HAJEE KARUTHA ROWTHER HOWDIA COLLEGE (AUTONOMOUS)

UTHAMAPALAYAM

Choice Based Credit System
M.Sc., Chemistry (Semester)

Course Scheme & Scheme of Examinations

(Effective from the academic year 2013 – 2014 onwards)

Qualification : B.Sc.,as the major subject with physics as one ancillary. The other ancillary subject may be Mathematics or Botany or Zoology.

Duration of the Course: M.Sc., Chemistry - 2years (4– Semesters)

Medium of instruction: English

OBJECTIVES OF THE COURSE:

1. To gain knowledge on the basic and advanced level aspects in the different disciplines of chemistry.
2. To get an exposure to the basics in Nanochemistry and Biochemistry.
3. To gain knowledge on the basic and advanced level experimental techniques.
4. To get an exposure on some current trends in chemistry.

Question Paper: Three Parts A, B and C

Section – A - 10 x 1 = 10 marks (multiple choice, True or False)

Section - B - 5 x 7 = 35 marks (either A or B)

Section – C - 3 x 10 = 30 marks (3 out 5 questions)

Passing minimum for theory paper (External)-34 marks

Internal and external put together-50 marks

Mode of evaluation of Internal Assessment for the theory papers:

Seminar - 5 Marks Assignment - 5 Marks

Test - 15 Marks (Three tests: Best of Two)

Scheme of Examination

Year	Semester	Code	Paper	Credit	Internal	External	Total
I	I	13PCHC11	Introduction to organic Reactions	5	25	75	100
		13PCHC12	Structure and Bonding	4	25	75	100
		13PCHC13	Thermodynamics, Chemical Equilibrium and Electrochemistry	4	25	75	100
		13PCHE11	**Major Elective:** Medicinal and pharmaceutical Chemistry	5	25	75	100
		13PCHC1P	Inorganic Qualitative and quantitative analyses and Preparations	5	40	60	100
I	II	13PCHC21	Stereochemistry and Organic Reactions	4	25	75	100
		13PCHC22	Coordination and Organo metallic Chemistry	5	25	75	100
		13PCHC23	Group theory and Spectroscopy	4	25	75	100
		13PCHE21	**Major Elective:** Analytical Chemistry	5	25	75	100
		13PCHC2P	Organic Qualitative and quantitative analyses and Preparations	5	40	60	100
II	III	13PCHC31	Organic Spectroscopy and Natural products	4	25	75	100
		13PCHC32	Inorganic Spectroscopy and Nano chemistry	4	25	75	100
		13PCHC33	Quantum, Nano and Macromolecular Chemistry	5	25	75	100
		13PCHE31	**Non-Major Elective:** 1.Computer Applications 2.Environmental Science	5	25	75	100
		13PCHC3P	Conductometric and potentiometric Titrations and Kinetic, Adsorption and spectral Measurements	5	40	60	100
II	IV	13PCHC41	Biomolecules, Rearrangements and Synthetic methods.	4	25	75	100
		13PCHC42	Nuclear and Analytical Chemistry	4	25	75	100
		13PCHC43	Chemical Kinetics, Surface, Biophysical and Photochemistry	4	25	75	100
		13PCHE41	**Major Elective:** Polymer Chemistry	5	25	75	100
		13PCHC4P	Project Project- Viva- Voce	4	60	40	100
			Total	90			2000

Semester I

13PCHC11	Introduction to Organic Reactions	Hours-5 / Credits – 5

Objectives:

- **To create an idea about the minute studies of electron displacement**
- **To develop the synthetic aspect among the students**
- **Make the students to enter the gate way of mechanisms**
- **To learn how an organic reaction is takes place and how the rate Changes correspondingly**

Unit I: Electron displacement: Inductive and field effects-Bond distances- Bond energies-delocalized bonds-Cross conjugation-rules of Resonance-Resonance energies-Resonance effects-Steric inhibition of resonance-Hyper conjugation-Hydrogen bonding-Addition compounds-EDA Complexes-Crown ether complexes-Inclusion compounds-Effect of Structure on the dissociation constants of acids and bases-concepts of hard and soft acids and bases.

Introduction to reaction mechanism: Reaction Intermediates-Free radicals, Carbenes, Nitrenes, carbanions, carbocations-formation and stability of reaction intermediates-Methods of determination of reaction mechanism – kinetic and thermodynamic control of Chemical reactions. Kinetic and non-kinetic methods for determining organic reaction mechanism – principle of microscopic reversibility-energy profile diagram-Hammond postulate.

Unit II: Aliphatic Nucleophilic substitutions: Nucleophilicity and basicity-SN1 and SN2 Mechanisms-Effect of substrate structure-Effect of the attacking Nucleophile -Effect of the leaving group - Effect of the reaction medium-ambident nucleophiles- ambident substrate-Neighbouring group participation of n, π and σ electrons-SNi mechanism-Nucleophilic substitution at an Aliphatic trigonal carbon-Nucleophilic substitution at allylic carbon-Nucleophilic substitution at a Vinyl carbon.

Aliphatic electrophilic substitution: Electrophilic substitution at saturated carbon-SE1 mechanism, SE2 and SEi mechanism.

UNIT III: Sterochemistry – 1: Symmetry elements and point group classification-concept of chirality, necessary and sufficient condition for chirality- relationship between substrate symmetry and chirality. Projection formulae -Wedge, Fischer, Sawhorse and Newmann. Optical isomerism due to centre of chirality. Molecules with one stereogenic center (Chiral centre) and

molecules with more than one chiral centre. Properties of enantiomers and disastereoisomers. Erythro and Threo nomenclature. Configuration - determination of configuration. Cahn, Ingold and Prelog system of designation of configuration.

Geometrical Isomerism: E-Z nomenclature-determination of configuration of geometrical isomers using physical and chemical methods- stereoisomerism in monocyclic compounds (upto six membered rings)

UNIT IV: Aromatic character: Aromatic character in Benzene, six membered rings, five, seven and eight membered rings- other systems with aromatic sextets-Huckel's rule- Craig's Rule- concept of Homoaromaticity and Antiaromaticity-Systems with 2, 4, 8 and 10 electrons-systems with more than 10 electron- Alternate and Non-alternate hydrocarbons. Chemistry of Cyclopentadienyl anion Fulvene, Azulene, tropolone, sydnones, annulenes.

Novel ring systems: Nomenclature of Bicyclic and tricyclic systems-Chemistry adamantane, Diamantane, (congressane), cubane and catenanes.

UNIT V: Oxidation and Reduction: Elimination of hydrogen and aromatization reactions – catalytic dehydrogenation-mechanism, applications and stereochemical aspects of the following oxidations- reduction reactions: Oxidation reactions involving CrO_3, SeO_2, OsO_4, Lead Tetraacetate, Periodic acid, N-Bromosuccinimide, H_2O_2-Oppenauer oxidation.

Catalytic hydrogenation-reactions involving lithium aluminum hydride, Triisobutylalumino hydride, DIBAL and Sodium Borohydride-Birch reduction-Meerwin-pondoff-verley reduction-wolff-krishner reduction-Huang minlon modification-Hydroboration-Selectivity in Oxidation reduction.

Regents in organic synthesis: Gilman's reagents (Lithium dimethyl cuprate), lithium diisoproylamide (LDA), Dicyclohexylcarbodiimide, 1,3-dithane, Trimethyl silyl iodide, Tri-n-butyl tin hydride, Wood and Prevost hydroxylation, DDQ, Merrifield resin, Phase transfer catalyst, Peterson's synthesis. Baker yeast.

Suggested Readings:

1. P. Skyes, Guidebook to Mechanism to in organic chemistry, Orient Longman, 1976.
2. Jerry March, "Advanced Organic Chemistry: Reactions, Mechanisms and Structure", 5th Edition, Wiley (2000).
3. E.S. Gould, Mechanism and structure in Organic chemistry, Henry Halt & Co. Newyork, 1959.
4. J. Shorter, Correlation analysis in organic chemistry, Clarendon press, Oxford, 1973
5. R. T. Morrison, R.N. Boyd, Organic chemistry, Prentice-Hall, 6th edn, 2001.
6. I. L. Finar, "Organic Chemistry", Volume-II, 5th Edition (1975).
7. T. H. Lowry and K. S. Richardson, "Mechanism and Theory in Organic Chemistry", 2nd Edition, Harper and Row, 1981.

8. Reinhard Bruckner, Advanced Organic chemistry, Reaction mechanisms, Academic Press, 2002.
9. F. A. Carey and R.J. Sundberg, Advanced Organic chemistry, Part B, 4th Edition. Plenum Publishers, 2001.
10. R.O.C. Norman, Organic synthesis, 3rd Edition, 1993.
11. W. Carruthers, some modern methods of organic synthesis, Cambridge university press, 2nd edition, 1982.
12. Ho. House, Modern synthesis reactions, W.A. Benkjamin, Inc., California 2nd Edition, 1972.
13. P. S. Kalsi, "Stereochemistry", Wiley Eastern Ltd, 1990.
14. P. Ramesh, Basic principles of Organic stereochemistry, Meenu publications, Madurai, 2005.

