenium ion mechanism – orientation and reactivity in monosubstituted benzene rings – benzene rings with more than one substituent – **effect of leaving group**– o/p ratio.

Aromatic Nucleophilic substitution – mechanism – S_NAr – S_N1 – Benzyne – reactivity – effect of substrate, leaving group and attacking nucleophilie.

REFERENCE BOOKS:

Carey F.A., **Organic Chemistry**, Second Edition, McGraw-Hill, Inc., 1992.

Edwin S. Gould , **Mechanism and Structure in Organic Chemistry**, Holt Rinehart and Winston, Inc. 1959.

Jerry March, Advanced **Organic Chemistry**, Wiley eastern limited, Fourth Edition, New Delhi, 1999.

Raj. K. Bansal, **Organic Reaction Mechanism**, Tata McGraw Hill, New Delhi, 1990.

Solomons T.W.G., **Organic Chemistry**, John Wiley & Sons, Inc., U.S.A., 1976.

UNIT V: SELECTED ORGANIC NAME REACTIONS **15 hrs**

Favorskii reaction, Stark enamine reaction, Michael addition, Mannich reaction, Sharpless asymmetric epoxidation, Ene reaction, Hofmann – Loffler –Freytag reaction, Shapiro reaction, Baeyer-villegar reaction, Chichibabin reaction, Skraup synthesis, Fischer-Indole synthesis, Bischler-Napieralski reaction, Robinson annelation.

REFERENCE BOOK:

Jerry March, Advanced **Organic Chemistry**, Wiley eastern limited, Fourth edition, New Delhi, 1999.

PCH 1525M - QUANTUM CHEMISTRY AND GROUP THEORY

SEMESTER I (THEORY)

5 hrs/week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	Recognize the concepts of Quantum Mechanics.
II	Illustrate the Quantum Mechanics of simple systems.
III	Appraise the concepts of Chemical bonding and Molecular Spectroscopy through Quantum Mechanics.
IV	Recognize the symmetry of the molecules using Group Theory.
V	Interpret molecular bonding and vibrations in terms of Group Theory.

COURSE OUTLINE:

UNIT I : FUNDAMENTALS OF QUANTUM CHEMISTRY **15 hrs**

Introduction to quantum mechanics-Black body radiation, photoelectric effect, de Broglie equation and its verification, Interpretation of Bohr's first postulate in terms of wave nature of electron, Heisenberg Uncertainty principle- **Setting up the Schrodinger equation**- operators, algebra of operators, linear operators, setting up operators of linear momentum, angular momentum, kinetic energy, and total energy of systems- **Writing the Hamiltonian for H and He atoms**- eigen functions and eigen values , proving that linear momentum and angular momentum operators are linear, Hermitian operator and its properties, commutator theorem and its converse, Expansion theorem-**Postulates of quantum mechanics**

UNIT II: QUANTUM MECHANICS OF SIMPLE SYSTEMS **15 hrs**

The Schrödinger wave equation- particles in 1D and 3D boxes, harmonic oscillator, rigid rotator, Hydrogen atom, Hydrogen orbital - **Time dependent Schrödinger wave equation**- **Approximation methods** - Pertubation Theory (first order and non-degenerate), The Variation method, linear variation principle, **Helium**- Hartree- Fock self consistent field method.

UNIT III: APPLICATIONS OF QUANTUM CHEMISTRY **15 hrs**

Chemical bonding- VB & MO theory as applied to H_2^+, Conjugated hydrocarbons and Aromatic hydrocarbons, Huckel MO theory - **Molecular Spectroscopy and quantum mechanics**- Born

Oppenheimer approximation, Schrodinger equation for rotational, vibrational and electronic components and their selection rules.

REFERENCE BOOKS:

Chandra A.K., **Introductory Quantum Chemistry**- 5th edn, Tata McGraw –Hill.

Goodisman.J, **Contemporary Quantum Chemistry,** Plenum Press, New York, 1977.

Hanna M.W., **Quantum Mechanics in Chemistry**, Benjamin Inc., N.Y.

Horia Metiu, **Quantum Mechanics,** Taylor & Francis, New York, 2006.

Ira. N. Levine, **Quantum Chemistry**, 5th edn., Prentice Hall of India, 2000.

McQuarrie, Donald A., **Quantum Chemistry**, Viva Books Private Limited, Chennai, 2003

Powell and Crassman, **Quantum Mechanics**, Narosa Publishing house, 1988.

Prasad R.K., **Quantum Chemistry through Problems and Solutions**, New Age International Publishers, 1997.

Prasad R.K., **Quantum chemistry**, Wiley Eastern, 1992.

UNIT IV: PRINCIPLES OF GROUP THEORY 15hrs

Introduction-groups, subgroups, classes, Group multiplication table-**Molecular symmetry-** Symmetry elements and operations– products of symmetry operations- Classes of symmetry operations and classification of molecules, point groups. **Representations of groups**-– matrix representation of symmetry operations – reducible and irreducible representations-Statement of Great Orthogonality theorem-character tables and their constructions – C_{2v}, C_{3v}, D_{3h}, $C_{\infty v}$, C_4 point groups

UNIT V: APPLICATIONS OF GROUP THEORY 15 hrs

Symmetry and chemical bonding- Formulating SALC's with projection operators, LCAO and Huckel approximation-Naphthalene system, Molecular Orbital theory for inorganic compounds-tetrahedral and octahedral compounds, Ligand field theory- **Molecular vibrations-** symmetry of vibrations in non-linear molecules – selection rules for IR and Raman vibrations.

REFERENCE BOOKS: (For Units IV & V)

Bhattacharya P.K., **Group Theory and Its Chemical Applications**, Himalayan Publishing House, 1986.

Douglas B.E., and Hollingsworth C.A., **Symmetry in Bonding and Spectra – An Introduction**, Academic Press, New York, 1985.

F.A. Cotton, **Chemical Applications of Group Theory**, edn.Wiley Eastern Ltd, 1990.

Kettle S.F.A., **Symmetry and Strucutre,** John Willey & Sons, Chichester, 1985.

Lowell H. Hall, **Group Theory and Symmetry in Chemist**

Ramakrishnan V. and M.S. Gopinathan, **Group Theory In Chemistry**, Vishal Publications, 1998.

Raman K.V., **Group Theory and Its Applications to Chemistry**, Tata McGraw-Hill, 1990.

PCH1526M - BASIC CONCEPTS IN INORGANIC CHEMISTRY

SEMESTER I (THEORY)

5 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit

I
- Explain the periodic properties of atoms.
- Apply the theory of hard and soft acids and bases.

II
- Demonstrate the structure of different types of molecules.
- Apply VSEPR theory to predict the shapes of inorganic compounds.

III Relate the structure and electrical, mechanical properties of solids.

IV Discuss the applications of radioactivity.

V Describe the special aspects of non-metal chemistry.

COURSE OUTLINE:

UNIT I: PERIODIC PROPERTIES AND THEORY OF ACIDS AND BASES 15 hrs

Periodic properties of atoms – ionization energy – electron affinity – Pauling's and modern scales of electronegativity – Acid-base concept – measure of acid and base strength – non-aqueous solvents NH_3,H_2SO_4,HF,N_2O_4,SO_2 – superacids – hard and soft acids bases – theory and applications.

UNIT II: STRUCTURE AND BONDING 15 hrs

Ionic bonding – Born-Lande equation and Born-Haber cycle – lattice types – lattice energy – radius ratio – typical crystal structures – covalent bonding –resonance– MO theory –Walsh diagram– MO diagrams for A_2, AB (NO,CO - conventional and Coulson method) and AB_2 (linear $BeCl_2$) -AB_3-(NH_3) molecule – bond energy – bond order – polarizability – VSEPR theory with applications to inorganic compounds- Bent's rule and energies of hybridization.

UNIT III: SOLID STATE CHEMISTRY AND CRYSTALLOGRAPHY 15 hrs

Symmetry – point groups and its application – space groups (H.M notation) –lattices, planes-x-ray diffraction – experimental methods of crystal structure determination (single crystal and powder partteren) – structure factor calculation – indexing of lattices – defects, point and plane dislocatins – non-stoichiometry – experimental methods of study of non-stoichiometry –Hume Rothery rule– electrical and mechanical properties of solids – metallic bond – band model – semi conductors and super conductors –BCS theory– solid state reactions. Neutron diffraction, Electron diffraction basic principles and applications.

UNIT IV: NUCLEAR CHEMISTRY 15 hrs

Radioactivity – decay constant – half-life period – artificial transmutation – G.M. Counter – Scintillation counter – nuclear forces – nuclear fission and fussion reactions – nuclear models-single particle –liquid drop – nuclear accelerators – linear accelerators – cyclotron, synchrocyclotron, betatron – nuclear reactors – fast breeder reactors – power reactors - radioisotopes and their applications-radioactive isotopes as tracers, analytical, medicinal, agriculture.

UNIT V: INTRODUCTORY NON-METAL CHEMISTRY 15 hrs

Catenated compounds – range – energies of homonuclear bonds – synthesis – catenated compound of group IV, V, VI – heterocatenation – isopolyacids of vanadium, molybdenum and tungsten – 12-heteropoly acids – inclusion compounds – clathrates – intercalation compounds – host – guest complexation involving crowns and cryptands.

REFERENCE BOOKS:

Azaroff.L. **Introduction to Solids**, Tata McGraw Hill Publishing Company, 1995.

Cotton F.A.and G.Wilkinson, **Advanced Inorganic Chemistry,** Fifth edition, John Wiley & Sons, Inc., 1988.

Freidlander, Kennedy et al**., Nuclear and Radiochemistry**, John Wiley and Sons, 1964

Glasstone, **Source Book of Atomic Energy**.

Greenwood N.N. and Earnshaw A., **Chemistry of the Elements**, Pergamon Press, Oxford, 1984.

Greenwood N.N., **Ionic crystals, Lattice Defects and Non-stoichiometry**, Buterworths and Co Ltd., 1968.

Gurdeep Raj **Advanced Inorganic Chemistry** Vol. 1

Jaffe H.H. Milton Orchin, **Symmetry in Chemistry**, John Wiley and Sons, New Delhi,

James E.Huheey, **Inorganic Chemistry,** Fourth edition, HarperCollins College Publishers, 1993.

Jolly, William L., **Modern Inorganic Chemistry**, Mcgraw-Hill, New York, 1985.

Keith F. Purcell and John C.Kotz, **Inorganic Chemistry**, W.B.Saunders Company, 1997.

