SRI KALISWARI COLLEGE, SIVAKASI

(An Autonomous Institution, Affliated to Madurai Kamaraj University,
Reaccredited with 'A' Grade by NAAC with CGPA 3.30)

DEPARTMENT OF CHMEISTRY

Programme Scheme of Examinations and Syllabi

(with effect from June, 2015)

PG Programme – M.Sc. (CHEMISTRY)

Programme Outcome for Postgraduate programmes

Knowledge

PO 1: Acquisition of advanced knowledge for higher studies and research.

PO 2: Synthesis of knowledge and critical thinking

Skills

PO 1: Life Skills and Skills for contribution to nation building.

PO 2: Acquisition of specialized skills for entrepreneurship/employability.

Attitude

PO 1: Acquisition of professional ethics and human values.

PO 2: National Integration and Social Commitment to Society.

Programme Specific Outcome for M.Sc Chemistry

- Students are supposed to have an advanced depth and detailed functional knowledge of theoretical concepts and experimental methods of chemistry.
- Broaden their professional foundations through activities such as teaching, internships, and fellowships.
- Capable to conduct analysis and interpretation of experimental data
- Able to communicate scientific results in writing and in oral presentation.
- Achieve the basic tools needed to carry out independent chemical research.
- Proficient in specialized area of chemistry and successfully complete an advanced research project.
- Proficient to conduct risk assessments concerning the use of chemical substances and laboratory procedures.
- Self awareness, to interact with other people in team working, and to work independently.
- Ability to work in a chemical, analytical and other related field.
- Gain knowledge of specific skills in planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques.
- Enable the students to be well prepared for the CSIR/UGC-JRF, NET, GATE, SET, TRB examinations.

Sri Kaliswari College (Autonomous) - Sivakasi
Choice based credit system
PG Programme - M.Sc (Chemistry) - 2015-2017
Semester-I
Core paper – I: CONCEPTS-REACTION MECHANISM AND STEREO CHEMISTRY-15PCHC11

Duration: 75 Hrs **Credits : 5**

Aim and Objectives

- Understand the basic concepts of electronic effects and their correlation analysis.
- Understand the mechanistic evidence for organic reactions.
- Know the concept of stereochemistry.
- Understand the mechanism of aliphatic electrophilic and nucleophilic substitution reactions.
- Understand the conformation of organic molecules.

Course Outcome:

- Get an idea about the basic concepts of organic chemistry
- Enhance the knowledge on chemical reactivity by theoretical approach
- Study the organic reaction mechanism by non kinetic methods
- Enhance the ideas about order, molecularity, kinetics of organic reactions and its kinetic measurement
- Gain knowledge about various aliphatic and aromatic substitution reactions
- Deepen the ideas of electrophilic substitution reactions
- Understand the concepts of chirality and its operations in organic molecules
- Knowing the concepts of asymmetric synthesis and geometrical isomerism
- Understand the concepts of conformation and its application to various organic molecules
- Enhance the knowledge on stereo chemical aspects of organic compounds

Unit I **(15 Hrs)**

Basic concepts

Electronic effects: Inductive and field effects- resonance - Hyperconjugation-hydrogen bonding and steric effect-influence of these effects on the acidity of organic acids, basicity of organic bases, stability of carbocations and carbanions.

Linear free energy relationship – Hammett equation-significances of reaction and substituent constants-application–limitations and deviations – Taft equation.

Unit II **(15 Hrs)**

Introduction to Reaction Mechanism

Kinetic methods of determining organic reaction mechanism- order – molecularity – rate – Activation energy - Energy profile diagram - Hammond postulate - kinetic isotopic effect.

Non kinetic methods, Reaction intermediates- Trapping of intermediates – isotopic labeling – cross over experiments – Principle of microscopic reversibility.

Unit III **(15 Hrs)**

Aliphatic nucleophilic and electrphilic substitution

Aliphatic nucleophilic substitution-Nucleophilicity and basicity- S_N1, S_N2, S_Ni, S_N1' , S_N2' and S_Ni' mechanisms- effect of substrate, attacking nucleophile, leaving group and solvents on S_N1 and S_N2 reactions- Neighbouring group participation of Π and σ electrons.