Semester I

13PCHC12	Structure and Bonding	Hours-5 / Credits – 4

Objectives

- **To identify the geometry of the molecules.**
- **To know the properties of various bonds.**
- **To study the different types of solids and their electrical conductivity.**
- **To evaluate the chain, ring and cage structures in certain inorganic compounds.**
- **To study about metals in detail.**

Unit I: Nature of chemical bonds

Covalent bond: Hybridization - calculation of s and p characters-Bent's rule-M.O. theory; LCAO approximation-application of MOT to heteronuclear diatomic molecules like $BeCl_2$, BeH_2 and H_2O-concept of multicentered bond as applied to electron deficient molecules like diborane and metal alkyls - VSPER theory - Walsch diagram.

UNIT II: Bond properties and ionic bonding: Ionic radii-covalent radii-van der Waals radius-bond length-Bond order-bond energy, bond polarity-partial ionic character of covalent bonds-electronegativity-electron affinity-lattice energy-Born Haber cycle-Covalent character in Ionic compounds-Different types of electrostatic interactions -Hydrogen Bond.

UNIT III: Solid state chemistry: Crystal defects-points, line and plane defects- Colour centers - Non-stoichoimetry on physical properties-Electronic structure of solids- Free electron and band theories-Types of solids-Electrical conductivity and superconductivity-High temperature superconductors-Types of semiconductors-Thermo-electric power and Hall effect-Photovoltaic effect-Semiconductors in solar energy conversion.

UNIT IV: Inorganic chains - Rings and cages: Silicates: Various silicate structures-structure, property, correlation-silicones.

Poly acids: Classification-isopolyacids like polymolybdate, polyvanadate and polytungstate-their structures - heteropolyacids: 12A, 12B, 9 and 6 heteropolyacids- preparation and structures.

Phosphazenes and its polymers -Phosphonitrile compounds-S_4N_4-Polymeric sulphur nitride (Polythiazyl) cage compounds: Nomenclature of Boranes and carboranes-Wades rule-STYX number- preparation and structure of B_4H_{10}, $C_2H_{10}H_{12}$, $(B_{12}H_{12})_2$-- Boranzine.

UNIT V: Occurrence, isolation, purification, properties and uses of the following metals as well as their important compounds: Be, Ge, Ti, Zr, Th, V, Pu, U and Platinum.

Suggested readings:

1. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry", 5th Edition, John Wiley & Sons, Singapore, 1998.
2. K.M. Mackay and R. A. Mackay, Introduction to Modern Inorganic chemistry, 4th Edn. Prentice Hall, New Jersy, 1989.
3. James E. Hugheey, Ellen A. Keitler and Richard L. Keitler, Inorganic Chemistry, 4th Edn, Harper COllins COllege Publishes, New York, 1993.
4. P. W. Atkins, D. k. Shriver and C. H. Langfood, Inorganic Chemistry, Oxford ELRS, UK, 1990.
5. K.F. Purcell and J.C. Koltz, An introduction to Inorganic Chemistry, W.B. Saunders Company, Philadelphia, 1980.
6. N.B. Hanny, SOlid State chemistry.

Semester I

13PCHC13	**Thermodynamics, Chemical Equilibrium and Electrochemistry**	**Hours-5 / Credits – 4**

Objectives

- **To get an idea about the concepts of second law of thermodynamics, derivation of equations & absolute entropy.**
- **To enable the students to understand the effect of pressure and temperature on phase equilibrium.**
- **To study phase rule.**
- **To understand about statistical thermodynamics.**
- **To learn about Electro chemistry and its applications.**

UNIT I: Thermodynamics: Second law thermodynamics-concept of entropy-Gibbs function-Gibbs Helmholtz equation-Maxwell relations-Thermodynamic equation of state-Thermodynamics of systems of variable composition- Partial molar quantities, partial molar volume- chemical potential, Gibbs-Duhem equation-Experimental determinations of fugacity of real gases and its determination-Third law of thermodynamics - Absolute entropies-Determination of absolute entropies-Exception to third law- Unattainability of absolute Zero.

UNIT II: Chemical and Phase Equilibria: Reaction free energy/Reaction potential-Reaction isotherm and direction of spontaneity - Standard reaction free energy-its calculation from thermo chemical, electrochemical and equilibrium data-Temperature coefficient of reaction free energy and equilibrium constant.

Gibbs phase rule-its thermodynamic derivation - Application of phase rule to three component systems - Formation of one pair, two pairs and three pairs of partially miscible liquids-Systems composed two solids and a liquid.

UNIT III: Statistical Thermodynamics: Aims of statistical thermodynamics -definition of state of system - ensembles (micro, macro and grand canonical)-Boltzmann distribution law and its deviation-Boltzmann-Planck equation-Partition functions-Thermodynamic properties from partition functions-partition function and equilibrium constant-Quantum statistics- Fermi-Dirac and Bose- Einstein's statistics-Photon gas and electron gas according to such statistics-population inversion-Einstein's and Debye's theories of heat capacities of solids. Nuclear spin statistics-

Statistical basis of entropy of H_2 gas - Ortho and Para nuclear states- Calculation of residual entropy of H_2 at 0K in terms of ortho-para ratio.

UNIT IV: Electrochemistry I: Theory of electrolytic conductance -inter-ionic attraction-ionic atmosphere -thickness of ionic atmosphere-The Debye-Huckel-Onsager conductance equation-its deviation and experimental verification - deviations and modifications -Debye Falkenhagan and Wein effects-mean ionic activity and activity coefficients of strong electrolytes.

The role of electrodes- the electrochemical potential -types of electrodes-the gas/inert metal electrode-ion/insoluble salt/metal electrode-oxidation-reduction electrode-liquid junction potential and membrane potential-Electrochemical cells -kinds of cells-notation-electrochemical cell reactions -EMF of cells -Nernst equation- Application of EMF measurements -determination of equilibrium constant, dissociation constant, solubility product and potentiometric titrations.

UNIT V: Electrochemistry II: The electrical double layer and Zeta potential -perrin, Gouy-Chappman and stern models-polarisable and non-polarisable interfaces-electrokinetic phenomena-dynamic electrochemistry-electrode processess and non-equilibrium electrode potential -over potential -Butler Volmer equation -Tafel equation-Current-potential curves-hydrogen over voltage.

Application of electrochemical processess -power generation and storage- Fuel cells-storage batteries and dry cells-Principles of inhibition of corrosion-cyclic voltammetry-Photo electrochemistry and electrochemiluminescence.

Suggested Readings:

1. S. Glasston, Thermodynamics for chemists, East-west Press Private Ltd., New Delhi.
2. J. Rajaram and J.C. Kuriakose, Thermodynamics (III Edn.) Shoban Lal Nagin, Chand & Co., Ltd., New Delhi (1999)
3. B.R. Puri, L.R. Sharma and M.S. Pathania, Priciples of Physical Chemistry (Millenium Edn.) Vishal Publishing Co., (2003)
4. Gurdeep Raj, Advanced Physical Chemistry (25th Edn.,) Goel Publishing Co., (2001)5. D. A. McQuarrie and J.D. Simons, Physical Chemistry - A Molecular Approach, viva Books (P) Ltd., New Delhi (1998)
6. P.W. Atkins, Physical Chemistry. VI Edn., ELPS and Oxford University Press (1996)
7. S.H. Maron and J. B. Lando, Fundamentals of Physical Chemistry, MacMillan Publishing Co., New York (1974)
8. D. N. Bajpai, Advanced Physical Chemistry, S. Chand & Company Ltd., New Delhi (1998)
9. A. Findlay, The Phase Rule and its Applications, Campbell and Smith.
10. A. W. Adamson. Physical Chemistry of Surfaces, 5th Edn., John wiley & Sons, New Delhi (1990).

11. D. Attwood and A. T. Florence, Surfactant Systems-Their chemistry, Pharmacy and Biologyl, Chapman and Hall, New York (1983)

Semester I
Major Elective

13PCHE11	**Medicinal and Pharmaceutical Chemistry**	**Hours-5 / Credits – 5**

Objectives:

- **To study about the drugs and their interactions with various organs of humans.**
- **To learn the synthesis of new drug molecules and their biological activities.**
- **To ascertain the elucidations of drugs interactions with receptors viz., DNA and enzymes.**
- **To know the therapeutic uses of steroids, antibiotics, antihistamines, antihypertensive drugs, anti inflammatory drugs and CNS stimulants etc.**

UNIT I: Fundamentals of Medicinal Chemistry: Definitions of Medicinal Chemistry, Pharmacology and Molecular Pharmacology-major process involved in drug action-pharmacokinetics phase –Quantitative structure –Activity relationship (QSAR)-Hansch approach –concept of bio-isomerism pharmacodynamics phase –receptors and classification of membrane bound receptors-enzyme inhibitors as drugs (illustrated with one example).

UNIT II: Medicinally useful antibiotics and steroids: Structural features and mode of action of the following antibiotics –penicillin G, cephalosporin and their semi synthetic analogs (β-lactum), streptomycin (aminogylcoside), terramycin (tetracyclin), erythorymycin (macrolide) and chloramphenicol.

Physiologically active steroids - their structural features and therapeutic use. Oral contraceptives, anabolic steroids, anit-inflammatory steroids.

UNTI III: Chemotheraopeutic agents:

Antineoplastic agents: Classification, synthesis, Assay e.g., Cyclophosphamide, Ifofamide, Chlorambucil, Busulfan, Decarbazine, Methotrexate, Azathioprine, 6-Mercaptopurine, 5-

fluorouracil, Cisplatin, Carnplantin, Anti-tubercular drugs: Classification, synthesis, Assay, e.g., Isoniazid, Rifampicin, Pyrazinamine, Ethambutol, Thiacetoazone, Paramino salicylic acid and Ethionamide.