Lindoy L.F., **The chemistry of macrocyclic ligand complexes**, Cambridge University Press 1989.

Powell P. and P.Timmas, **The chemistry of the Non-metals, chapman and Hall**, 1974.

Shriver, Atkins, Langford, **Inorganic Chemistry**, Oxford University Press, 1990.

PCH 1421M - ANALYTICAL CHEMISTRY

SEMESTER I (LAB CUM THEORY)

4 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	Employ the various methods to handle and analyze the data scientifically.
II	Collect and systematically arrange information in chemistry through literature survey.
III	Compose an article through computer aided tools.
IV & V	Review the different instrumental techniques.

COURSE OUTLINE:

UNIT I: DATA HANDLING **12 hrs**

Accuracy and precision- -significant figures – Ways of expressing accuracy - Statistical analysis of data- -mean, median and mode standard deviation - Determinate and indeterminate errors - propagation of errors – Control chart- confidence limit – tests of significance – rejection of result - linear least square fit – correlation coefficient - use of computer for data handling.

REFERENCE BOOKS:

Gary D. Christian, **Analytical Chemistry,** 6th edition, John Wiley & Sons, Inc., 2004.

UNIT II : LITERATURE SEARCH IN CHEMISTRY **12 hrs**

Literature survey - Primary sources – Journals, Patents- **Secondary sources** - Listing of titles , Absracts , Beilstein, reviews and annual reviews, monographs and treatise, textbooks- **Online literature search** – Web browsing, search engines, popular websites in chemistry, e-library and e-journals, science citation index, locating journal articles.

REFERENCE BOOKS:

Jerry March, **Advanced Organic Chemistry**, Wiley eastern limited, Fourth Edition, New Delhi, 1999.

UNIT III: LAB WORK **12 hrs**

Use of computer for Text or article preparation, presentation and Data analysis – MS Office – Word, Powerpoint, Excel - Sigma plot – ISIS draw, Marvin sketch and Marvin view – online literature search – preparation of an article and thesis writing.

UNIT IV : OPTICAL SPECTROSCOPIC AND THERMOANALYTICAL TECHNIQUES 12 hrs

Optical spectroscopic methods - Principle, working & Applications of Atomic absorption spectrometry, Inductively coupled plasma atomic emission spectroscopy (ICPAES), Atomic fluorescence spectroscopy, X-ray fluorescence spectroscopy. **Mass spectrometry**- Introduction, Basic theory, Instrumentation, the mass spectrometer, Ionisation methods (EI & CI), desorption ionization(FAB, Laser, Plasma thermospray methods), Separation methods(Magnetic sector,quadrapole, TOF analyzers). **Thermoanalytical methods**- Thermogravimetry, Differential thermal analysis, Thermometric titrations.

UNIT V : ELECTROANALYTICAL TECHNIQUES 12 hrs

Potentiometry – Types of electrodes, reference, Glass pH, membrane indicator, ion selective electrodes – potentiometric measurements and titrations – **Coulometry**- current – voltage relationships during an electrolysis , coulometric methods of analysis, coulometric titrations- **Voltammetry** – Cyclic & pulse voltammetry, applications of voltammetry and stripping methods.

REFERENCE BOOKS:

Adon A. Gordus, **Theory and Problems of Analytical Chemistry,** Schaum's Outline Series, Tata McGraw- Hill, New Delhi, 1987.

Douglas A.Skoog, F. James Holler, Stanley R. Crouch, **Instrumental Analysis,** Brooks / Cole Cengage Learning,, 2007.

Ewing, **Instrumental Methods of Chemical Analysis**, 5th edition, MacGraw-Hill, Tokyo, 1985.

Frank Settle ed., **Handbook of Instrumental Techniques for Analytical Chemistry**, Pearson Education, 2004.

Khopkar S.M., **Basic concepts in Analytical Chemistry**, Wiley Eastern, New Delhi, 1984.

Sharma B.K., **Instrumental Methods Of Analysis**, Goel publishing House, Meerut, 1994.

Straughen and Walker, editors**, Spectroscopy, Vol I,** John W

Willard, Dean, Merritt and Settle, **Instrumental Methods of Analysis**, CBS Publishers and Distributors, 6th edition, New Delhi, 1986.

PCH 0423P EXPERIMENTAL CHEMISTRY I

ORGANIC CHEMISTRY PRACTICALS

SEMESTER I & II

5 hrs/ week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

- Identify the functional groups
- Design experiments to prepare, purify and characterize organic compounds
- Record the method of quantitative analysis of organic compounds

COURSE OUTLINE:

GENERAL LAB SAFETY MEASURES 2 Hrs

SPECIAL TECHNIQUES IN ORGANIC SYNTHESIS: 10 Hrs

1. Purification of solvents (General discussions related to Nature, toxicity etc)
2. Steam distillation – Isolation of clove oil from cloves
3. Solid – liquid extraction – using Soxhlet apparatus.
4. Recrystallisation techniques

REFERENCE BOOK:

Addison Ault "Techniques and Experiments in Organic Chemistry", 6 th edition, University Science books

SEPARATION AND ANALYSIS OF WATER SOLUBLE / INSOLUBLE ORGANIC COMPOUNDS 30 hrs

1. Mixture of a solid and a liquid.
2. Mixture of two organic liquids.
3. Mixture of two organic solids

PREPARATION and CHARACTERIZATION OF ORGANIC COMPOUNDS 23 hrs

Two- Stage Preparations:

1. Any one asymmetric synthesis

Three- Stage Preparations:

1. p-bromoaniline from aniline.

One Green Chemistry Experiment – Choice of the student

ESTIMATION OF ORGANIC COMPOUNDS 10 hrs

1. Estimation of ketone.
2. Estimation of glucose (Bertrand's method & Lane and Eynon method).
3. Estimation of glycine.

REFERENCE BOOKS

Arthur I. Vogel, **Elementary Practical Organic Chemistry,** Part I – Small scale preparations, 2nd edition, CBS publishers and distributors, New Delhi, 1987.

Arthur I. Vogel, **Elementary Practical Organic Chemistry**, Part II – Qualitative organic analysis, 2nd edition, CBS publishers and distributors, New Delhi, 1987.

Arthur I. Vogel, **Elementary Practical Organic Chemistry**, Part III – Quantitative organic analysis, 2nd edition, CBS publishers and distributors, New Delhi, 1987.

Furniss B.S.et al, **Vogel's Textbook of Organic Chemistry**, ELBS, 5th edition, London, 1989.

Vishnoi N.K., **Advanced Practical Organic Chemistry**, VIKAS publishing house private Ltd, New Delhi, 1990.

PCH0425P - PHYSICAL CHEMISTRY LAB

SEMESTER I & II

5 hrs/ week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

- Experiment the theoretical knowledge in laboratory
- Operate the instruments and collect the necessary data
- Design an experiment based on the theoretical background
- Evaluate the data collected through an experiment

COURSE OUTLINE:

UNIT I: ELECTROCHEMISTRY

Concept

1. Construction of Galvanic cell and determination of single electrode potential.
2. Redox titrations
3. Precipitation titrations

Methodology –Potentiometry, Conductometry

UNIT II: PHOTOCHEMISTRY

Concept

1. Verification of Beer-Lambert's Law
2. Job's Continuous Variation Method
3. Estimation of individual ions in a mixture of two

Methodology

Spectrophotometry

UNIT III: SURFACE CHEMISTRY

Concept

1. Determination of critical Micellar concentration
2. Verification of Adsorption isotherm (using the adsorption characteristics of dyes on various adsorbents)

Methodology

Spectrophotometry,Conductometry

UNIT IV: CHEMICAL KINETICS

Concept

1. Kinetics of iodination of acetone
2. Determination of order of persulphate-iodide reaction
3. Verfification of Brϕnsted-Bjerrum equation

Methodology –Spectrophotometry, Titrimetry

UNIT V: ELECTROLYTIC CONDUCTANCE AND IONIC EQUILIBRIA

Concept

1. Verification of Kohlrausch's Law
2. Conductometric Titrations
3. Acid-Base titrations

Methodology - Conductometry

UNIT VI: THERMODYNAMICS

Concept Determination of Thermodynamic parameters of a reaction

Methodology Potentiometry

UNIT VII : NANOMATERIALS

Concept: Surface Plasmon Oscillations of colloidal nanoparticles

Methodology : Absorption Spectroscopy

UNIT VIII: DEMONSTRATION ON THE FOLLOWING INSTRUMENTAL TECHNIQUES/ SOFTWARE PACKAGES

Flame photometer, Atomic Absorption Spectrometer, Nephelometer, Cyclic Voltametry, UV- Visible Spectrophotometer, Fluorescence spectrometer, Gaussian software.

The student has to design and carry out an experiment based on any of the above demonstrations and submit it as an applied project towards the end of the course.

REFERENCE BOOKS:

Jeffery, Bassett & et al., **Vogel's Text Book of Quantitative Chemical Analysis,** Fifth edn. ELBS.

Viswanathan B.& Raghavan P. S., **Practical Physical Chemistry**, Viva Books Pvt. Ltd., New Delhi

PCH 0426P INORGANIC CHEMISTRY LAB

SEMESTER I & II

5 hrs/ week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

- Design experiments for the separation of mixtures by chromatography
- Plan the method of preparation, characterization of inorganic complexes
- Analyze the inorganic cations in a mixture

COURSE OUTLINE:

CHROMATOGRAPHIC SEPARATIONS **15 hrs**

Separations using, column (adsorption)- separation of Zn & Mg, Cu & Ni) – paper(ascending and radial) – TLC- Electrophoresis.

PREPARATION AND CHARACTERISATION OF INORGANIC COMPLEXES **25 hrs**

Tetramminecopper(II) sulphate monohydrate, mixed ligand complex (Cu^{2+} oxine/ phenanthrolene/DMG).

ESTIMATION OF CATIONS IN A MIXTURE (ANY TWO)

Copper and Iron

Copper and Nickel

Copper and Zinc

Iron and magnesium

ANALYSIS OF FOUR - CATIONS MIXTURE **35 hrs**

Qualitative analysis of mixture of salts containing common and rare cations like Tungsten, Thallium, Selenium, Tellurium, Molybdenum, Cerium, Vanadium, and Zirconium.

REFERENCE BOOKS

Gurtu J.N and Kapoor. R., **Advanced Experimental Chemistry,** S. Chand & Co., New Delhi, 1989.