Aliphatic electrophilic substitution- - S_E1, S_E2 and S_Ei mechanisms.

Unit IV **(15 Hrs)**

Stereochemistry-I

Symmetry elements - Concept of chirality, prochiral center - prochiral face – homotopic, enantiotopic and diastereotopic faces and ligands - Optical isomerism of compounds with one and two chiral centers.

Cahn, Ingold and Prelog system of designation of configuration.

Asymmetric synthesis: Cram's rule – Prelog rule.

Geometrical Isomerism-E-Z nomenclature- determination of configuration of geometrical isomers using physical and chemical methods.

Unit V **(15 Hrs)**

Conformational Analysis

Configuration and conformation – conformation of simple acyclic compounds like 1,2 dichloroethane, ethylene glycol, butane-2,3-diol. Conformation of cyclohexane - monosubstituted and disubstituted cyclohexanes- cyclohexanone – α-halocyclohexanone – Decalin – aldohexopyranoses - conformational free energy- Curtin-Hammett Principles.

Reference:

1. P.Sykes, Guidebook to Organic Chemistry, Orient Longman, 1976.
2. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 4th edn., 2000.
3. E.S.Gould, Mechanism and Structure in Organic Chemistry, Henry Holt & Co., New York, 1959.
4. J.Shorter, Correlation Analysis in Organic Chemistry, Clarendon Press, Oxord, 1973.
5. R.T.Morrison and R.N.Boyd, Organic Chemistry, Prentice-Hall, 6th edn., 2001.
6. I.L.Finar, Organic Chemistry, Vol. II and II, 5th edn., ELBS, 1975.
7. Reinhard Brucker, Advanced Organic Chemistry, Reaction Mechanisms, Academic Press, 2002.
8. F.A.Carey and R.J.Sundberg, Advanced Organic Chemistry, Part B, 4th edn., Plenum Puplishers, 2001.
9. H.O.House, Modern Synthetic Reactions, W.A.Benjamin Inc., Califoria, 2nd edn., 1972.
10. P.Ramesh, Basic Principles of Organic Stereochemistry, Meenu Publications, Madurai, 2005.

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015-17
Semester – I

Core paper –II: Bonding and Solid state chemistry -15PCHC12
Duration -60 hrs **Credits: 4**

Aim and Objectives

- Understand the basic concepts of Inorganic chemistry.
- Know the characters of chemical bonds.
- Study the principles of solid state chemistry.
- Understand the concepts of polymer of inorganic material.

Course Outcome:

- Know the periodic properties and its trend in physical and chemical properties of inorganic compounds
- Enhance the knowledge on acid, base concepts and non aqueous solvents
- Understand the concepts of various types of solids and its properties
- Deepen the ideas of properties of solid into its various applications
- Gain knowledge on conductor, semiconductor and its application
- Idea about the defects of crystals and its application
- Understand the concept of theories on chemical bonding and its usage in the structure detection of inorganic molecules
- Enhance the ideas of ionic bond and its nature in crystal
- Know the concepts involved in the inorganic polymer and conducting inorganic polymers
- Increase the ides of electron deficient molecules, cluster compounds and its chemical reactions

Unit I **(12 Hrs)**

Basic concepts of Inorganic Chemistry

The Modern long form of periodic table - Periodic properties of elements - ionic radius - ionization potential - electron affinity - electro negativity scales.

Acids and Bases – Bronsted & Lewis concepts - pH, pK_a, buffer - Acid, base concept in non aqueous solvent - liq.ammonia, HF, anhydrous H_2SO_4 and N_2O_4.

Super acids - HSAB principle – Symbiosis – measurement and theoretical basis - application.

Unit II **(12 Hrs)**

Nature of Chemical bonds

Ionic bond: Lattice energy, Born-Haber cycle, Born-Lande equation (problems on Born-Lande expression to be worked out). Calculation of lattice energies of NaCl and MgO, effect of lattice energy on solubility of ionic compounds.