Antimalarial drugs: Classification, synthesis, assay, e.g., Chloroquin, Primaquine, Amaodiaquine, Mefloquine, Proguanil Pyrimethamine, Diuretics: Classification, Synthesis, Assay e.g., Furesemide, Acetazolamide, Chlorothiazide.

UNIT IV: Synthesis and Therapeutic action and SAR of certain drugs:

Antihypertensive drugs: Nifedipine, Captopril, Hydralazine, Sodium nitropruside, clonidine, methyldopa and guanothidine.

Antihistamines: H1-Antagonists: Pheniramine, Chlorpheniramine, Diphenylhydramine, Mepyramine, Promethazine, H2-Antogonist: Cimetidine, Ranitidine and Fomotidine.

UNIT V:

Anti-inflammatory drugs: Antipyretics & Non-narcotic analgestics; Aspirin, sodium salicylate, Paracetamol, phenylbuttazone, Oxypheylbutazone, Ibuprofen, Mefenamic acid, Dichlofenac sodium.

CNS stimulant Drugs: Amphetamine, Caffeine, Therobromine, Theophylline, Bemegride, Nikethamide, Methy Phenidate and peracetum.

CNS Depresent Drugs: Phenelazine, Isocarboxazide, Imipramine, Nortiptyline, Amitriptyline, Desipramine.

Suggested Reading:

1. G.L. Patrick, An introduction to Medicinal chemistry, II Edn. Oxford University Press, 2001.
2. T. Nagradi, Medicinal Chemistry – A Biochemical Approach, Oxford University Press-2004.
3. J. B. Taylor and P.D. Kennewall, Introductory Medicinal Chemistry, Ellisworth Publishers, 1985.
4. C. Laxmi, Medicinal Chemistry.
5. B. Jeyasree Ghosch, Pharmaceutical chemistry
6. Ashutoshkar Medicinal Chemistry.

SEMESTER II

13PCHC21	Stereochemistry and Organic Reactions	Hours-5 / Credits – 4

Objectives:

- **To study about the stereochemistry of organic compounds and their nomenclature.**
- **To assign the conformation and configuration of simple acyclic, monosubstituted and disubstituted cyclohexanes.**
- **To understand the mechanism of electrophilic, nucleophilic and free radical addition reactions and also know about E1, E2 AND E1CB elimination reactions.**
- **To get knowledge about terpenoids and vitamins.**

Unit I: Stereochemistry II – Prochirality and prostereoisomerism, enantiotopic and disatereotopic ligands and faces and their nomenclature – pro-R and pro-S and Re and Si faces. Stereospecific and stereoselective reactions. Asymmetric synthesis; Cram's rule and Prolog rules. Optical isomerism due to axial chirality – biphenyl, allenes and spiranes. Molecules with planar chirality- paracyclophanes, trans cyclooctene and ansa compounds.

Unit II: Conformational analysis: Configuration and conformation – conformations of ethane and n-butane – conformation analysis – stereo-electronic and steric-factors – conformation of simple acyclic compounds – conformation of monosubstituted and disubstituted cyclohexane – correlation of the conformation of acyclic and cyclic systems with their physical and chemical properties – conformational free enery – Curtin- Hammett principle- Quatitative treatment of mobile system – Eliel-Ro equation – conformation and reactivity of cyclohexanones- conformational analysis of aldohexaopyranoses.

Unit III: Addition to multiple bonds: Electrophilic, nucleophilic and free radical additions – addition to conjugated systems – orientation of the addendum – stereochemical factors in reactions like addition of hydrogen, halogen, hydrogen halide and hypohalous acids. Hydroboration and hydroxylation – epoxidation.

Addition to carbonyl groups – mechanism – Aldol condensation – Perkin reaction- Knoevenagel reaction- Mannich reactions – Cannizaro reaction – Benzoin condensation- Claisen ester condensation – Darzen's reaction – Reformatsky reaction – Wittig reaction- Grignard reactions.

Addition to α, β-unsaturated carbonyl groups – addition of Grignard reagent to α, β-unsaturated carbonyl compounds – Michael addition – Diels- Alder reaction – addition to carbenes and carbenoids to double and triple bonds.

Esterification of acids and hydrolysis of esters – decarboxylation of carboxylic acids.

Elimination: α-elimination - β-elimination – E1 and E2 and E1CB mechanisms- Stereochemistry of elimination – orientation of the double bond – effect of changes in the substrate, base, leaving group and medium on E1, E2 and E1CB reactions- elimination vs. substitution- pyrolytic cis elimination- Bredt's rule.

Unit IV: Terpenes: Classification of terpenoids-struture, stereochemistry and synthesis of α-pinene, camphor, zingeberene, codinene, α-santonin, abietic acid and sqalene.

Vitamins: Struture and synthesis of Vitamins A, B1, B2, B6 and B12 (Strutural features only) C, E, and H and K.

Unit V: Aromatic electrophilic substitution – orientation –reactivity-mechanism of nitration, halogenations, Friedel-Craft's reaction and sulponation –partial rate factors- ortho/para ration – Quantitative treatment of reactivity of reactivity of the electrophile (the selectivity relationship) – Aromative nucleophilic asubstitituon reactions - SNAr, SN1 and benzyne mechanisms.

Quatitative treatment of the effect of structure on reactivity – The Hammett relationship – significance of reaction and substituents constants – application of the Hammett equation in reaction mechanism –limitations and deviations.

Suggested Readings:

1. E. L. Eliel, S.H. Wilen & L.N. Mander, Stereochemistry of carbon compounds, John Wiley & Sons, 2003.
2. V.M. Potapov, Stereochemistry, MIR Publishers, Moscow, 1979.
3. I.L.Finar, Organic Chemistry, vol. II, 5th edn. ELBS, 1975.
4. D. Nasipuri, Stereochemistry of organic compounds. Principles and Applications, New Age International (P) ltd., 2nd edn. 1994.
5. P.S. Kalsi, stereochemistry, conformation and mechanism, New Age international (p) ltd., 4th 1997.
6. T.H. Lowry and K. S. Richardson, Mechanism and Theory in Organic Chemistry.
7. E.S. Gould, Mechanism and Structure in Organic chemistry, Henry Holt & Co., New York, 1959.
8. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 4th edn., 2000.

9. Reinhard Bruckner, Advanced organic chemistry, Reaction mechanism, Academic press, 2002.
10. F. A. Carey and R.J. Sunderberg, Advanced Organic chemistry, part B, 4th edn., Plenum Publishers, 2001.
11. Paul de Mayo, chemistry of Tenpenoids, vol. I & II, academic Press.
12. L. Fieser and Mary Fieser, Steroids, Methuen & Co., New York, 1965.
13. S.F. Dyke, Chemistry of vitamin, Interscience Publishers, 1965.

Semester II

13PCHC22	**Coordination and Organometallic Chemistry**	**Hours-5 / Credits – 5**

Objectives:

- **To ascertain theories of bonding and geometries in coordination Compounds.**
- **To understand the reaction mechanism of coordination compounds.**
- **To study the role of metal ions in biological systems.**
- **To know the role of enzymes and co enzymes in biological systems.**
- **To learn the reaction mechanism, structure, synthesis of inorganic Complexes.**

UNIT I – Coordination compounds: IUPAC Nomenclature of coordination compounds- isomerism in coordination compounds –Types of ligands –monodentate , ambidentate and macro cyclic ligands – Stability constants – Factors affecting Stability constant in solution – Determination of Stability constant Spectrophotometrically, polarographic and potentiometric methods.

Theories of bonding – VB –CFT – MO theories – Splitting of d-orbitals in Octahedral, Tetrahedral and Square planar and trigonal bipyramidal geometries –CFSE calculation in terms of Dq-Factors affecting crystal field splitting – Spectrochemical series –Magnetic properties of transition metal complexes – Calculation of spin-only magenetic moments –Quenching of orbital magnetic moments.

UNIT II – Reaction mechanism of coordination compounds: Substitution reactions of octahedral complexes – labile –inert complexes –mechanisms of acid hydrolysis –base hydrolysis and anation reactions. Substitition reactions of Square planar complexes – Factors

affecting reactivity of Square planar complexes – The trans effect and its applications – electron transfer reactions – completementary reactions – outer sphere and inner sphere electron transfer mechanism – Synthesis of coordination compounds using electron transfer and substitution reactions.

UNIT III – Bioinorganic chemistry I: Porphyrin ring system – metalloporphyrins –hemoglobin and myoglobin structures and work functions – synthetic oxygen carriers –cytochromes – structures and work functions in respiration – chlorophyll- structure – photosynthetic sequence – iron-sulphur proteins (non-heme iron protein) – Copper containing proteins – classification – blue copper proteins – structure of blue copper electron transferases – copper proteins as oxidases –Cytochrome C oxidase – mechanism studies of C oxidase – Hemocyanin.

UNIT – IV: Bioinorganic chemistry II: Carboxypeptidase A: structure, function – carbonic anhydrase – inhibition and poisoning – corin ring system-vitamin B_{12} coenzyme –in-vivo and in-vitro nitrogen fixation – essential and trace elements in biological systems – metal ion toxicity and detoxification –molecular mechanism of ion transport across the membrane – sodium and potassium ions pumps –chelate therapy – *cis*-plantin.