Jeffery G.H., J.Bassett, J.Mendham and R.C.Denney, **Vogel's Textbook of Quantitative Chemical Analysis**, 5th edition, ELBS, London, 1989.

Pass and Sutcliffe.H, Practical **Inorganic Chemistry**, 2nd edition, Chapman and Hall, London, 1974.

Venkateswaran V., R. Veeraswamy, A.R.Kulandaivelu; **Basic Principles of Practical Chemistry**, 2nd edition, Sultan Chand & Sons, New Delhi, 1997.

PCH 2623M - CHEMICAL KINETICS AND CATALYSIS

SEMESTER- II (THEORY)

5 hrs/ week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit

I Differentiate the theories of various reactions rates.

II Describe the kinetics in solutions and fast reactions.

III Apply the concepts of catalysis to different systems.

IV Review the chemistry of macromolecules.

V Apply the concepts of kinetics to polymerization reactions.

COURSE OUTLINE:

UNIT I: THEORIES OF REACTION RATES **15 hrs**

Basic kinetic concepts-rate of reaction, order, rate constants, reactions having no order, elementary, composite, chain reactions-**Theories of reaction rates-**collision theory, Transition State theory-Temperature effects, Arrhenius equation and its applications, composite rate constants, isokinetic relationships, pressure effects and volume of activation, chemical interpretation of activation parameters, principle of microscopic reversibility- **Gas-phase reactions-**Lindemann, Hinshel wood, RRK, RRKM and Slater treatments-**Oscillating reactions**-B-Z reaction,mechanism, Brussellator and Oregonator models.

UNIT II: REACTIONS IN SOLUTIONS AND FAST REACTIONS **15hrs**

Reactions in solutions- nature of reactions in solvent- diffusion controlled reactions, applications of transition state theory, solvent effects on polar and ionic reactions, salt effects, kinetic isotope effect.

Fast reaction kinetics- Need for sophisticated techniques to study very fast reactions, Stopped flow methods, chemical relaxation methods, kinetic equations for chemical relaxation, NMR line shape analysis, flash and laser photolysis, pico second and femto second methods, pulse radiolysis.

REFERENCE BOOKS:

Dove R.K., **Chemical Kinetics**, Campus Books, 2000.

Espenson, James H., **Chemical Kinetics and Reaction Mechanisms**, McGraw-Hill, Inc, Singapore, 1995.

Horia Metiu, **Physical Chemistry-Kinetics,** Taylor & Francis, New York, 2006.

Houston, Paul L., **Chemical Kinetics and Reaction Dynamics**, McGraw-Hill, Inc, Singapore, 2001.

Isadore Amdur, Gordon G, Hammes, Chemical kinetics: principles and selected topics McGraw-Hill, 1966.

Laidler, Keith J., **Chemical Kinetics**, Third edition, Harper &Row Publishers, Inc,.

Steinfeld J.J., Franciso J.S. and Hase W.L., **Chemical Kinetics and Dynamics,** 2nd edition, Prentice Hall, New Jersey, 1999.

Stephen Berry R., Rice S.A., and Ross J., **Physical Chemistry**, 2nd edition, Oxford University press, New York, 2000.

UNIT III: CATALYSIS AND SURFACE CHEMISTRY **15 hrs**

Homogenous catalysis-Acid-Base catalysis and enzyme catalysis-**Heterogenous catalysis**-adsorption, Physisorption and chemisorptions, Langmuir and BET adsorption, Gibbs adsorption isotherm, insoluble surface films, electrokinetic phenomena, zeta potential-**Surface Active agents**-classification, micellization,hydrophobic interaction, CMC and factors affecting CMC, counter-ion binding to micelles, thermodynamics of micellization, reverse micelles.

REFERENCE BOOKS:

Adamson A.W., **Physical Chemistry of Surfaces,** 4th edition, John Wiley and Sons, New York, 1982.

Fendler J.H., **Membrane Kinetic Chemistry,** John Wiley & Sons, Inc., 1982.

Gratzel and K. Kalyanasundaram, **Kinetics and Catalysis in Microheterogenerous systems**, Marcel Dekker, Inc. 1998.

Kuriacose J.C., **Catalysis,** MacMillan India Ltd., 1991.

UNIT IV: MACROMOLECULES **15 hrs**

Introduction- Definitions, functionality, classification of polymers-**Molecular forces and chemical bonding** – primary & secondary forces– **Molecular weight** – number, weight, viscosity and sedimentation average molecular weights, molecular weight and degree of polymerization , polydispersity and molecular weight distribution, polydispersity index –**Determination of molecular weight** -osmometric, light scattering, sedimentation and viscosity methods- **Glass transition temperature** – factors influencing T_g, crystallinity in polymers- **Polymer degradation**.

UNIT V: KINETICS OF POLYMERISATION

a) Condensation (step or self-growth) polymerization

Flory Equal reactivity principle – kinetics of self-catalysed and acid-catalysed, condensation polymerization – Carother's equation – gelation and gel point.

b) Addition (or vinyl) polymerization

a. Radical (or chain) polymerization –
b. Ionic – cationic, anionic, co-ordination, stereo regular polymerization.

c) Co-polymerisation

Kinetics of free radical copolymerisation – Mayo and Lewis equaton, reactivity ratios and co-polymerization behaviour – Q-e scheme of Alfred and Price.

Characterisation techniques– chemical (end group analysis) , spectral, X-ray diffraction, thermal and physical (analysis and testing) methods.

REFERENCE BOOKS:

Bahadur P., Sastry N.V., **Principles of polymer science**, 2nd edition, Narosa Publishing house, Chennai, 2005.

Billmeyer, Fred.W., **Text Book of Polymer Science**, John Wiley and Sons, New York, 1994.

Flory P.J., **Principles of Polymer Chemistry,** Cornell University Press, Ithaca, 1971.

Ghosh P., **Polymer Science and Technology**, 2nd edition,Tata Mc-Graw-Hill Publishing company, Ltd., New Delhi, 2002.

Gowariker, Viswanathan, Jayadev Sreedhar, **Polymer Science**, New Age International, New Delhi, 1986.

Misra, **Introductory Polymer Science**, Wiley Eastern Ltd., Chennai, 1993.

PCH 2624M - MOLECULAR SPECTROSCOPY

SEMESTER II (THEORY)

6 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

- Recognize the spectroscopic techniques in terms of interaction of EMR with molecules
- Describe the principles of the rotational, vibrational, electronic, magnetic resonance spectroscopic and mass spectrometric techniques
- Apply the principles of spectroscopy to understand the structure of compounds
- Interpret the spectroscopic data for any given compound
- Propose the structure of a new compound based on the spectroscopic data

COURSE OUTLINE:

UNIT I: INTRODUCTION AND MICROWAVE SPECTROSCOPY 18 hrs

Electromagnetic radiation –interaction of EMR with molecules-types of molecular spectroscopy-principles and instrumentation of rotational, vibrational and NMR spectroscopic techniques- factors affecting line width and intensity - signal to noise ratio and resolving power - absorption and emission spectroscopy

Microwave Spectroscopy - Rotation of molecules-Rotational Spectra of rigid rotator, Intensities of rotational lines, Effect of Isotopic substitution - Rotational spectrum of non-rigid rotator-linear & symmetric top molecules- Stark effect.

Applications of Microwave spectroscopy - determination of bond length, bond angle dipole moment and atomic mass from microwave spectra.

UNIT II: INFRA RED AND RAMAN SPECTROSCOPY 18 hrs

The Vibrating Diatomic Molecule - harmonic and anharmonic oscillators- Diatomic Vibrating Rotator-Vibrations of polyatomic molecules-Molecular vibrations, types of molecular vibrations, Rotational Vibrational Spectrum of Linear and Symmetric- top molecules.

Applications- Skeletal vibrations of organic and inorganic molecules- Factors influencing vibrational frequency of bonds- hydrogen bonding, electronic effect, mass effect, conjugation, ring-size - identification of functional groups (both organic and Inorganic) using IR data.

Raman Spectroscopy- classical and quantum theory of Raman effect- **Rotational Raman spectra**- Linear, Symmetric Top molecules-**Vibrational Raman Spectra**- Raman activity of vibrations, Rule of Mutual Exclusion, polarisability ellipsoids-Rotational Fine structures- polarized and depolarized Raman lines-

Combined application of IR and Raman spectral data for in structural study of simple molecules and ions like N_2O, ClF_3, ClO_4^- and NO_3^-.

UNIT III: UV- VISIBLE SPECTROSCOPY AND MASS SPECTROMETRY 18 hrs

Electronic Spectra of diatomic molecules- The Born-Oppenheimer Approximation, Vibrational Coarse structure:Progressions, Intensity of vibrational-Electronic spectra: Franck-Condon Principle,Dissociation Energy and Dissociation Products, Rotational Fine Structure 0f Electronic-Vibration Transitions, The Fortrat Diagram, Predissociation

Applications electronic transitions in organic molecules- solvent effects- Woodward rules for calculation of λ_{max} for dienes, polyenes and carbonyl compounds

Mass Spectrometry-Mass spectrum, Determination of molecular weight, molecular formulae, isotopic abundance- molecular ion - metastable ions- fragmentation routes- fragmentations associated with hydrocarbons- hydroxyl compounds, ethers, ketones, aldehydes, acids, amines, nitro compounds , halogen compounds with more than one Cl /Br atoms (both aliphatic and aromatic compounds to be done simultaneously).

UNIT III: Proton NMR **18 hrs**

Nuclear spin states and NMR active nuclei, nuclear magnetic moments-Mechanism of resonance absorption- Population of nuclear spin states, Proton nmr- interaction of spin magnetic moment of a proton with external magnetic moment, chemical shift and shielding, chemical equivalence, chemical environment and chemical shift, magnetic anisotropy, spin-spin splitting, coupling constant, geminal, vicinal , long-range, trans, aromatic, allylic coupling, factors influencing coupling constant, splitting of nmr signals- AX and AMX types - Proton NMR spectra of organic molecules.

Applications : Structural elucidation of organic molecules using Proton NMR spectral data.

UNIT V: ^{13}C NMR AND COMPOSITE SPECTRAL PROBLEMS **18 hrs**

^{13}C nucleus – chemical shifts, calculation of ^{13}C chemical shifts, spin-spin splitting of ^{13}C signals, proton decoupled ^{13}C spectra, NOE, Off-resonance decoupling, DEPT, molecular relaxation in ^{13}C NMR. (9 hrs)

Use of IR, UV-visible, NMR and Mass spectral data for structural elucidation of organic compounds. (9 hrs)

REFERENCE BOOKS

Aruldhas G**., Molecular Structure and Spectroscopy**, Prentice-Hall of India Pvt. Ltd., New Delhi, 2001.