Covalent bond: Valence bond approach: hybridization and directional characteristics of sp, sp^2, sp^3, sp^2d, sp^3d^2.Shapes of $BeCl_2$, BF_3, $SiCl_4$, PCl_5, SF_6, Bent's rule. VSEPR theory: shapes and geometry of molecule containing only bond pairs of electrons, containing bond pair and lone pair of electrons of molecules and ions. Molecular orbital theory: Basic principles – MOT of H_2, He_2^+, Li_2, Be_2, N_2, O_2, O_2^-, O_2^{2-}, O_2^+ and CO, NO and its ions, HF, HCl (bond order, stability and magnetic properties to be discussed)

Unit III **(12 Hrs)**

Solid state Chemistry – I

Crystal systems and lattice types.Bravais lattices.Crystal symmetry.Introduction to point groups and space groups.Miller indices.Reciprocal lattice concept. Close packed structures: BCC, FCC and HCP,Voids. Coordination number.Ratius ratio rule and its applications.

X- Ray diffraction by crystals, Bragg's equation. of cubic crystals Diffraction methods: Powder, rotating crystal, Indexing and determination of lattice type and unit cell dimensions.

Crystal defects: Perfect and imperfect crystals. Point, line and plane defects. Thermodynamics of Schottky and Frenkel defects. Colour centers in alkali halide crystals. Defect clusters. Extended defects: Crystallographic shear structure and stacking faults. Dislocations and crystal structure. Structure of compounds of AX (Zinc blende, Wurtzite), AX_2 (Rutile, fluorite, antifluorite), A_mX_2 (Nickel arsenide), ABX_3 (Perosvskite, Ilmenite). Spinels: Inverse, spinel structures.

Unit IV **(12 Hrs)**

Solid State Chemistry-II

Electronic structure of solids. Free electron theory, band theory. Band structure of conductors, insulators and semiconductors and their applications. Colour in inorganic solids. Intrinsic and extrinsic semiconductors, doping of semiconductors and conduction mechanism, the band gap, temperature dependence of conductivity, carrier density and carrier mobility in semiconductors, synthesis and purification of semiconducting materials, single crystal growth, zone refining, fractional crystallization, semiconductor devices, rectifier transistors, optical devices, photoconductors, photovoltaic cells, solar batteries.

Unit V **(12 Hrs)**

Inorganic polymers

Sulphur-nitrogen compounds: Tetrasulphurtetranitride, disulphurdinitride and polythiazyl SxNy compounds. Sulphur-posphorous compounds: Molecular sulphides such as P_4S_3, P_4S_7, P_4S_9 and P_4S_{10}.

Phophorous-nitrogen compounds: Phosphazines, Cyclo and linear phosphazines.
Other P-N compounds.

Boron-nitrogen compounds: Borazine, and boron nitride. Boron hydrides: Reactions of diborane. Structure and bonding. Polyhedral boranes: Preparation, properties, structure and bonding. The topological approach to boron hydride structure.*Sytx*numbers, Wade's rules, Structural study by NMR. Carboranes. Metallocarboranes. Organoboron compounds and hydroboration.

Reference:

1. James E.Huheey, Ellen A.Keitler and Richard L.Keitler, Inorganic Chemistry, 4th Edn. Harper Collins College Publishers, New York, 1993.
2. P.W. Atkins, D.K. Shriver and C.H. Langfood, Inorganic Chemistry, Oxford ELBS. U.K, 1990.
3. K.F.Purcell and J.C.Koltz, An Introduction to Inorganic Chemistry. W.B.Saunders Company, Philadelphia, 1980.
4. Satya Prakash, G.D. Tuli, S.K. Basu and R.D. Madan, Advanced Inorganic Chemistry, Vol II , S. Chand & Company LTD, 2004 .
5. Y.Mido, Chemistry in Aqueous and Non-aqueous Solvents, Discovery

Publishers House, New Delhi, 1969.

6. N.B. Hanny, Solid State Chemistry

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015-17
Semester – I

Core paper –III : Chemical Thermodynamics and Electrochemistry – 15PCHC13
Duration -60hrs **Credits: 4**

Aim and Objectives :

- Understand the basic concepts of Chemical Thermodynamics.
- Know the basic principles of electrochemistry.