UNIT – V Complexes of π-acceptor ligands: Synthesis, structure and bonding in metal carbonyls, nitrosyls, dioxygen complexes and dinitrogen complexes-Application of EAN rule. Synthesis, properties, structure and bonding Ferrocene, Arene, Olefin, acetylene and allyl complexes.

Catalysis using organometallic compounds: Oxidative addition – reductive elimination – insertion reaction-Catalytic mechanism in the following reactions-hydrogenation of olefins (Wilkinson catalytic) – Tolmann catalytic loops-hydroformylation (oxo process) – acetic acid from ethanol-oxidation of alkenes to aldehydes and ketones (Wacker process)- catalysis in the formation of synthesis of gas-olefin polymerization (Ziegler-Natta) – Cyclo oligomerization of acetylenes (Reppe's catalyst or Wilke's catalyst) Olefin isomerization using Ni catalyst.

Suggested Readings:

1. W. E. Addison, Structural Principles of Inorganic Chemistry, Wiley, 1961.
2. A.F. Wells, Structural Inorganic Chemistry, 4th Ed, Oxford, New York, 1975.
3. F.A. Cotton and G. Wilkinson, Advances Inorganic Chemistry, 5th Ed, John Wiley & Sons, Singapore, 1988.
4. K.F. Purcell and J.C. Kotlz. An Introduction to Inorganic Chemistry, W. B. Sanders. Company, Philadelphia. 1980.
5. James E. Hugheey, Ellen A. Keitler and Richard, L. Keitler, Inorganic chemistry, 4th Ed, Harper Collins college Publishers. New York, 1993.

6. Y. Mido, Chemistry in Aqueous and nonaqueous solvents, Discovery publishers house, NewDelhi, 1969.

SEMESTER II

13PCHC23	Group theory and spectroscopy	Hours-5 / Credits – 4

Objectives:

- **To identify and concerned with the symmetry found in molecules and solids.**
- **To assign the modes of molecular vibrations to irreducible representations of point groups to which a molecule belongs.**
- **To determine which orbital's used for hybridization in chemical bondings and selection rules.**
- **To deals with the transitions that a molecule undergoes between its energy levels.**
- **To verify Quantum mechanical calculations on atoms, molecules.**

UNIT I: Group Theory: Molecular Symmetry elements and symmetry operations- Vector and matrix algebra- Symmetry operations and transformation matrices- Group- definition and properties of a group- Symmetry point groups- representation of a group- reducible and irreducible representations- Great orthogonality theorem- characters- construction of character tables- C_{2V}, C_{3V}, C_{4V} and D_{2d}- Direct product concept.

UNIT II: Application of Group Theory to spectroscopy and Molecular Problems:

Symmetry of normal modes of vibrations, application of group theory to normal modes of vibrations and to normal mode analysis- Symmetry properties of integrals- application for spectral selection rules of vibration spectra- IR and Raman active fundamentals. Symmetry of molecular orbitals and Symmetry selection rules for electronic transitions in simple molecules like ethylene, formaldehyde and benzene. Group theory and quantum mechanics- wave functions as the basis of irreducible representations- Group theory applied to hybridization- HMO theory- HMO calculations and delocalization energy for cyclopropenyl, butadiene and benzene systems.

UNIT III: Molecular Spectroscopy I: Electromagnetic spectrum- Types of molecular energies- Absorption and emission of radiation- Einstein's coefficient- induced emission and

absorption- Rotational spectra of rigid diatomic molecules- isotope effect in rotational spectra- Microwave spectrometer-Informations derived from rotational spectra.

Infrared spectroscopy- vibrational energy of a diatomic molecule- Infrared selection rules- diatomic vibrating rotator- vibrations of polyatomic molecules- overtone, combination and difference bands- concept of group frequencies- coupling interaction- Fermi resonance- Fourier transform infrared spectroscopy

UNIT IV: Molecular Spectroscopy II: Raman spectroscopy- Theories of Raman scattering- Rotational Raman spectra- Vibrational Raman spectra- Mutual exclusion principle- Laser Raman spectra- Electronic spectra of diatomic and polyatomic molecules-intensity of vibrational electronic spectra- Franck-Condon principle- rotation fine structure of electronic vibrational spectra- the Fortrat parabola- Dissociation and predissociation spectra.

NQR- principles and applications- quadrupole moment and electric field, nuclear quadrupole resonance, nuclear quadrupole coupling in atoms and molecules- identification of ionic character and hybridization.

UNIT V: Spin Resonance Spectroscopy: Magnetic properties of nuclei- Resonance condition- NMR instrumentation- Relaxation processes- Bloch equations- chemical shift- spin-spin splitting, relaxation times, line shape and line width experimental techniques- double resonance techniques, ENDOR, Overhauser effect, FT-NMR spectroscopy, Lanthanide shift reagents- NMR imaging.

ESR- principles of ESR- total Hamiltonian-hyperfine structure- ESR spectra of free radicals in solution- Anisotropic systems-systems in triplet state- Zerofield splitting in ESR and Krammers degeneracy**.**

Suggested Readings:

1) F.A.Cotton, Chemical Applications of Group Theory, 3nd Edn., John Wiley & Sons, New York (1999).
2) G.Davidson, Introduction to Group Theory for chemist, Applied Science Publishers Ltd, London(1971).
3) V. Ramakrishnan and Gopinath, Group Theory in Chemistry, 2nd edn.,Vishal publications,1991.
4) K.V.Raman, Group Theory and its application to chemistry. Tata McGraw-Hill (1990).
5) A. Streitweiser, Molecular Orbital Theory for Organic chemistry,John Wiley & Sons.
6) C.N.Banwell and E.M.Mccash, Molecular Spectroscopy, Tata McGraw-Hill,4th Edn.,(1995).

7) G. Arulhas, Molecular Structure and Spectroscopy, Prentice- Hall of India Pvt.,Ltd, New Delhi(2001).
8) R. S. Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977).
9) D.C.Harris and M.D. Bertolucci, Symmetry and Spectroscopy- An introduction to vibrational and electronic Spectroscopy, Oxford University Press, New York (1978).
10) G.H. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill.
11) R.Chang, Basic principles of Spectroscopy, McGraw-Hill, London (1976).
12) B.F.Straughan and S.Walker(eds), Spectroscopy, Vol 1,2 and 3,chapman & Hall, London(1976).
13) P.W.Atkins, Physical Chemistry, 6th edn., Oxford University Press, Tokyo (1998).
14) E.B.Becker, High Resolution NMR, 2nd edn.,Academic Press,1990.
15) A.Carrignton and A.D. McLachian, Introduction to Magnetic Spectroscopy, Harper and Row.
16) D. Shaw, Fourier Transform NMR Spectroscopy, Elsevier.

Semester II

Major Elective

13PCHE21	**Analytical Chemistry**	**Hours-5 / Credits – 5**

Objectives :

- **To recollect the mathematical significant among the students**
- **Make the students to infers the various laboratory techniques**
- **Create the knowledge to manipulate the electro chemical system**
- **To know the temperature dependent substances**

UNIT I: Precipitation Techniques: Introduction –properties and precipitating reagents-Colloidal precipitates-Co-precipitation –Post-precipitation –Precipitates from homogenous solutions – Surface adsorption –Drying and ignition of precipitates – Application of gravimetric methods.

UNIT II: Error Analysis: Error analysis: Classification of errors –accuracy and precision – minimization of errors – significant figures – significant figures in computation – statistical treatment of data- mean, median, standard deviation, variance, relative standard deviation – spread, errors – standard deviation of computed results-reliability of results-Q test, T-test –

confidence limit-comparision of results- Student's test –F-test T-test – comparison of the means of tow samples- correlation and regression: linear regression (least square analysis).

UNIT III: Electroanalytical Methods: Electroanalytical Techniques: Electrogravimetry: Theory of electrogravimetric analysis- Electro analytical separation and determination of metal ions, Coulometry: Electrolytic cell-work electrodes-auxilliary electrode and reference electrode – Coulometric titrations. Voltammetry; Cyclic voltammetry – stripping voltammetry – chromopotentiometry. Amperometry; Amperometric titrations.

UNIT IV: Thermoanalytical Methods: Thermal analysis; Theory and principles of DTA and TGA – factors affecting the position of DT and T G traces- application of DTA and TGA to the thermal behavior of the following compounds- crystalline copper sulphate, calcium oxalate monohydrate, calcium acetate monohydrate, ammonium nitrate, potassium chlorate with without catalyst, ammonium metavanadate, zinc hexafluorosilicate-complementary nature of DTA and TGA – principle and application of DSC –determination of degree of conversion of high alumina cement – purity determination –phase transition study – in forensic laboratory.

Unit-V: Spectroanalytical Methods: Colorimetry: Beer and Lambert's law –terminalogy – conditions for a satisfactory colorimetric analysis –methods of colour measurement or comparison -principles of colorimetric determinations of NH_3, Cr, Fe, Mn –simultaneous spectrophotometric determination of Cr & Mn.

Nephelometry and turbidometry :-determination of sulphate and phosphate – fluorimetry:principle –application of flourimetry in the determination of Ca ,Cd and Zn and determination of codein and morphine in a mixture –flame spectrometry :theory- interferences-AAS-applications in the determination of Mg^{2+}, Ca^{2+} in tap water, V in lubricating oil, trace lead in a Ferrous alloy and trace elements in contaminated soil.