Banwell C.N. and E.M.McCash, **Fundamentals of Molecular Spectroscopy**, Tat McGraw-Hill Publishing Co. Ltd., 7th Edition, New Delhi, 1999 .

Barrow G.M.,**Introduction to Molecular Spectroscopy,** McGraw Hill, New York, 1964.

Bellamy L.J., **The Infrared Spectra of Complex Molecules, vol 2,** Chapman and Hall, 3rd Edition, London, 1975.

Dyer J.R., **Applications of Absorption Spectroscopy of Organic Molecules,** Prentice-Hall of India Pvt. Ltd., New Delhi, 1987.

Ghosh P.K., **Introduction to Photoelectron Spectroscopy,** John Wiley , New York, 1989.

Jag Mohan, **Organic Spectroscopy, Principles and Applications**, Narosa Publishing House, Chennai, 2004

Kemp W., **Organic Spectroscopy**, Macmillan Press Ltd., London, 1991.

Russel S. Drago, **Physical Methods in Inorganic Chemistry**, Affiliated East-West Press Pvt. Ltd., New Delhi, 1968.

Russel S.Drago, **Physical Methods in Chemistry,** Saunders, Philadelphia, 1977.

Silverstein R.M., G.C. Bassler, T.C. Morill, **Spectrophotometric Identification of Organic Compounds**, 6th edition, John Wiley & Sons, New York & London, 1998.

Straughan and Walker**, Spectroscopy-Volume I, & II,** Chapman and Hall, London, 1976.

PCH2523O - COORDINATION CHEMISTRY

SEMESTER II (THEORY)

5 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	• Explain the bonding in coordination compounds.
	• Describe the stereochemistry and isomerism exhibited by the complexes
	• Use a simplified CFT to rationalize the structure and reactivity of metal complexes
	• Compare the various theories of bonding in complexes
II	• Analyse the electronic spectra of complexes
	• Calculate Δ_0 and β.
III	• Explain the principle of EPR
	• Interpret the EPR spectra of inorganic complexes
IV & V	• Identify the different types of reactions of complexes.
	• Discuss the mechanical aspects of the reactions of complexes.

COURSE OUTLINE:

UNIT I. COORDINATION CHEMISTRY **15 hrs**

Recall the nomenclature of coordination compounds- types of ligands - coordination number – geometries– stereochemistry and isomerism–constitutional, geometrical and optical-coordination numbers 4 and 6 –theories of bonding - CFT – crystal field splitting in octahedral, square planar, tetrahedral complexes – CFSE- factors influencing the magnitude of Δ_0 – applications of CFT – Jahn-Teller distortions - limitations - LFT and MOT- applications to octahedral complexes – (σ - bonding) – tetrahedral, square planar complexes – comparison of different theories - stabilization of unusual oxidation states by coordination, applications of ORD.

REFERENCE BOOKS:

Cotton F.A.and G.Wilkinson, **Advanced Inorganic Chemistry,** Fifth edition, John Wiley & Sons, Inc., 1988.

Gary Wulfsberg, **Inorganic chemistry** ,Viva books pvt.Ltd, 2002

James E.Huheey, **Inorganic Chemistry,** Fourth edition, HarperCollins College Publishers, 1993.

Lee J. D., **Concise Inorganic Chemistry**, Fifth edition, ELBS, 1994.

UNIT II: MAGNETIC PROPERTIES AND ELECTRONIC SPECTRA OF METAL COMPLEXES **15 hrs**

Magnetic properties of tetrahedral and octahedral complexes- spin and orbital contribution quenching –spin cross over rule -microstates of electron configuration in free atoms and ions –term symbols for equivalent and non-equivalent electrons- possible term symbols for given configuration – p^2 - d^2 – splitting of terms in square planar, tetrahedral , octahedral fields- Electronic spectra of various complexes – selection rules - spin orbit coupling -assignment and intensities of transitions – Orgel (d^1 to d^9 octahedral and tetrahedral complexes) and Tanabe Sugano diagrams(d^1 ,d^6 complexes and its applications)- calculation of Δ_0 and β and Racah parameters – examples from d^2 , d^3 d^7, d^8 octahedral complexes- CT spectra of metal complexes.

REFERENCE BOOKS:

Cotton F.A, and G.Wilkinson, **Advanced Inorganic Chemistry,** Fifth edition, John Wiley & Sons, Inc., 1988.

Day, M. Clyde, Jr.; Selbin, Joel **Theoretical inorganic chemistry**

Gary Wulfsberg, **Inorganic chemistry**, Viva books pvt.Ltd, 2002.

James E.Huheey, **Inorganic Chemistry**. Fourth edition, HarperCollins College Publishers, 1993.

Lee J. D., **Concise Inorganic Chemistry**, Fifth edition, ELBS, 1994.

Sarkar R., **General and inorganic chemistry Part II** , Books and allied publishers, 2002.

UNIT III: ELECTRON SPIN RESONANCE SPECTROSCOPY 15 hrs

Electron Spin Resonance Spectroscopy-Introduction- position of ESR absorption- g factor and its applications- zero field splitting – Kramer's degeneracy – hyperfine structure- electron nucleus coupling- hyperfine splitting due to more than one nucleus- anisotropic effects- fine structure of ESR spectra- electron-electron coupling- hyperfine splitting constant from MO theory- McConnell equation- instrumentation- ESR study of H, D atoms; CH_3 and naphthalene radicals-applications of EPR in the structural study of Bis- salicylaldimine copper(II) , and metal complexes of Cu, Cr and Mn.

REFERENCES BOOKS:

Aruldhas G**., Molecular Structure and Spectroscopy**, Prentice-Hall of India Pvt. Ltd., New Delhi, 2001.

Kaur H, **Spectroscopy,** Pragati Prakashan, Uttar Pradesh, 2010

Russel S. Drago, **Physical Methods in Inorganic Chemistry**, Affiliated East-West Press Pvt. Ltd., New Delhi, 1968.

Russel S.Drago, **Physical Methods in Chemistry,** Saunders, Philadelphia, 1977.

UNIT IV: REACTION MECHANISM OF METAL COMPLEXES – I 15 hrs

Ligand substitution reactions in octahedral, square planar complexes- labile and inert complexes (application of VBT,MOT) – dissociation, association mechanism – Mechanism of hydrolysis reactions – acid hydrolysis – base hydrolysis – anation reactions – trans effect –trans influence–trans effect and its application-theories of trans effect- Thermodynamic and kinetic stability of complexes – factors affecting stability of metal complexes – experimental determination of stability constant of complexes.

REFERENCE BOOKS:

Gary Wulfsberg, **Inorganic chemistry** ,Viva books pvt.Ltd, 2002

James E.Huheey, **Inorganic Chemistry,** Fourth edition, HarperCollins College Publishers, 1993.

Malik, Tuli, Madan, **Selected topics in inorganic chemistry**, fifth edition, S.Chand.

Shriver, Atkins, Langford, **Inorganic Chemistry**, Oxford University Press, 1990.

UNIT V: REACTION MECHANISM OF METAL COMPLEXES – II 15 hrs

Electron transfer reactions – one electron transfer reactions – inner sphere mechanism – outer sphere mechanism - two electron transfer reactions – complementary and non – complementary electron transfer reactions -synthesis of coordination compounds using electron transfer reactions- – metal assisted reactions – Aldol condensation – ester hydrolysis – phosphate ester, aminoesters and amide hydrolysis – template effect – synthesis of macrocyclic ligands – reaction of coordinated ligand .

REFERENCE BOOKS:

Basolo, and Pearson, Ralph. G, **Mechanism of Inorganic Reactions- A study of metal complexes in solution**. Wiley Eastern, New Delhi,1984.

James E.Huheey, **Inorganic Chemistry**. Fourth edition, HarperCollins College Publishers, 1993.

Keith F. Purcell and John C.Kotz, **Inorganic Chemistry**, W.B.Saunders Company, 1997.

Malik, Tuli, Madan, **Selected topics in inorganic chemistry,** fifth edition, S.Chand & Co., New Delhi.

Shriver, Atkins, Langford, **Inorganic Chemistry**, Oxford University Press, 1990.

PCH 3623M - ORGANIC SYNTHETIC METHODS

SEMESTER III (THEORY)

5 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	Illustrate the various types of molecular rearrangements
II	Demonstrate the retro synthetic plan
III	Design the consecutive steps for the synthesis of Novel compounds
IV	Relate the appropriate reagents for the conversion of organic compounds
V	• Recognize the significance of green technology in organic synthesis • Apply the green technology in organic synthesis

COURSE OUTLINE:

UNIT I: MOLECULAR REARRANGEMENTS **15 hrs**

Introduction, nucleophilic arrangements- actual nature of migration, migratory aptitude, memory effects, longer nucleophilic rearrangements, free radical rearrangements, electrophilic rearrangements -

1,2 – rearrangement - Wagner – Meerwein and related reactions.

Acid –catalysed rearrangement - Arndt-Eistert synthesis

Carbon to Carbon migration of other groups - Neber rearrangement

Carbon to Nitrogen migration - Hofmann rearrangement, Curtius rearrangement, Lossen rearrangement, Schmidt rearrangement, Beckmann rearrangement

Nitrogen to carbon, oxygen to carbon, sulphur to carbon migration of groups-Stevens, Wittigs

REFERENCE BOOKS:

Gould E.S., **Mechanism and Structure in Organic Chemistry**, Hold, 1959.

Jerry March, **Advanced Organic Chemistry**, Wiley eastern limited, Fourth edition, New Delhi, 1999.

Kalsi P.S., **Stereochemistry**, Wiley eastern limited, New Delhi, 1990.

Lowry T.H. & Richardson K.S., **Mechanism and Theory in Organic Chemistry**, Harper and Row, 1976.

Miller B. & Prasad K. J. R., **Advanced Organic Chemistry: Reactions and Mechanisms**, 2nd edition, Pearson Educations, **2006**.

UNIT II: ORGANIC SYNTHESIS - I **15 hrs**

The synthetic process – preliminary planning, molecular characteristics, stereochemical control - functional group transformation-**retro synthetic analysis** – order of events - one group c-x disconnection –1,1- 1,2 – 1,3-1,4-1,5- and 1,6 -two group c-x disconnections

UNIT III: ORGANIC SYNTHESIS: II **15 hrs**

Chemo selectivity - reversal of polarity – cyclisation reactions – protecting groups–one group disconnection C-C, alcohols, C=O, stereo selectivity – regio selectivity – use of acetylenes – aliphatic nitro compounds in synthesis – **Retrosynthetic analysis of** multistriatin – Pirindol – *cis*-jasmone – Dienoestrol.