Course Outcome:

- Understand the concept of laws of thermodynamics and its need in chemistry
- Increase the knowledge on the need of partial molar properties and its derivation
- Apply the concepts of thermodynamics into quantum based thermodynamics
- Deepen the ideas of statistical thermodynamics by various statistical theory and heat capacity theories
- Gain knowledge on various types of conductance, conductance measurements and its application
- To know the concepts of electrolyte, electrolysis and its law
- To understand the various concepts such as common ion effect, pH measurement using electrochemistry
- To gain the knowledge on indicators and the theories behind indicator
- To deepen the idea of theory of strong electrolyte and its derivation
- To know the concepts of equilibrium and electrochemistry

Unit I **(12 Hrs)**

Chemical Thermodynamics-I

Second law of thermodynamics–Statement–Entropy-Definition and derivation of the concept of entropy-Physical significance (illustrations with unavailable energy, disorder and probability)-Work and Gibbs function-Variation of free energy change with temperature and pressure-Gibbs-Helmholtz equations Maxwell relations-partial molar properties-Physical significance-chemical potential-Gibbs Duhem equation-variation of chemical potential with temperature and pressure-Clapeyron-Clausius equation-concepts of fugacity and activity-determination of fugacity by graphical method-third law of thermodynamics-Statement-Determination of absolute entropies of Solids, liquids and gases-Test of the third law- Exception to third law-residual entropy-calculation of residual entropy of CO, NO, N_2O and H_2-Unattainability of absolute zero.

Unit-II **(12 Hrs)**

Statistical Thermodynamics

Aims of Statistical thermodynamics – definition of state of a system – ensembles(micro, macro and grand canonical)- Boltzmann distribution law and its derivation – Boltzmann – Planck equation – partition functions – thermodynamics properties from partition functions – partition function and equilibrium constant – Quantum statistics Fermi Dirac and Bose – Einstein 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.

Unit III **(12 Hrs)**

Electrochemistry – I

Electrolysis – movement of ions during electrolysis – Faraday's law of electrolysis – conductance – Resistance- Specific conductance – Electrolytic conductance -equivalent Conductance – Relation between molecular Conductance and specific Conductance – equivalent Conductance at infinite dilution – conductance in non – aqueous – effect of dielectric Constant – Effect of viscosity – Walden's rule -Onsager's equation – Conductometric titrations – Advantage of Conductometric titration – Types of Conductometric titrations – Replacement titration – precipitation titration - complexometric titrations.

Unit IV **(12 Hrs)**

Electrochemistry – II

Strength of an acid – methods of comparing relative strength of two acids – Thomson's thermal method -conductivity method – Dissociation constants method – Ostwald's volume method- Dissociation constant of polybasic acids- common – ion effect – Applications of common –ion effect – solubility product – Ionic product of water – pH value – Determination of pH value – colorimetric method – EMF method – indicators – Theories of indicators – Ostwald's theory – Modern Quinoid theory – indicators and acid – base titrations – Buffers – Buffer capacity – Action of Buffers – theories of Buffer.

Unit V **(12 Hrs)**

Electrochemistry – III

Absolute ionic velocities - Experimental determination of Ionic velocities- Ostwald's dilution law – Experimental verification of the dilution law - Limitations of Ostwald's dilution law - Degree of dissociation - Dissociation constant - Arrhenius theory of electrolytic dissociation – evidence in favour of the theory – limitations of Arrhenius theory - Theory of Strong electrolytes – Debye-Huckel theory- Test of Debye-Huckel theory- limiting law - Debye-Huckel – Onsager's equation - Relaxation effect - electrophoretic effect – Applications of Debye-Huckel equation - Determination of thermodynamic equilibrium – Effect of ionic strength on ion reaction rate in solution- Debye – Falkenhagen effect – Wien effect.