Suggested Reading:

1. D. A. Skoog, D. M. West and F. J. Holler, Fundamentals of Analytical Chemistry, 7th Edition, Saunders College Publishing, Philadelphia, 1996.
2. Willard HH, Merritt LL, Dean JA, Settle PA. Instrumental Methods of Analysis, 6th Ed. New York: Van Nostrand, 1988.
3. J. Basset et al., Vogel's Text book of Qualitative Inorganic Analysis, Longman, 5th Edition, ELBS, Essex, 1989.
4. J. G. Dick, Analytical Chemical, Tata-McGraw Hill, 1973.

SEMESTER III

13PCHC31	Organic Spectroscopy and Natural Products	Hours-5 / Credits – 4

Objective

- **To study the different spectroscopes such as UV spectroscopy, IR spectroscopy and mass spectroscopy.**
- **To study about NMR spectroscopy through various aspects.**
- **To know chiro optical and analytical techniques in organic compounds and to study about chromatography**
- **To know about steroids and prostaglandins, also about certain alkaloids and antibiotics.**

Unit I : Spectroscopy I :

UV Spectroscopy: Principle – absorption spectra of conjugated dienes- α,β-unsaturated carbonyl compounds- Woodward-Fischer rules.

IR Spectroscopy: Molecular vibrations – vibrational frequency – factors influencing group frequencies – quantitative studies.

Mass Spectroscopy : Principle – type of ions – base peak – parent ion , meta stable and isotopic peaks – fragmentation – general rules – pattern of fragmentation for various classes of compounds - McLafferty rearrangement – Retro Diels-Alder reaction.

Unit II: Spectroscopy II:

^{1}H NMR Spectroscopy: Origin of NMR spectra – chemical shift – spin-spin coupling – coupling constant- first and second order spectra – spin-spin splitting – influence of stereo chemical factors on chemical shift or protons- simplification of complex spectra- deuterium substitution – spin decoupling – double resonance – shift reagents – Nuclear overhauser effect – CIDNP-NMR concept of aromaticity.

^{13}C NMR Spctroscopy: Basic principle of FT technique – Relaxation time – assignment of signals – Off resonance decoupling – additivity relationship- calculation of chemical shifts for aromatic and aliphatic compounds – DEPT ^{13}C spectra - ^{13}C-^{13}C correlation COSY, HETCOR, ROESY, NOESY and TOCSY- technique.

Unit III: Chiro optical and Analytical techniques:

ORD and CD – Principle- cotton effect- type of ORD curves- α-halo ketone rule- octant rule- applications to determine the configuration and conformation of simple mono cyclic and bi cyclic ketone and comparison of ORD and CD.

Chromatographic techniques: column- TLC, paper, GLC, HPLC, exclusion and ion exchange.

Unit IV : Steroids: Classification – configurational and conformational aspects of A/B cis and A/B trans steroids- complete chemistry and stereo chemistry of cholesterol (includes bile acids) chemistry of ergosterol and vitamin D – male sex hormones – androsterone- testosterone- female sex hormone- oestrone, equilenin and progesterone – a basic idea about adrenocortical hormones – cortisone (synthesis not included)

Prostaglandins. General study of prostaglandins- structure – chemistry of PGE1 and PGF1 α

Unit V alkaloids and antibiotics: general methods of structural determination – Hoffmann, Emde and Von Braun degradations. Structure and synthesis of quinine, papaverine, atropine , norcotine, morphine, reserpine and lysergic acid.

Antibiotics: definition, classification of antibiotics, structure, stereochemistry and synthesis of penicillin, chloramphenicol.

Suggested Readings:

1. John R. Dyer. Application of adsorption Spectroscopy, Prentice- Hall.
2. William Kemp, Organics Spectroscopy. ELBS, 3rd Edn.
3. Robert M. Silverstein, Francis X. Webster, Spectrometric Identification of Organic compounds, 6th Edn., John Wiley & Sons, Inc., 2004.
4. I. L. FInar, Organic chemistry, Vol. II. ELBS, 1975.
5. Paul de Mayo, Chemistry of Terpenoids, Vol. I & Vol II, academic Press.
6. L. Fieser and Mayr Fieser, Steroids, Reinhold, 1953.
7. W. Klyne, The chemistry of steroids, Methuen & Co., Newy York, 1965.
8. E.L. ELiel, Stereochemistry of carbon compounds, McGraw Hill, 1962.
9. P. Crabbe, ORD and CD in chemistry and Biochemistry, Academic Publishers 1972.
10. A, Brainth Waite and F.J. Smith. Chromatographic Methods, Chapman and Hall., 4th Edn. 1985.
11. K.W. Bently, Alkaloids, Vol I & II, Intersicence, 1957.

Semester III

13PCHC32	Inorganic Spectroscopy and NanoTechnology	Hours-5 / Credits – 4

Objectives;

- **To undertand the rearrangement mechanisms.**
- **To grow their spectroscopic knowledge about how to find out the NMR , ESR,IR ,UV active compounds**
- **To know the shift reagent's uses**
- **To compare the orbital degeneracy of various molecules**
- **To improve their ability to understand the spectral data's**

Unit I: Electronic spectra of transition metal complexes and photochemistry – d-d transition-charge transfer transition-selection rules-mechanism of breakdown of selection rules-bandwidths and shapes-John Teller effect-Tanabe-sugano Diagram-evaluation of 10Dq and β for Octahedral and Tetrahedral complexes of d^3, d^6 d^7 d^6 and d^8 configurations-Photochemistry-photoredox and photosubstitution reactions occurring in Co(III) and Cr(III) complexes-photochemistry of ruthenium polypyridyls.

Unit II: Application of Spectroscopy to the study of Inorganic compounds I:

Application of IR and Raman spectra in the study of coordination compounds-application to metal carbonyls and nitrosyls- geomentrical and linkage isomerism-detection of inter and intramolecular hydrogen bonding-stretching mode analysis of metal carbonyls.

Mossbauer and Photoelectron spectroscopy (PES): Mossbauer effect resonance absorption-Doppler effect –Doppler velocity –Experimental technique of measuring resonance absorption-isomer shift-magnetic hyperfine splitting –application of Mossbauer spectroscopy in the study of Iron and Tin complexes.

Photoelectron spectroscopy: Theory –XPEX-UV-PES- Instrumentation evaluation of Ionization potential –chemical identification of elements –Koopmann's theorem –chemical shift-UPS-XPES of N_2, O_2 and HCI-evaluation of vibrational constants from UPS – spin- orbit coupling –Auger spectroscopy –principles and its applications.

UNIT III: Application of spectropscopy to the study of Inorganic compounds II:

NMR Spectroscopy: ^{31}P - ^{19}F and ^{15}N –NMR –Introduction-applications in structural in problems –evaluation of rate constants –monitoring the course of reaction –NMR of Fluxional molecules –NMR of paramagnetic molecules –contact shifts and shifts Reagents

ESR spectroscopy: Principles –presentation of the spectrum –hyperfine splitting –evaluation of g and A tensors –factors affecting magnitude of g values –zero field splitting –Kramer's degeneracy-ESR of d^3 Octahedral complexes –anisotropy –hyperfine splitting constants-application of ESR in the study of transition metal complexes – John Teller distortion studying in Cu(II) complexes – Evaluation of spin orbit coupling

UNIT IV: Nano chemistry

Basic Idea of nano chemistry –defining nanoassemblies-measurements-examples-potential **uses** –Zero dimensional, one dimensional and two dimensional arrangements.
Nano tubes: Structure and characterization single walled carbon nano tubes –Nano tubes properties –applications of Nano tubes.
Nano Wires: Vapour phase-oxide assisted – carbo thermal growth of Nano wires- properties.
Nano Rods: Seed mediated growth of inorganic Nano tubes and Nano rods.
Nano structured Polymers: Conducting polymers –block –copolymers-Nano cages

UNIT V: Molecular Rearrangements and reaction of coordinated ligands
Molecular rearrangement of four coordinated complexes –six coordinated complexes-reation at coordinated ligands-reaction due to metal ion polarization of coordinated ligands-hydrolysis of amino acids –esters , amides and of peptides-Aldol condensation –Imine formation –hydrolysis and substituent exchange-the template effect and Macrocyclic ligands.

Suggested Readings:

1. F. Basalo and R.G. Pearson, Mechanism of Inoganic reaction, 2nd Edn., Wiley, New York, 1967.
2. Adamson, Concept of Inorganic Photochemistry, Wiley, New York, 1975.
3. S.F. Kettle, Coordination chemistry. An approach, Spectrum Academic Publishers, Oxford, 1996.
4. R.S. Drago, Physical Methods in chemistry, Sanders Golden Sunburst series, W.B. Saunders company, London, 1977.
5. I. Bertini et al. Bioinorganic chemistry, Viva Books Pvt Ltd, Chennai, 1998.
6. Chatwal Bhagi and Agarwal, Bioinorganic chemistry, sultan chand co., New delhi, 2001.

7. M.A. O. Hill and P. Day (Eds), Physical Methods in Advanced Inorganic chemistry, Interscience, Newyork, 1968.
8. R. S. Drago, Physical Methods in Chemistry, W.B. Saunders Co., London (1977).
9. K.F. Purcell and J.C. Kotlz. An Introduction to Inorganic Chemistry, W. B. Sanders. Company, Philadelphia. 1980.