REFERENCE BOOKS:

Ahluwalia V.K.and Renu Aggarwal, **Organic Synthesis**, Narosa Publishing House, New Delhi.

Clayden, Greeves, Warren, **Organic Chemistry**, Oxford University Press, 2001.

Herbert O.House, **Modern Synthetic Reactions**, 2nd Edition, The Benjamin/ Cumming Publishing Company, U.S.A., 1972.

Mackie R.K.& D.M. Smith, **Guidebook to Organic Synthesis**, ELBS, England, 1985.

Norman R.O.C., **Principles of Organic Synthesis**, 2nd Edition, Chapman and Hall, London, New York, 1978.

Robert E. Ireland, **Organic Synthesis**, 2nd edition, Prentice- Hall of India Private Limited, New Delhi, 1988.

Stuart Warren, **Organic Synthsis**, The Disconnection Appraoch , John Wiley & Sons 2004.

Wyatt P. & Warren S., **Organic Synthesis: Strategy and Control**, John Wiley & Sons Ltd, UK, 2007.

UNIT IV : REAGENTS IN ORGANIC SYNTHESIS **15 hrs**

Oxidation:

Selenium dioxide, periodic acid, DMSO, aluminium t-butoxide, $Pb(OAC)_4$, $Hg(OAC)_2$, I_2 / AgOAc (dry and wet), peroxides and peroxyacids, PCC (Corey's reagent), PDC, Etards reagent, MnO_2, OsO_4, N_2O_4, Jones reagent, copper chromite Ruthenium tetraoxide, Iodobenzene diacetate and Thallium (III) nitrate, Synthetic utility of Silanes.

Reduction:

Catalytic hydrogenation – hydrogen in presence of platinum, Wilkinson's catalyst and Lindlar catalyst – Complex metal hydrides such as $LiAlH_4$, $NaBH_4$, $Na(CN)BH_3$, $Zn(BH_4)_2$ and trialkyl tin hydride. $SnCl_2$ and Lawessonn reagent – $TiCl_4$ / Zn-Cu (McMurrays reagent) – $TiCl_4$ / Mg-Hg and Dicyclopentadienyltitanium dichloride. BH_3 / THF, 9-BBN and optically active boranes. Dissolving metal reduction – Clemenson and Wolff-Kishner reduction, Meerwin- Ponndorf-verly reduction. Enantioselective reductions: Noyoris catalyst, Corey-Bakshi-Sibhata catalyst, Brown's Ipc_2BH and Ipc_2BCl reagents.

REFERENCE BOOKS:

Carey and Sundberg, **Advanced Organic Chemistry Part – A Structure and Mechanism, Part-B Reactions and synthesis**, Plenum press, 5th edition 1997.

Carruthers W., **Some Modern Methods of Organic Synthesis**, Cambridge Univ Press 3rd Edition,1988.

Graham Solomons, **Organic Chemistry**, John Wiley and Sons INC 5th edition, 1992.

Herbert O.House, **Modern Synthetic Reactions**, 2nd Edition, The Benjamin/Cumming Publishing Company, U.S.A., 1972

Mackie R. K. & D.M. Smith, **Guidebook to Organic Synthesis**, ELBS, England, 1985.

Michael B. Smith, **Organic Synthesis,** M.C.Graw Hill, International Edn, 1994.

Norman R.O.C., **Principles of Organic Synthesis**, 2nd Edition, Chapman and Hall, London, New York, 1978.

Smith M. B. & March J., March's Advanced **Organic Chemistry: Reactions, Mechanisms, and Structure**, 6th edition, John Wiley & Sons, 2007.

UNIT V: NOVEL SYNTHETIC ROUTES AND REAGENTS **15 hrs**

Reagents:

Gilman`s reagent, lithium diisoprpylamide (LDA) dicyclohexylcarbodiimide, 1,3-Dithiane, tri-n-butyltinhydride, Woodward and Prevost hydroxylation, DDQ, Cr and V complexes, Peterson's synthesis Baker's yeast.

Green synthesis:

Principles of green synthesis, green catalysts, Green solvents – Water, Dimethylcarbonate, supercritical CO_2, Solventless reactions, Ionic liquids. Solid supported organic synthesis, Phase transfer catalysts, microwave assisted green synthesis, ultra sound assisted synthesis.

REFERENCE BOOKS:

Ahluwalia, Kidwai**, NewTrends in Green Chemistry**, 2nd edition, Anamaya Publishers, New Delhi, 2006.

Desai. K. R., **Green chemistry**, 1St edition, Himalaya Publishing House, Mumbai, 2005.

Graham Solomons, **Organic Chemistry**, John Wiley and Sons INC 5th edition, 1992.

Herbert O.House, **Modern Synthetic Reactions**, 2nd Edition, The Benjamin/Cumming Publishing Company, U.S.A., 1972

Michael B. Smith, **Organic Synthesis,** M.C.Graw Hill, International Edn, 1994.

Norman R.O.C., **Principles of Organic Synthesis**, 2nd Edition, Chapman and Hall, London, New York, 1978.

Rashmi sanghi, Srivastava M.M, **Green chemistry**, Narosa Publishing House, Chennai, 2003.

PCH 3624 M – ORGANIC STEREOCHEMISTRY & PHOTOCHEMISTRY

SEMESTER III (THEORY)

5 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	• Construct molecular representations for organic compounds • Define the terms stereoisomerisms, chirality, racemic mixture, configuration isomers. • Discuss the significance of chirality of allenes, spiranes and biphenyls
II	• Judge the topic ligands and faces • Analyze the the confirmations of cyclic compounds
III	Compose asymmetry in organic molecules with suitable molecules Interpret the ORD & CD curves
IV	Interpret the various pericyclic reactions.
V	• Describe the various photochemical reactions • Solve the photochemical reactions.

COURSE OUTLINE:

UNIT I: FUNDAMENTALS OF STEREOCHEMISTRY **15 hrs**

Stereoisomerism – definitions and classification - **Molecular representation** – interconversion of sawhorse, Fischer and Newman projection formulae- classification of stereoisomers – racemic modifications – **configurational nomenclature** – E,Z nomenclature – chirality – **molecules with more than one chiral centre** – erythro, threo, like, unlike – brewster's system. - **stereoisomerism in cyclic compounds** axial chirality, planar chirality and helicity principles of axial and planar chirality – molecules with axial chirality – **stereochemistry of** allenes – spiranes – Biphenyls

UNIT II: PROSTEREOISOMERISM AND CONFORMATIONAL STUDY **15 hrs**

Topicity and Prostereoisomerism-Homotopic ligands and faces – enantiotopic ligands and faces – diasterotopic ligands and faces, **Nomenclature of** stereoheterotopic ligands and faces. Molecules with one prochiral center – Re and Si system of Nomenclature for ligands- **Conformations of typical and atypical examples** of disubstituted cyclohexanes, decalins, **Conformational study** of perhydrophenanthrenes, perhydroanthracenes, **Structure and nomenclature of bridged ring systems**

UNIT III: ASSYMETRIC SYNTHESIS & CHIROPTICAL PROPERTIES **15 hrs**

Principles of asymmetric synthesis, enantiomeric excess - **asymmetric induction** Cram and Prelog's rule**-** Felkin-Ahn model and Texler-Zimmerman model **–**- biochemical asymmetric transformations- first, second, third and fourth generation processes **– generation of optically pure molecule through** classical resolution, Kinetic resolution, Dynamic Kinetic Resolution.

Chiroptical properties:

Optical activity, anisotropic refraction, optical rotatory dispertion, circular dichroism, cotton effect, anisotropic absorption, applications of ORD and CD- determination of configuration and conformation, - The octant rule - axial haloketone rule – solvent effects

REFERENCE BOOKS:

Ernest L.Eliel, **Stereochemistry of Carbon Compounds**, 22nd Reprint, Tata- McGrawHill, New Delhi, 1997.

Finar I.L., **Organic Chemistry**, V.2, 6TH Edition, ELBS, Singapore, 1994.

Kalsi P.S., **Stereochemistry**, Wiley eastern limited, New Delhi, 1990.

Nasipuri D, Stereochemistry **of Organic Compounds – Principles and applications**, 2nd edition, New Age International, 2002.

UNIT IV: PERICYCLIC REACTIONS 15 hrs

Definition – types – FMO treatment, and correlation approaches and diagrams of typical electrocyclic reactions – Woodward-Hoffmann rule - PMO method - cycloadditions, sigmatropic reactions, ene reaction ans chelotropic reactions – Cope, Aza-cope , Sommelet - Hauser and Claisen rearrangement – Fluxional tautomerism.

REFERENCE BOOKS:

Chatwal G. R., **Organic Photochemistry**, 1st edition, Himalaya publishing house, Mumbai, 1998.

Coxon J. M., Halton B., **Organic Photochemistry**, Camb.Univ. Press 2nd edition 1987.

Depuy C.H.and Chapmann O.L., **Molecular Reactions and Photochemistry**, Eastern Economic Edition Tata- McGraw Hill 1975.

Finar I.L., **Organic Chemistry**, V.1, 6TH Edition, ELBS, Singapore, 1994.

Gilchrist T.L.& R.C.Storr, **Organic Reactions and Orbital Symmetry**, Cambridge University press, 1972.

Jagdamba Singh, Jaya Singh, **Photochemistry and Pericyclic reactions,** New Age International Pvt. Ltd., New Delhi, 2010.

Lowry T.H. & Richardson K.S., **Mechanism and Theory in Organic Chemistry**, Harper and Row, 1976.

Nasipuri D, **Stereochemistry of Organic Compounds – Principles and applications**, 2nd edition, New Age International, 2002.

UNIT V: ORGANIC PHOTOCHEMISTRY 15hrs

Introduction – Interaction of electromagnetic radiation with matter – electronic excitations – excited states –

transfer of excitation energy – sensitization and quenching - **photochemical eliminations**, Norrish type I and II reactions, Barton reaction -Paterno-Buchi reaction, oxidations -reductions- cis-trans isomerisation, rearrangements (di-pi- methane or Zimmerman rearrangement), photochemistry of arenes.

REFERENCE BOOKS:

Chatwal G.R., **Organic Photochemistry**, 1st edition, Himalaya publishing house, Mumbai, 1998.