SEMESTER III

13PCHC33	**Quantum Mechanics and Macro Nanochemistry**	**Hours-5 / Credits – 5**

Objectives;

- **To assign the formulation of Quantum mechanics for wave mechanical treatment of atom.**
- **To know about the probabilities of finding the particles at various locations in space.**
- **To get a key factors of which is the quantization of energy.**
- **To get a knowledge about the instrumentation used in nanoscience.**
- **To give a detailed notes about the large molecules and their properties.**

Unit I: The Birth of Quantum Mechanics Plank's explanation about Black body radiation – de Broglie concept of matter waves, Compton effect- Heisenberg's uncertainty principle and complementarity- operators- linear operator – method of getting the following quantum mechanical operator- position, momentum, kinetic energy, potential energy, total energy, angular momentum, raising and lowering and spin angular momentum

Postulates of quantum mechanics- hermicity and proving the quantum mechanical operators are hermitian- commutators – eigen function and eigen value- introducing dirac notation- expansion theorem. Orthogonality and normalization of wave function

Unit II: Application of Quantum mechanics to simple systems: Derivation of schrodinger wave equation –application of SWE to simple systems- free particle moving in one dimensional box- physical interpretation of the one dimensional problem- characteristics of wave function- average momentum of a particle in a box is zero- particle moving in 3-D box- degeneracy –

distortion – particle moving in a ring- rigid rotator – spherical harmonics- simple harmonic oscillator – Hermite polynomials- hydrogen atom problem- radial wave function- radial probability distribution – shapes of various atomic orbitals- Term symbols- LS coupling scheme- spectroscopic states.

Unit III: Approximation methods in Quantum mechanics: Need for approximation methods- schrodinger equation for He atom and other many electron system- the time independent perturbation theory(first order only)- application to hydrogen atom- variation theorem- application to hydrogen and helium atom- Hartee- fock- self consistent field (HFSCF) method of many electron system and its application to helium atom- electron spin and Pauli's principle- antisymmetric nature of the wave functions- Slater determinants- electronic configuration of many electron system- Born-Openheimer approximation –VB and MO theories, MO treatment of hetero nuclear and homo nuclear diatomic molecules.

Unit IV: Instrumentation in nano chemistry

Microscopic techniques for the characterization of nano materials- UV-VISIBLE and Fluorescence spectroscopy- AFM, SEM, TEM, X-RAY diffraction and micro analysis

Unit V: Macro molecules over view of polymers- types and properties of polymers- kinetics and mechanism of free radical, ionic , condensation and Zeigler-Natta polymerization process- emulsion and suspension polymerization techniques- polymer molecular weight and its distribution- molecular weight determination- osmotic pressure method- light scattering g method- ultra centrifuge method and viscosity method-conducting polymers.

Suggested Readings:

1. A. K. Chandra, Introductory Quantum Chemistry, 3rd Edn., Tata McGraw Hill Publishing Co., New Delhi, 1988.
2. M.W. Hanna, Quantum Mechanics in Chemistry, 2nd Edn., The Benjamin/Cummings publishing Co., London, 1969.
3. D.A. McQuarrie, Quantum Chemistry, 1st Indian Edn., Viva Books Pvt Ltd, New Delhi, 2003.
4. P.W. Atkins, Molecular Quantum Mechanics, 2nd Edn., Oxford University Press,, 1986.
5. C.P. Poole and F.J. Owens. Introduction to nanotechnology, 2004.
6. C.C. Koch Nano structured Materials.

Semester IV

13PCHC41	**Biomolecules, Photochemistry, Rearrangement and Synthetic methods**	**Hours-5 / Credits – 4**

Objective

- **To get a knowledge about carbohydrates, amino acids and nucleic acids.**
- **To analyse photochemistry and free radical formation in organic compounds.**
- **To understand the mechanisms involved in certain molecular rearrangements.**
- **To know about green chemistry and micro wave synthesis.**
- **To study about methods involved in various synthesis.**

UNIT I: Proteins, amino acids, Nucleic acids and Carbohydrates:

Classification of proteins – peptides – structure of peptides- synthesis of peptides – chemistry of glutathione and oxytocin – an elementary treatment of enzymes, coenzymes and nucleic acids- biosynthesis of amino acids.

Introduction to carbohydrates

Pyronose and furanose, forms of aldohexoses and keto hexoses – methods used for determination of ring size – conformation of aldohexopyranoses- structure and synthesis of maltose, lactose, sucrose and cellobiose.

UNIT II: Photochemistry & Free radicals:

Conservation of orbital symmetry – electrocyclic reactions – cycloaddition reactions and sigmatropic rearrangement – applications of correlation diagram approach, Frontier molecular orbital approach, Huckel-Mobius approach and Pertubation molecular orbital approach to the above reactions.

Photochemical reactions of ketones – photosensitization – Norrish I and II type reactions- Patternobuch reactions – Photooxidation – Photoreduction – Photochemistry of arenes.

Free radicals: Formation, detection and stability of free radicals – Free radical reactions- halogenation, addition, oxidation, reduction and rearrangement reactions- Barton, Sandmeyer , Gomberg-Bechmann, Ullmann, Pschorr and Hundicker reactions.

UNIT III: Molecular rearrangements:

Mechanism of the following rearrangement reactions: Wagner-Meerwin, Pinacol-Demzanov, Bechmann, Hoffmann, Curtius, Wolff, Baeyer-villiger, Stevens, Sommellet-Hauser, Favorskii, Benzil-bezillic acid, Claisen, Cope, Fries, Dienone-phenol, di-pi methane, hydroxiamino-p-aminephenol and benzidine rearrangement –Photochemical rearrangement.

UNIT IV: Green Chemistry I:

Principles of green chemistry – planning a green synthesis in a laboratory – general interest for solvent free processes- solvent free technique -Microwave synthesis: Introduction and characteristics of microwave heating – interaction of microwave radiation with the material – difference between conventional heating and microwave heating. Dielectric poloarization – dipoloar polarization – application and advantages of microwave heating over conventional heating.

UNIT V: Synthetic methods:

Planning a synthesis – Relay approach and convergent approach to total synthesis – Retro-synthetic analysis of simple organic compounds – functional groups interconversions –use of activating and blocking groups in synthesis – stereoselective problems of geomentrical and optical isomerism – steric crowding – Transition metals complexes in organic chemistry – Homogeneous hydrogenation –Regioselectivity-Diastereoselectivity –Enantioselectivity – Umpolung synthesis.

Suggested Readings:

1. A.I. Lehninger, Biochemistry, Nath Publications.
2. C.H. Depuy and O.L. Chapman, Molecular Reactions and Photochemistry, Prentice Hall, 1972.
3. S.M. Mukherji and S.P. Singh, Reaction Mechanism in Organic Chemistry, McMilan India Limited, 1978.
4. R.B. Woodward and R. Hofmann, The Conservation of Orbital Symmetry, Verlog Chemie GMBH and Academic Press, 1971.
5. Hung, The Chemistry of Free Radicals.
6. I.L. Finar, Organic Chemistry, Vol. II, ELBS, 1975.
7. P.De. Mayo, Molecular Rearrangements.
8. Jerry March, Advanced Organic Chemistry, John Wiley&Sons, 4thedn., 2000.
9. K.R. Desai, Green Chemistry (Microwave Synthesis) Himalaya Publishing House, Mumbai, 2005.
10. R.Sanghi and M.M. Srivastava, Green Chemistry (Environmental Friendly Alternatives), Narosa Publishing House, India, New Delhi, 2003.

11. A.k. Ahluwalia, Green Chemistry (Environmentally Benign Reactions) Aru Books India, New Delhi 2006.
12. R.E. Ireland, Organic Synthesis, Prentice-Hall of India Pvt. Ltd., 1975.
13. R.D. Morrison and R.N. Boyd, Organic Chemistry, Prentice-Hall, 6th edn., 2001.

Semester IV

13PCHC42	**Nuclear and Analytical chemistry**	**Hours-5 / Credits – 4**

Objectives:

- **To understand the fission and fusion mechanisms**
- **To grow their computer knowledge about browsing, programming**
- **To know the radioactive element's uses**
- **To compare the processes of Nuclear power reactor and breeder reactor**
- **Classify the various reactors**

Unit I: STRUCTURE OF NUCLEUS AND RADIO ACTIVE DECAY

Composition of the nucleus-nuclear size, shape and density –principal, radial and magnetic quantum numbers- magnetic and electric properties of nucleus –elementary treatment of shell (independent particle) model –nuclear configuration-parity and its conversion –mass defect and binding energy-nuclear forces theory.

Relative decay : Group displacement law –decay series –rate of disintegration – half life –average life –units of radio activity-secular and transient equilibria-theories of alpha decay, beta decay, gamma emission ,positron decay, nuclear isomerism, internal conversion and electron capture –Auger effect.

Unit II: NUCLEAR FISSION AND FUSION AND APPLICATION OF RADIOACTIVE ISOTOPES

Bethe's notation of nuclear process –nuclear reaction energies (Q value)-fission-energy release in nulear fission-mass distribution of fiision products-theory of nuclear fission – fissile and fertie isotopes-energy from nuclear fission –thermonuclear reactions in stars-classification of stars-power nuclear reactor-breedor reactor –nuclear reactors in India.

Applications of radioactive isotopes: characteristics of tracer isotopes – chemical investigations – age determination – medical field –agriculture –industry -analytical applications-isotope dilution analysis-neutron activation analysis –biological effects of radiation-waste disposal management

Unit III: ACTINIDES & LANTHANIDES: Chemistry of lanthanides and actinides : Lanthanides –Occurrence, extraction from ores –seperation procedure-ion exchange method – solvent extraction method .physical and chemical properties – Electronic configuration - common oxidation state –lanthanide contraction and its consequences- colour of lanthanide ions –magnetic properties of lanthanides-seperation of actinide elements - separation of pu from fission products -electronic configuration –oxidation state –comparision of lanthanides and actinides –position in the periodic table.

Unit IV: ELECTROANALYTICAL & THERMOANALYTICAL METHODS:

Electrogravimetry : Theory of electro gravimetric analysis –electrolytic separation and determination of metal ions. Coulometry: Electrolytic cell-working electrodes- auxiliary electrode and reference electrode-coulometric titrations .Voltammetry :Cyclic voltammetry-stripping voltammetry –chronopotentiometry.Amperometry: Amperometric titrations.

Thermoanalytical methods : Instrumentation and applications of thermogravimetry – Differential Thermal Analysis and Differential scanning colorimetry.

Spectroanalytical Methods: Spectroanalytical methods :Laws of absorption and quantitative law of luminescence –principles and applications of colorimetry and spectrophotometry, fluorimetry ,nepheleometry and turbidometry –emission spectroscopy and flame spectroscopy-atomic absorbtion , atomic emission and and atomic fluorescence spectroscopy –Optical rotator dispersion and circular dichorism

Unit V: COMPUTERS IN CHEMISTRY: History and development of computers, Mainframe ,micro and super computer systems -CPU and other peripheral devices –Evolution of programming language and higher level language .Syntax and structure of C language.

Internet –History of internet –the working of internet and internet services- applications of internet in chemistry –websites in Literature survey in chemistry –popular web sites in chemistry –data base in chemistry –downloading the attachment/ PDF files –opening,browsing and searching a web site –literature searching online .

E-mail: Introduction –working way –mailing basics e-mail ethics –advantages and disadvantages –creating e-mail id –receiving and sending e-mails.

Suggested Readings:

1. S. Glasstone, Source Book on Atomic energy, 3rd edn., Van Nostrand Reinhold Company, NewYork, 1967.
2. G. Friedlander, J.W. Kannedy, E.S. Macias and J.M. Miller. Nuclear and Radiochemistry, John Wiley & Sons Inc., New York, 1981.
3. H.I. Arnikar, Essentials of Nuclear Chemistry, 3rd Edn., Wiley Eastern Ltd.
4. U.N. Dash, Nuclear Chemistry, Sultan Chand and sons, New Delhi, 1991.
5. J. Basset et al. Vogel's Text book of Quantitative Inorganic Analysis, Longman, 5th Edn., ELBS, Essex, 1989.
6. H. H. Wilard, LL. Merritt and J.A. Dean, Instrumental Methods of Analysis, East-West Press, New Delhi, 1988.
7. D.A. Skoog and D.M. West, Fundamentals of Analytical Chemistry, Saunders College Publishing Co., Philadelphia, 1982.
8. J.G. Dick, Analytical Chemistry, Tata-McGraw Hill, 1973.
9. Alexis Leon and Mathews Leon, Fundamentals of Information Technology", Leon Vikas, Chennai, 1999.
10. Barbara Kasser, Using the Internet, 4th Edn., EE edition, New Delhi, 1998.
11. Sathyaprakash, Advanced Chemistry of Rar Elements, S. Chand & Col., 4th Edn., 1986.
12. T.Modlar, The chemistry of Lanthanides, Chapman and Hall, London, 1963.
13. H. D. Mathur and O.P. Tandon, Chemistry fo Rare Eleements, 3rd edn., S. Chand & Co., New Delhi, 1986.

Semester IV

13PCHC43	Chemical kinetics, Surface, Biophysical and Photochemistry	Hours-5 / Credits – 4

Objectives:

- **To concerns with measurements of rates of reactions.**
- **To determine the factors which influence rate of reactions.**
- **To study the rates of catalyst in rate of reactions.**
- **To get the knowledge about the adsorption on solids and liquid surface.**
- **To study the various chemical reactions by absorption of light radiations.**

UNIT I: CHEMICAL KINETICS I

Potential energy surfaces: Chain reactions-general characteristics- Steady state approximations-Study of kinetics of Chain reactions like H_2-Br_2 reaction-decomposition of N_2O_5 and acetaldehyde.

Unimolecular reaction rate theories-the simple Lindemann treatment- Hinshelwood's theory-Rice, Ramsperer and Kessel (RRK) theory-Advanced Unimolecular theory-Marcus theory or Rice, Ramsperer Kessel and Marcus (RRKM) theory-Slater's theory. Principle of microscopic reversibility and detailed balancing- Reactions in solution- influence of solvent dielectric constant, ionic strength (Bronsted-Bjerrum equation)-primary and secondary salt effects and pressure on reaction rates in solution-Significance of volume of activation.

UNIT II: CHEMICAL KINETICS II AND CATALYSIS:

Fast reactions techniques-chemical relaxation methods, temperature and pressure jump methods, ultrasonic absorption techniques, reactions in flow system, continuous and stopped flow, shock wave tube methods., chemical kinetics in crossed molecular beams- Flash photolysis- Spin resonance techniques in study of reaction kinetics.

Catalysis in biological systems-Enzyme catalysis-Michaelis-Menton kinetics-Lineweaver and Burk plot-Eadie's plot-influence of pH on the Enzyme catalysis. Heterogeneous catalysis-chemical reactions on solid surfaces- Kinetics and mechanism of Unimolecular and bimolecular

reaction- Langmuir, Hinshelwood's theory and Langmuir-Rideal mechanism-ARRT of surface reactions.

UNIT III: SURFACE CHEMISTRY

Introduction-Adsorption of gases on solids-Physisorption and chemisorptions-adsorption isotherm- Freundlich- Langmuir-BET- Temkin adsorption isotherm- Adsorption on liquid surface-surface tension-Gibbs adsorption isotherm-surface area determination- Electro kinetic phenomena at interfaces including electro osmosis and electrophoresis- Spreading of a liquid on another surfactant-monolayers-preparation of LB films- Micelles- Critical micellar concentration(CMC)-structure-bimolecular reaction occurring in a micellar solution-reverse micelles-micro emulsion- Application of photoelectron spectroscopy- ESCA and Auger spectroscopy to the study of surfaces.

UNIT IV: BIOPHYSICAL CHEMISTRY

Basic concepts of non-equilibrium thermodynamics- Onsager reciprocal relationship- Its application to biological systems- High energy metabolites- ATP and its role in bioenergetics-transfer of potential and coupled reaction- Biological energy conversion in catabolism and anabolism- role of singlet oxygen in biology- Biophysical applications of Mossbauer effect-NMR imaging- Applications of spin labeling in membrane research- Molecular recognition – An introduction to supra- molecular chemistry and photochemistry.

UNIT V: PHOTO AND RADIATION CHEMISTRY:

Physical properties of the electronically excited molecules- excited state dipole moments, pKa and redox potentials- photo physical processes in electronically excited molecules-fluorescence, phosphorescence and other deactivating processes. Stern-Volmer equation and its applications- electronically energy transfer mechanisms –photosensitisation and chemiluminescence. Experimental techniques in photochemistry- light sources-chemical actinometry- Elementary aspects of photosynthesis, photochemical conversion and storage of solar energy.

Radiation chemistry-source of high energy- interaction of high energy radiation with matter-radiolysis of water- definition of G value- mode of reactions of hydrated electrons- OH- and H+. Experimental techniques of radiation chemistry- Dosimetry- Elementary aspects of radiation chemistry in biology and industry.

Recommended Books:

1) K.J.Laidler, Chemical kinetics,3rd Edn.,Harper International Edn,London(1987).
2) K.J.Laidler,Theories of Chemical Reaction Rates, McGraw Hill Book Co., London(1969).
3) F.Wilkinson, Chemical kinetics and Reaction mechanism, Van Nostrand Reinhold Co.,New York(1980).
4) C.Kalidas, Chemical kinetic Methods, New Age International, 1996.
5) Margaret Robson Wright, Fundamental Chemical kinetics-An Explanatory introduction to the concepts,Horwood Publishing Ltd.,West Sussex 1999
6) A.W.Adamson, Physical Chemistry of surfaces,5th Edn., John Wiley & Sons, New York(1990).
7) D.Attwood and A.T.Florence, Surfactant Systems- Their chemistry, Pharmacy and Biology, Chapman and Hall, New York (1983).
8) K.K. Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern.
9) N.J. Turro, Modern Molecular Photochemistry,Benjamin Cummings.
10) Hamil, Williams and Mackay, Pronciples of physical Chemistry II Edn.,Prentice- hall of India,Pvt., Ltd., New Delhi(1968). (Radiation Chemistry)

Semester IV

Major Elective

13PCHE41	POLYMER CHEMISTRY	Hours-5 / Credits – 5

Objectives:

- **To know the types of polymers and mechanism of polymerization.**
- **To ascertain the preparation and uses of individual polymer.**
- **To study the properties and molecular weight determination of polymers**
- **To understand polymerization techniques**
- **To know the polymer processing**

Unit – I CLASSIFICATION OF POLYMERS AND CHEMISTRY OF POLYMERISATION

Classification of polymers: linear polymers, non-linear polymers, branched polymers, cross linked polymers, homo chains, hetero chains, homo polymers, co polymers, block polymers and graft polymers.