Coxon J. M., Halton B., **Organic Photochemistry**, Camb.Univ. Press 2nd edition 1987.

Coyle J.D., **Organic Photochemistry**, Wiley, 1985.

Depuy C.H.and Chapmann O.L., **Molecular Reactions and Photochemistry**, Eastern Economic Edition Tata- McGraw Hill 1975.

Finar I.L., **Organic Chemistry, V.1,** 6TH Edition, ELBS, Singapore, 1994.

Gilchrist T.L &.Storr R.C, **Organic Reactions and Orbital Symmetry**, Cambridge university press, 1972.

Jagdamba Singh, Jaya Singh, **Photochemistry and Pericyclic reactions,** New Age International Pvt. Ltd., New Delhi, 2010.

Lowry T.H. & Richardson K.S., **Mechanism and Theory in Organic Chemistry**, Harper and Row, 1976.

Nicholass J. Turro, Scaiano J.C., Ramamurthy V., **Modern Molecular Photochemistry of Organic Molecules,** 1st edition, University Science Books, 2010.

PCH3625M - ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY

SEMESTER III (THEORY)

5 hrs/week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	Describe the structure and bonding in π-complexes
II	• Explain the reactions of organometallic compounds • Report on the catalytic properties of organometallic compounds.
III & IV	• Review the importance of metallobiochemistry • Recognize the role of metals in medicine
V	• Explain the photochemistry of coordination compounds

COURSE OUTLINE:

UNIT I: π COMPLEXES–STRUCTURE AND BONDING 15 hrs

Theoretical basis of sixteen and eighteen electron rule- structure and bonding in metal carbonyls- Nitrosyl complexes –metal alkyl, carbenes, carbyne and carbide complexes – Non aromatic Ziese's salt and alkyne complexes- Allyl, benzenoid and cyclopentadienyls - dinitrogen and dioxygen complexes – synthesis , structure and chemical properties of alkene, chemical properties of metallocenes like ferrocene, cobaltocene.

REFERENCE BOOKS:

Cotton F.A.and Wilkinson G., **Advanced Inorganic Chemistry**, Fifth edition, John Wiley & Sons, Inc., 1988.

Greenwood and Earnshaw, **Chemistry of the Elements,** Pergamom press, Oxford, 1984.

James E.Huheey, **Inorganic Chemistry,** Fourth edition, HarperCollins College Publishers, 1993.

Purcell and Kotz. **Inorganic Chemistry**, Saunders, Philadelphia, 1977.

UNIT II: ORGANOMETALLIC COMPOUNDS - CATALYSIS 15 hrs

Substitution reaction- Nucleophilic and electrophilic ligand substitution - oxidative addition and reductive elimination reactions- insertion reactions - co-ordinative unsaturation and rearrangement- ligand protonation-stereochemical non rigidity -activation of small molecules by complexation- Homogeneous catalysis- hydrogenation- (using Wilkinson , Monsanto acetic acid process) hydroformylation-(oxo process)-oxidation of alkene (Wacker process)-carbonylation of methanol**-** Syn-gas, water gas reaction -olefin isomerisation and cyclooligomerisation reactions-heterogeneous catalysis–polymerization of olefin–Ziegler–Natta catalysis.

REFERENCE BOOKS:

Cotton F.A.and G.Wilkinson, **Advanced Inorganic Chemistry**, Fifth edition, John Wiley & Sons, Inc., 1988.

Gary Wulfsberg, **Inorganic chemistry** ,Viva books pvt.Ltd, 2002.

Greenwood and Earnshaw, **Chemistry of the Elements**, Pergamom press, Oxford, 1984.

James E.Huheey, **Inorganic Chemistry**. Fourth edition, HarperCollins College Publishers, 1993.

Purcell and Kotz, **Inorganic Chemistry**, Saunders, Philadelphia, 1977.

Shriver, Atkins, Langford, **Inorganic Chemistry**, Oxford University Press, 1990.

UNIT III: BIOINORGANIC CHEMISTRY I **15 hrs**

Introduction –metallophorphyrins- cytochromes- respiration – Dioxygen carriers- heme proteins – hemoglobin, myoglobin, Hemocyanin, hemerythrin, Zinc finger proteins, enzymes-carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase- vitamin B_{12} dependent enzymes.

REFERENCE BOOKS:

Bertini, Gray, Lippard, Valentine, **Bioinorganic Chemistry**, VIVA books private Ltd., 1998

Chatwal G.R., A.K. Bhagi, **Bioinorganic Chemistry**, Himalaya Publishing House, 1996

Das A.K., **A Text Book on Medicinal Aspects of Bio- inorganic Chemistry,** CBS Publishers,1990

James E.Huheey, **Inorganic Chemistry,** Fourth edition, HarperCollins College Publishers, 1993.

UNIT IV: BIOINORGANIC CHEMISTRY II **15 hrs**

Elementary principles of photosynthesis- chlorophyll – electron transfer agents – Iron- sulphur proteins (Ferredoxins and Rubredoxins) – blue copper proteins- classification –type of proteins- blue copper electron transfer protein –plastocyanin- azurin-blue copper proteins as oxidases- cyctochorme C oxidase, nitrogenase enzyme - Nitrogen fixation – in vitro and in vivo fixation, metal ion transport across the membrane- sodium ion pump, Au,Pt,Cu metals in medicine - diagnosis and chemotherapy.

REFERENCE BOOKS:

Bertini, Gray, Lippard, Valentine, **Bioinorganic Chemistry**, VIVA books private Ltd.,1998.

Chatwal G.R., A.K. Bhagi, **Bioinorganic Chemistry**, Himalaya Publishing House, 1996.

Das A.K., **A Text Book on Medicinal Aspects of Bio- inorganic Chemistry**, CBS Publishers,1990

James E.Huheey, **Inorganic Chemistry,** Fourth edition, HarperCollins College Publishers, 1993.

UNIT V: PHOTOINORGANIC CHEMISTRY **15 hrs**

Photochemistry of coordination compounds- types of photochemical reactions – photochemistry of Chromium(III) and Ruthenium(II)- polypyridine complexes,Photochemistry of heavy metal complexes-Rhodium(II) and Platinum(II), role of spin orbit coupling, life times of excited states in these complexes, photochemistry of metallocene and metal carbonyls- $Mn_2(CO)_{10}$,$Cr(CO)_6$,$Fe(COT)(CO)_3$.

REFERENCE BOOKS:

Arunachalam.S, **Inorganic photochemistry**, Kala publications, Tamil nadu, 2002

Rohatgi K.K. -Mukherjee**, Fundamentals of Photochemistry**, New Age International Publisher, New Delhi, 1978.

Russel S. Drago, **Physical Methods in Inorganic Chemistry**, Affiliated East-West Press Pvt. Ltd., New Delhi, 1968.

Russel S.Drago, **Physical Methods in Chemistry,** Saunders, Philadelphia, 1977.

PCH 3523O - CHEMICAL THERMODYNAMICS AND PHOTOCHEMISTRY

SEMESTER III (THEORY)

5 hrs/ week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I & II	Recognize the principles that govern equilibrium and non-equilibrium thermodynamics.
III & IV	• Describe the different types of thermodynamic statistics. • Identify the statistical approach to describe the thermodynamics of a system
V	Apply the concepts of photochemistry to define the various photochemical processes.

COURSE OUTLINE:

UNIT I: EQUILIBRIUM THERMODYNAMICS 15 hrs

General review of enthalpy, entropy and free energy concepts-genesis of third law and its limitations-thermodynamics of systems of variable compositions-partial molar quantities and their determination- chemical potential-Gibbs-Duhem equation- Gibbs-Duhem-Margules equation-fugacity and its determination- choice of state- Activity and activity coefficients- electrolytes and non electrolytes- equilibrium thermodynamics-Gibbs phase rule and its application to three component system.

UNIT II: NON-EQUILIBRIUM THERMODYNAMICS 15hrs

Non-equilibrium thermodynamics-introduction-conservation of mass and energy-entropy production-entropy production in chemical reactions-entropy production and entropy flow in open systems-transformation properties of rates and affinities-Onsager's theory- validity of Onsager theory and its verification- the principle of microscopic reversibility and Onsager reciprocal relations-thermoelectricity-electro kinetic effects- thermomolecular pressure difference-thermomechanical effect-transference of electrolytes in aqueous solutions-stationary non-equilibrium states-irreversible thermodynamics of biological systems-irreversible thermodynamics of non linear regime.

REFERENCE BOOKS:

Atkins P.W., **Physical Chemistry,** Oxford University Press, 1998.

Klotz, **Chemical Thermodynamics**, Prentice Hall, 1950.

Kuriakose and Rajaram, **Thermodynamics for students of Chemistry**, Shoban Lal Nagin Chand, 1986.

McQuarie D.E. & J.D. Simon, **Physical Chemistry**, University Science Book, California, 1977

Samuel Glasstone, **Thermodynamics for Chemists**, Affiliated East West Press Ltd, 1947.

Horia Metiu, **Physical Chemistry – Thermodynamics,** Taylor & Francis, 2006.

Sears and Salinger, **Thermodynamics, Kinetic Theory and Statistical Thermodynamics**, Narosa Publishing House, 1975.

UNIT III: STATISTICAL THERMODYNAMICS I 15 hrs

combinatory rule - probability theorem - Permutations and combinations- concept of ensembles energy states and energy levels- Macro states and micro states - **Maxwell-Boltzmann statistics** -- thermodynamic probability, Sterling's approximation, Legrange's undetermined multilplier,

distribution functions – **Partition function and thermodynamic functions**- molar partition function- entropy and third law – separation of partition function- translational, rotational, vibrational and electronic partition functions, combined partition function- equilibrium constant and partition function.

UNIT IV: STATISTICAL THERMODYNAMICS II **15 hrs**

Quantum statisitics-Bose-Einstein and Fermi-Dirac statistics- photon gas - Bose Einstein condensation, degeneracy and Bose Einstein condensation, application to liquid He. Electron gas, degeneracy and electron gas. Heat capacities- principle of equipartition of energy -rotational degrees of freedom- specific heat capacity of diatomic gas- heat capacities of solids- paramagnetism- population inversion- negative kelvin temperature .

REFERENCE BOOKS:

Atkins P.W., **Physical Chemistry**, Oxford University Press, 1998.

Gupta M.C., **Statistical Thermodynamics**, Wiley Eastern, 1990.

Kuriakose and Rajaram, **Thermodynamics for Students of Chemistry**, Shoban Lal Nagin Chand, 1986.

McQuarrie D.A., and Simon A., **Physical Chemistry: A Molecular Approach,** Viva Books Pvt. Ltd., New Delhi, 2003.

Science Reporter, **Article on Probability**, August 2000.

Sears and Salinger, **Thermodynamics, Kinetic Theory and Statistical Thermodynamics**, Narosa Publishing House, 1975.

UNIT V: Photochemistry **15 hrs**

Introduction –Laws of Photochemistry (Recall) **Photophysical processes**- Jablonski diagram- types of photophysical pathways, fluorescence, phosphorescence, delayed fluorescence, effect of Temperature on emission processes-**Photophysical kinetics**- unimolecular and bimolecular processes, quenching of fluorescence, Stern–Volmer equation, Principle of chemical actinometry – – **Photochemical processes** – classication and types, rate constants and life times of reactive energy states, Time resolved single photon counting techniques, effect of light intensity on the rate of photochemical reactions- Chemiluminescence and photosensitization-**Physical properties of electronically excited molecules** – potential energy diagram – Frank Condon principle – dipole moment – pk* values – redox potential –geometry - Wigner's spin conservation rule

REFERENCE BOOKS:

Houston, Paul L., **Chemical Kinetics and Reaction Dynamics**, McGraw-Hill, Inc, Singapore, 2001.

Robert A. Alberty, **Physical Chemistry**, John Wiley & Sons, 1987.

Rohatgi- K.K. Mukherjee, **Fundamentals of Photochemistry**, New Age International Publisher, New Delhi, 1978.

Wayne R.P., **Photochemistry,** Butterworths**,** London, 1970.

Sharma A., and Schulman S.G., **Introduction to Fluorescence Spectroscopy,** John-Wiley and Sons, Inc., New York, 1999.

PCH 4621M – CHEMISTRY OF NATURAL PRODUCTS

SEMESTER IV (THEORY)

6 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	Discuss the chemistry of heterocycles and supramolecules.
II	Compare the structures and functions of DNA and RNA
III, IV & V	Elucidate the structure of selected steroids, alkaloids, terpenoids, vitamins and carbohydrates.

COURSE OUTLINE:

UNIT I: HETEROCYCLICS AND SUPRAMOLECULES 18hrs

Heterocyclics – Nomenclature – compounds containing two hetero atoms – azoles - **the chemistry of** pyrazole, imidazole,oxazole, isoxazole, thiazole and isothiazole – diazines – **the chemistry of** pyridazine, pyrimidine and pyrazine.

Introduction to Supramolecular chemistry – Physical and chemical characteristics of supramolecules -**Preparation and structure** of catenanes and rotaxanes - molecular recognition – **Synthetic applications of** calixarenes and cyclodextrins – **organic reactions on solid supports like** zeolite, clay, alumina and silica – dendrimers.

REFERENCE BOOKS:

Acheson R M, **Chemistry of heterocyclic compounds**, Wiley Eastern, 1973.

Andre Loupy, **Solvent free reactions, Topics in Current Chemistry**, vol 206, page 155-173, 1999.

Bansal R K, **Heterocyclic Chemistry**, Wiley Eastern, 1990.

Dodziuk H., **Introduction to Supramolecular Chemistry**, Kluwer Academic, 2002

Finar I.L., **Organic Chemistry**, V.2, 6TH Edition, ELBS, Singapore, 1994.

Gilchrist T.L., **Heterocyclic Chemistry**, 1st edition, John Wiley & Sons, 1985.

Gupta R R, Kumar M, Gupta V, **Heterocyclic Chemistry**, Vol 2, Spriger Verlag, 2002

Joule J A and Mills K**, Heterocyclic Chemistry**, 4th edition, Blackwell Science, 2000.

Joule J.A. & G.F. Smith, **Heterocyclic Chemistry**, 2nd edition, ELBS, 1986.

Lehn J. M.**, Supramolecular Chemistry**, **Concepts and Perspectives**, VCH, 1995.

Nasipuri D**, Stereochemistry of Organic Compounds – Principles and applications**, 2nd edition, New Age International, 2002.

Steed J. W., J. L. Atwood, **Supramolecular Chemistry**, A Concise Introduction, John Wiley, 2000.

UNIT II : CHEMISTRY OF PROTEINS AND NUCLEIC ACID 18 hrs

Classification of amino acid – proteins – classification of proteins – peptide linkage – primary structure of peptides – synthesis of peptides – spatial arrangement of protein molecules – factors influencing the stability of protein secondary, tertiary and quaternary structure of protein – biosynthesis of protein.

Nucleic acid - structure of–nucleosides – nucleotides - **structure and function** of RNA – DNA – genetic code.

UNIT III : BIOORGANIC CHEMISTRY **18 hrs**

Steroids – Introduction, constitutional study of cholesterol, stereochemistry of steroids, Bile acids

Steroid hormones – structural elucidation of progesterone, Androsterone

Hormones in chemical communication.

Antibiotics:

Structural elucidation, synthesis and Biological activity of penicillins, chloramphenicol and streptomycin.

REFERENCE BOOKS:

Agarwal O.P., **Chemistry of Organic Natural Products, V.1& 2,** Goel Publishing House, 15th edition, 1992.

Finar I.L., **Organic Chemistry**, V.2, 6TH Edition, ELBS, Singapore, 1994.

UNIT IV: CHEMISTRY OF NATURAL PRODUCTS **18 hrs**

Structural elucidation and synthesis of **Terpenoids** - Monocyclic sesquiterpenoids – Zingiberene - Bicyclic sesquiterpenoids - Eudesmol

Alkaloids – General methods of determining the structure - Quinoline alkaloids- Quinine, - Opium alkaloids - Morphine.

Biosynthesis of alkaloids & Terpenoids.

Anthocyanins and Flavones

Natural occurrence – **structural elucidation** of cyanidine chloride– Quercitine

REFERENCE BOOKS:

Agarwal O.P., **Chemistry of Organic Natural Products**, **V.1,** Goel publishing house, 15th edition, 1992.

Finar I.L., **Organic Chemistry**, V.2, 6TH Edition, ELBS, Singapore, 1994.

UNIT V: LIPIDS, CARBOHYDRATES AND VITAMINS **18 hrs**

Classification – conformation of monosaccharides – Hudson's rule - Methods to determine the size of the ring – **disaccharides**- sucrose – maltose – **polysachharides** – cellulose – starch – chitosan

Lipids – Introduction – biological function – classification of lipids – chemical properties – analysis of oils and fats.

Structural elucidation and synthesis of vitamins A, B_1, B_2, B_6, C & D.

REFERENCE BOOKS:

Conn E.E, P.K Stumpf and Doi, **Biochemistry,** John Wiley ,1992.

Finar I.L., **Organic Chemistry**, V.2, 6th edition, ELBS, Singapore, 1994.

Wade L.G., **Organic Chemistry**, 5th edition, Pearson Publications, 2003.

PCH4622M - RINGS, CAGES AND CLUSTERS

SEMESTER IV (THEORY)

5 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I	Explain the chemistry of boranes.
II	Review the various aspects of hetero ring systems.
III	Describe the structural aspects of metal clusters.
IV & V	Apply B^{11}, N^{15}, F^{19}, Si^{29}, P^{31} NMR spectroscopic techniques to arrive at the structure of compounds.
	Explain the principle and applications NQR, Mossbauer, PES.

COURSE OUTLINE:

UNIT I: BORANES **15 hrs**

Boron and multicentre bonding – boron cages – vacuum technique of synthesis – lower and higher boranes (B_2H_6,B_4H_{10},B_6H_{10},$B_{10}H_{14}$,$B_{12}H_{12}^{2-}$) – reactions – structure and bonding – topological treatment – Wades rule – styx numbers – carboranes ($C_2B_{10}H_{12}$,$C_2B_8H_{10}^4$, $Na_3CB_{10}H_{11}$,$C_4B_2H_6$) – metallocarboranes ($C_2B_9H_{11}^{2-}$) – other hetero atom boron derivatives – borazines – boroxines.

UNIT II: Si-O, P-N and S-N SYSTEMS **15 hrs**

Silicates – principles of silicate structure – aluminates – zeolites – organosilicon compounds – polymerization of cyclic siloxanes – mechanism of polymerization reactions – silicones – silicones in technology .

Synthesis of P-N skeleton – hydrolysis of phosphazenes – reactions of halophosphazenes-theories of bonding – electronic structure and aromaticity.

S-N heteroatom systems – synthesis – S_4N_4 compounds and poly thiazyl $(SN)_x$.

UNIT III:.METAL CLUSTER **15 hrs**

Metal atom cluster – di,tri, tetra, and hexa nuclearity carbonyl clusters –cluster structure based on electron counting schemes – capping rule- isoelectronic and isolobal analogy – structure implications- relationship between fragments – their synthetic utility.

UNIT IV: **APPLICATIONS OF NMR,NQR and Mossbauer** **15 hrs**

B^{11} ,N^{15} ,F^{19}, Si^{29}, P^{31}NMR applications in the structural problem solving of inorganic compounds.

NQR – principle-effect of magnetic field (Zeeman effect) on spectral characteristics – relation between EFG and molecular structure – applications – phase transitions, hydrogen bonding, chemical bonding, biomolecules.

Mossbauer – theory – quadrupole interaction and magnetic interaction – applications to spin free, spin paired Fe complexes structure of carbonyls and nitrosyls- application to the compounds of tin.

UNIT V: PHOTOELECTRON SPECTROSCOPY **15 hrs**

Theory of XPS and UPS- determination of ionization potential –chemical

identification of elemtens-ESCA-koopman theorem,chemical shift – application of UPS in the energy level determination of NH_3,H_2,O_2,CO,H_2O and HCl vibrational fine structure and their orgin- evaluation of vibrational constant from UPS.

REFERENCE BOOKS:

Advances in Inorganic Chemistry, Radio Chemistry Volumes Review articles.

Allcock H.R., **Heteroatom ring systems and polymers**, Academic press, New York, 1967.

Allock H.R., **Phosphorus, Nitrogen compounds**, Academic press, New York, 1967.

Delhi 2005.

Gray L.Miessler and Donald A.Tarr **Inorganic chemistry,**Third edition,Pearson Education Ltd.,New

Greenwood N.N. and Earnshaw A., **Chemistry of the Elements**, Pergamon Press, Oxford, 1984.

Heal H.G., **The Inorganic heterocyclic chemistry of sulphur, nitrogen and phosphorus**, Academic press, New York, 1980.