Chemistry of polymerization: Types of polymerization-mechanism-chain, growth, free radical, ionic, co-ordination, ring opening, metathetical, group transfer, polyaddition and polycondensation polymerizations.

Unit – II: INDIVIDUAL POLYMERS

Individual polymers: monomers required general methods of preparation, repeat units and uses of the following polymers and resins- polyethylene, polystyrene, polyacrylonitrile, polymethymethacrylate, PVC, polytetrafluoroethylene, polyisoprenes, polybutadienes and polychloroprene, polyesters. Polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, polyethyleneglycols, phenol-formaldehyde, urea-formaldehyde, melamine-formaldehyde and epoxy resins-silicone polymers.

Unit – III: PROPERTIES OF POLYMERS

Intrinsic properties-processing properties-article properties-basic idea of isomerism of polymers-configuration of polymer chain-geometrical structure-syndiotatic, isotatic and atatic polymers

Glass transition temperature: Definition-factors affecting glass transition temperature-relationships between glass transition temperature and (a) molecular weight, (b) melting point and (c) plasticizer-importance of glass transition temperature- heat distortion temperature.
Molecular weight and size of polymers: Number average, weight average, sedimentation and viscosity average molecular weights-molecular weights and degree of polymerization-poly dispersity-molecular weight distribution in polymers-size of polymer molecules- kinetics of polymerization.

Unit IV: POLYMERIZATION TECHNIQUES, DEGRADATION AND USES OF POLYMERS

Polymerization techniques: Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation polymerizations.
Degradation: Types of degradation-thermal, mechanical, ultrasonic and photodegradation-photostabilizers-oxidative degradation-antioxidants-hydrolytic degradation- Uses of polymers in electronics and biomedicine.

Unit – V: POLYMER PROCESSING

Polymer processing: Plastics (thermo and thermosetting), elastomers, fibres, compounding, plasticisers, colorants, flame retardants. Compression and injection mouldings-film extrusion and calendaring-die casting and rotational casting-thermofoaming-reinforcing.

Reference Books

1. V.R. Gowariker, N.V. Viswanathan and Jayadev Sreedher, "Polymer Science", Wiley Eastern Ltd., New Delhi 1986.
2. G. Odian, "Principles of Polymerisation", 2nd edn., John Wiley and sons, New York, 1981.
3. D.W. van Krevelen and P.J. Hoftyrager, "Properties of Polymers", Elsevier, New York, 1976.
4. B.K. Sharma, "Polymer Chemistry", Goel Publishing House, Meerut, 1989.
5. P.J. Flory, "Principles of Polymer Chemistry", Cornell Univ. press, Ithaca, 1953.
6. F.W. Billmeyer, "Text Book of Poymer Science", 3rd edn., John Wiley and sons, New York, 1984.
7. Harry R. Allcock, F. W. Lampe and J.E. Mark, " Contemporary Polymer Chemistry", 3rd Edition, Pearson, Prentice Hall, New Delhi 2005.

Semester III

Non-Major Elective

13PCHE31	Environmental Science	Hours-5 / Credits – 5

Objectives:

- **To know the environmental chemistry and pollution**
- **To ascertain air pollution , acid rain, Green house effect**
- **To study about water pollution and waste water treatment**
- **To understand soil pollution and radioactive pollution**
- **To study different methods of analysis of pollutants**

Unit:I INTRODUCTION AND CLASSIFICATION

Introduction- Environmental Science- Environmental chemistry-Ecology-Definition-Eco System-Cycling of mineral elements and gases-phosphate cycle-Carbon cycle-Hydrogen cycle-Nitrogen cycle-Hydrological cycle- Environmental segments-pollution and its types: air pollution-water pollution-soil pollution-radioactive pollution-thermal pollution-noise pollution-marine pollution-other types of pollution- and its effects and control- remedial measures.

Unit:II AIR POLLUTION

Introduction-sources of air pollution-air pollutants-classification and effects of air pollutants-oxides of nitrogen,sulphur and carbon-acid rain-effects and control- hydrogen sulphide-effects and control- carbon mono oxide-effects and control-photochemical smog-effects and control- fly ash- effects and control- green house effects-global warming-effects and control-ozone layer-ozone depletion-chlorofluoro carbons--effects and control.

Unit:III WATER POLLUTION

Introduction-types of water- Water pollution-sources of water pollution-water pollutants-classification-physical,chemical and biological-inorganic pollutants and toxic metals-organic pollutants-radioactive pollutants in water- pesticides and fertilizers- suspended particles- water quality-water quality index- ill effects of water pollutants-fluorosis-water pollution control-water treatment- primary, secondary and tertiary treatment-desalination-reverse osmosis-sewage and industrial waste water treatment.

Unit:IV SOIL POLLUTION

Introduction-types of soil- Soil pollution-types-indicators of Soil pollution-plants as indicators of pollution-sources of Soil pollution- fertilizers and pesticides- radio active pollutants- solid wastes- soil sediments as pollutant-soil erosion-treatment of soil pollutants-treatment of solid wastes- thermal methods-land filling-composting- land protection-remedial measures for Soil pollution.

Unit:V ANALYSIS OF POLLUTANTS

Introduction- analysis of air pollutants- units-sampling-devices and methods for sampling-measurement: UV-Visible spectrometry-IR spectrometry- emission spectrometry-turbidimetry nephelometry- gas chromatograpy-HPLC-chemiluminescence of nitrogen oxides-IR photometry-conductometry-analysis of water pollutants-units-sampling- devices and methods for sampling- measurement: UV-Visible spectrometry-titration-analysis of different water quality parameters- BOD- COD analysis and monitoring of pesticides, carcinogens and industrial pollutants.

Suggested Readings:

1. B.K.Sharma and H. Kaur, Environmental chemistry,Krishna Prakashan,Meerut,1997.
2. A. K. De, Environmental chemistry,Wiley Eastern Ltd., Meerut,1994.
3. A. K.Mukherjee, Environmental pollution and Health Hazards- causes and control, Galgotia press, New Delhi, 1986.
5. N. Manivasakam,physio-chemical Examination of water, Sewage and Industrial Effluents,
6. Pragati Prakashan Publ., Meerut, 1985

Semester I

Inorganic qualitative and quantitative analysis and preparations

1. Semi micro qualitative analysis: analysis of mixtures containing one familiar and one less familiar cations from the following:

   W, Pb, Tl, Se, Te, Mo, Cu, Bi, Cd, Ce, Th, Zr, Ti, V, Cr, Mn, Al, U, Ni, Co, Zn, Ca, Ba,Sr, Li and Mg.

2. Estimation of one metal in the presence of another by EDTA (demonstration)
3. In organic preparations; Preparations of atleast 6 (six) in organic complexes.
4. Quantitative analysis: separation and estimation of mixture by volumetric and gravimetric methods.

   Cu, Ni; Cu,Zn: Ba,Ca; Fe,Ni; Fe,Cu.

5. Preparation of one Ni (II) octahedral complex-its UV-visible spectrum-evaluation of 10Dq, B and β (Demonstration only).

Semester II

Organic preparation, Qualitative and Quantitative analysis

Qualitative analysis

Separation and analysis of two component mixtures. Identification of the components and preparation of solid derivative.

Quanitative analysis:

a. Estimation of glucose by lane and Eynon method and Bertrand method
b Estimation of glycine
c. Estimation of formalin
d Estimation of methyl ketone

Organic preparationS: (only for class work)

About 3 (five) two-stage preparation:

a. P-Nitro aniline from acetanilide benzophenone
b. P-Bromo aniline from acetanilide Aniline
c. m-Nitro benzoic acid from methyl benzoate

Semester III

Physical chemistry practical: conductometric and potentiometric titrations and kinetic adsorption and spectral experiments.

I Conductometric experiments

i Double displacement & acid base titrations

a) NH_4cl →NaOH→Mixture of CH_3COOH & HCL

b) NH_4cl →NaOH→Mixture of NH_4cl & HCL

ii Precipitation titration

a) Na_2CO_3→$Pb(NO_3)_2$→Na_2CO_3

b) K_2SO_4→$BaCl_2$→ K_2SO_4

II Adsorption experiments

Adsorption of oxalic acid/acetic acid on charcoal

III. Kinetic experiments

i. Kinetics of alkali hydrolysis of ester by potentiometric method

ii. Perdisulphate and iodide ion reaction : Study of primary salt effect and determination of the concentration of given KNO_3

IV Potentiometric methods

i. Precipitation titration :Ag+vs halide mixture

ii. Redox titrations : a)permanganate vs iodide ion

b)ceric ammonium sulphate vs ferrous ion

iii) Determination of dissociation constant of weak acids and pH of buffer solutions

iv) Determination of soplubility product of sparingly soluble salts.

V Titrations using pH meter

Determination of first ,second and third dissociatioin constants of phosphoric acid.

VI Experiments based on UV-Visible and Infra red spectrophotometers.

Semester IV

Project.