James E.Huheey, **Inorganic Chemistry,** Fourth edition, HarperCollins College Publishers, 1993.

Keith F. Purcell and John C.Kotz, **Inorganic Chemistry**, W.B.Saunders Company, 1997.

New Delhi, 1968.

Ray N.H., **Inorganic Polymers**, Academic press, New York, 1978.

Relevant research articles from **Inorganic Chemistry** Journals.

Russel S. Drago, **Physical Methods in Inorganic Chemistry**, Affiliated East-West Press Pvt. Ltd.,

Russel S.Drago, **Physical Methods in Chemistry,** Saunders, Philadelphia, 1977.

PCH4623M - ADVANCED TOPICS IN CHEMISTRY

SEMESTER IV (THEORY)

5 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit

I
- Describe the various methods of representing molecules in a chemical database.
- Employ techniques for carrying out similarity searching
- Design new drug molecules using computational tools

II Explain the fundamentals principles of the various computational methods.

III Discuss the advanced concepts in magnetic resonance techniques.

IV Differentiate the concepts of macro, micro and nanoscale materials

Define the materials in nanoscale dimension

Identify a suitable characterization method for nanomaterials

V Describe the synthesis, characterization, properties and applications of nanomaterials.

COURSE OUTLINE:

UNIT I: ELEMENTS OF CHEMINFORMATICS **15 hrs**

History of chemoinformatics, Definition of Chemoinformatics, Computer representation of molecules, Introduction to chemical structure file formats. Linear, 2D and 3D representations. Connection Tables, Molecular structure Searching techniques – 2D substructure searching, 3D database searching- sources of data for 3D database- Introduction to Molecular Fingerprints,

Properties of similarity and distance coefficient- Tanimoto Coefficient, Eucledien distance - Molecular descriptors- pharmacophore keys, Applications of 3D database searching and Docking.

Chemical databases- Chembank, ChemPDB, Combichem, NCI- Pubchem (Compounds, Substances, Bioassay), PubMed, DrugBank, , ChemSpider .

Reference Books

Andrew R. Leach, Valerie J. Gillet. **An Introduction to Chemoinformatics,** revised edition, Springer, Netherland, 2007.

Larsen et al (ed), **Textbook of Drug Design and Discovery**, 3rd edition, Taylor and Francis, London and NewYork, 2004.

Leach A.R, **Molecular Modelling: Principles and applications**, 2nd edition, Prentice Hall, New Delhi, 2001.

UNIT II: COMPUTATIONAL CHEMISTRY **15 hrs**

Fundamental principles - Ab initio methods – Hartree Fock approximations – semi empirical methods – density functional theory – Basic theory – Linear scaling techniques – molecular mechanics - Basic theory – existing force fields – molecular dynamics and Monte Carlo simulations.

Reference Books

Ira. N. Levine, **Quantum Chemistry**, 5th edn., Prentice Hall of India, 2000.

Young D. C., **Computational Chemistry: A Practical Guide for Applying Techniques to Real-world Problems**, Wiley, 2001.

UNIT III: ADVANCED NMR SPECTROSCOPIC TECHNIQUES **15 hrs**

Non-first order spectra- AX_2, AB_2, A_2B_2, A_2X_2 and ABC spin systems- coupling in aromatic systems - coupling in heteroaromatic systems- simplification of non-first order spectra – spin-spin coupling and double irradiation techniques – INDOR, SPI - variable temperature NMR - multipulse techniques in NMR – 2D NMR – Application of the following techniques for structural elucidation ^{1}H-^{1}H COSY- ^{1}H-^{13}C COSY-HETCOR-HMQC-HMBC,NOSY,INADEQUATE – MRI - CIDNP.

Reference Books

Banwell & Mc Cash, **Fundamentals of Molecular Spectroscopy**, 7th edition, Tata Mc Graw Hill Publishing Co. Ltd. New Delhi, 1999.

Pavia, Chapman and Kriz, **Introduction to Spectroscopy**, 3rd edition, Thomson Asia Pte. Ltd, Singapore, 2001.

Silverstein R.M., G.C. Bassler, T.C. Morill, **Spectrophotometric Identification of Organic Compounds**, 6th edition, John Wiley & Sons, New York & London, 1998.

Straughan and Walker**, Spectroscopy-Volume I, & II,** Chapman and Hall, London, 1976.

William Kemp, **Organic Spectroscopy**, 3rd edition, ELBS, 1991.

UNIT IV : NANOMATERIALS I **15 hrs**

Introduction- Definition of the terms-nano, nanoscale, nanomaterials, nanoscience and nano technology. Scale of materials- natural and man-made-**History-**Nanoscience in ancient,

Medieval and modern times-**Fabrication Methods**-top-down and Bottom-Up approaches-**quantum confinement and quantum nanostructures**- 0D,1D and 2D nanomaterials-**Thermodynamics of small systems**- Surface energy and surface area of nanomaterials-**Characterisation Methods-**Electron Probe, scanning probe, spectroscopic methods and determination of particle-size by light scattering methods.

UNIT V : NANOMATERIALS II **15 hrs**

Synthesis, Characterization, properties of Nanomaterials-**zero-D materials**-C_{60}, metallic colloids and semiconductor quantum dots-**1D materials**-carbon nanotubes, gold nanorods- **2D materials**-self-assembled monolayers, graphenes-Applications of CNT(FET and as storage devices), self-assembled monolayers (sensor and catalysis applications), semi conductor quantum dots (imaging and diagnosis), metallic nanoparticles(medical and sensor applications), graphenes ( )

REFERENCE BOOKS:

Charles P. Poole Jr., Frank J. Owens, **Introduction to Nanotechnology**¸ John Wiley & Sons, New Delhi, 2006.

Hornyak, Dutta, Tibbals & Rao**, Introduction to Nanoscience,** CRC press, Boca Raton, 2008.

Klabunde J. (Ed.), **Nanoscale materials in Chemistry,** Wiley-Interscience, New York, 2001.

Lynn E. Foster, **Nanotechnology Science, Innovation and Opportunity**, Pearson Education, New Delhi, 2006.

Rao C.N.R., A. Müller, A.K. Cheetam, (Eds.), **Nanomaterials Chemistry**, Wiley – VCH, Weinheim, 2007.

PCH 4521M - PRINCIPLES AND APPLICATIONS OF ELECTROCHEMISTRY

SEMESTER – IV (THEORY)

4 hrs / week

LEARNING OUTCOMES:

On successful completion of this course, the student will be able to

Unit	
I & II	Differentiate the ionic and electrodic part of an electrochemical reactions.
III	Recognize the importance of electrochemistry in energy storage and conversion.
IV	Illustrate the significance of electrochemistry in carrying out organic reactions.
V	Identify the cause and control for corrosion.

COURSE OUTLINE:

Unit I: IONICS **12 hrs**

Ionic Interaction-Nature of electrolytes,Ion activity, Ion –ion interaction, activity coefficients, Ion-solvent interaction, Debye-Huckel theory, Debye-Huckel equation, limiting and extended forms, Applications of Debye-Huckel equation, Ion transport in solutions

UNIT II: ELECTRODICS **12 hrs**

Interfacial phenomena-Electrode electrolyte interface, Double layer structure, polarized and non-polarised electrodes, Helmoltz-Perrin theory, Guoy-Chapman theory, Stern theory-**Electrode Kinetics**-Non-equilibrium electrode potentials, exchange current density, Butler-Volmer equation, one-step-one-electron process, Symmetry factor and transfer co-efficient. Current density and Overvoltage, Tafel equation.

REFERENCE BOOKS

Bard and Faulkner, **Electrochemical Methods Fundamentals and Applications,** 2nd edition, John Wiley and Sons, 2004.

Bockris and Reddy, **Modern Electrochemistry, Vol I& II,** 2nd edition, Springer, New Delhi, 2000.

Samuel Glasstone**, An Introduction to Electrochemistry**, Affiliated East- West Press Private Limited, Chennai, 1942.

UNIT III: ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE 12 hrs

Batteries – Primary Batteries – Zn/MnO_2 batteries, primary lithium batteries – Zn-silver oxide batteries, zinc air cells. Secondary Batteries- lead-acid batteries – nickel-cadmium batteries, Modern Batteries – Nickel-metal hydride batteries, lithium secondary batteries. Fuel cells – History – Types of fuel cells – H_2 / O_2 fuel cells – Direct methanol fuel cells - types of H_2 / O_2 fuel cells – Alkaline fuel cells – phosphoric acid fuel cells - Molten carbonate fuel cells – Proton exchange membrane fuel cells (PEM Cells).

REFERENCE BOOKS:

Antrapov, **Theoretical Electrochemistry**, Mir Publishers, Lausanne, 1972

Bockris and Reddy, **Modern Electrochemistry, Vol I& II**, 2nd edition, Springer, New Delhi, 2000.

Crow (DR), **Principles and Applications of Electrochemistry**, 3rd edition, Chapman Hall, London, 1988.

Rieger (Philip – H), **Electrochemistry,** Ed(II), Chapman & Hall, London, 1994.

Samuel Glasstone**, An Introduction to Electrochemistry**, Affiliated East- West Press Private Limited, Chennai, 1942.

Sawyer (D.T) & Robert (J), **Experimental Electrochemistry for chemists**, John Wiley and Sons, New York, 1995.

Viswanathan B.,M.Aulice Scibioh, **Fuel Cells-Principles and Applications,** Universities Press, Hyderabad, India, 2006

Unit IV: ELECTRO ORGANIC CHEMISTRY 12 hrs

Chemically modified Electrodes – Introduction- Types of electrode modification – Electro catalysis at modified electrodes – Oxidation of small organic molecules at modified electrodes- **Introduction to electronanochemistry**.

REFERENCE BOOKS:

Allen J. Bard & Larry R. Faulkner, **Electrochemical methods,** 2nd edition, John Wiley & Sons (Asia) Pvt. Ltd. Singapore, 2004.

Bockris and Reddy,**Modern Electrochemistry, Vol IIB,** Plenum /Rossetta edn, 1970.

Unit V: CORROSION 12 hrs

Definition and importance of corrosion, causes of corrosion, Types of corrosion, Thermodynamics of corrosion and electrode potential– Poubaix diagrams, mechanism of corrosion, measurement of corrosion rate, Corrosion inhibition.

REFERENCE BOOKS:

Bockris and Reddy,**Modern Electrochemistry Vol. 2B,** Plenum /Rossetta edn, 1970.