Reference:

1. Introduction to Electrochemistry by Samuel Glasstone
2. Principles & Applications of Electrochemistry by D.R.Crow
3. Thermo dynamics for chemist by Samuel Glasstone.
4. Advanced Physical Chemistry by Bajpai. D.N, S.Chand and company private limited.2010.
5. Advanced physical chemistry by Gurdeep Raj – Thirty Ninth edition (2014)
6. Principles of physical chemistry by Puri, Sharma, Pathania – 45th edition (2011-2012)

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015 – 2017
Semester – I

Major Elective-I: Medicinal and Pharmaceutical Chemistry – 15PCHO11
Duration -75 hrs **Credits: 5**

Aim and Objectives :

- Understand the basics of medicinal Chemistry.
- Know the chemistry of antibiotics and steroids.
- Study the chemistry of chemotherapeutic agents.
- Learn synthesis and therapeutic action and SAR of certain drugs.

Course Outcome :

- Understanding the definitions of medicinal chemistry, pharmacology and molecular pharmacology
- Knowing the concept of pharmacokinetics, bioisomerism and pharmacodynamics
- Familiarity with medically useful antibiotics and steroids
- Acquire the ability to understand the structural features and mode of action of antibiotics
- Gain knowledge in classification and synthesis of antineoplastic agents.
- Knowing the various terms involved in the medicinal chemistry
- Analyse the drug action through QSAR study, Hansch approach
- Gainsssing the knowledge of mode of action of anti-inflammatory and CNS drug
- Proficiency of Anti-Histamines drug and Antihypertensive drug
- Role of Antibiotics and its derivatives in the treatment of generic diseases

Unit I **(15Hrs)**

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 bioisomerism – pharmacodynamics phase – receptors and classification of membrane bound receptors – enzyme inhibitors as drug (illustrated with example).

Unit II **(15Hrs)**

Medically useful antibiotics and steroids

Structural features and mode of action of following antibiotics – Pencillin G, cephalosphorin and their semisynthetic analogs (β-lactum), streptomycin (aminoglycoside), terramycin (tetracylin), erythromycin (macrolide) and chloroamphenicol.

Unit III **(15Hrs)**

Chemotherapeutic agents

Antineoplastic agents: classification, synthesis, assay, e.g., Cyclophosphamide, Ifosamide, chlorambucil, Busulfun, Decarbazine, Methotrexate, Azathioprine, 6-Mercaptopurine, 5-fluorouracil. Cisplatin.

Antitubulercular drugs classification, Synthesis, Assay, e.g., Isoniazid, Rifampicin, Pyrazinamine, Ethambutol, Thiacetazone, Para amino salicylic acid and Ethionamide.

Unit IV **(15Hrs)**

Synthesis and Therapeutic action and SAR of certain drugs

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

Antihistamines: H1 – Antagonists: Pheniramine, Chloropheniramine, Diphenyhydramine, Mepyramine, Promethazine, H2 – Antagonists: Cimetidine, Ranitidine and Fomotidine.

Unit V **(15Hrs)**

Anti – inflammatory drugs, CNS Stimulant Drugs and CNS Depresent Drugs

Anti – inflammatory drugs: Antipyretics and Non-narcotic analgestics: Asprine, sodium salicylate, paracetamol, phenylbutazone, oxyphenylbutaxone, Ibuprofen, Mephenamic acid, Diclofenac sodium

CNS Stimulant Drugs: Amphetamine, caffeine, Theobromine, Theophyllino, Bemegride, Nikethamide, Methyl phenidate and peracetum.

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

Reference:

1. G.L. Partrick, An introduction to Medicinal Chemistry, II end., Oxford University Press, 2001.
2. T. Nagradi, Medicinal Chemistry- A Biochemical Approach, Oxford University Press-2004.
3. J.B. Taylor and P.D.Kennewell, introductory Medicinal Chemistry, Ellisworth Publishers, 1985.
4. C.Laxmi, Medicinal Chemistry
5. B.Jeyasree Gosch, Pharmaceutical Chemistry.
6. Asutoskour, Medicinal Chemistry.

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015 – 2017
Semester – I

Major Elective-II : Polymer chemistry
Duration -75 hrs **Credit-5**
Aim and Objectives

- To understand the basics of classification of polymer.
- To know the chemistry of polymerization.
- To study the basics of Polymerization techniques.
- To learn Polymer processing**.**

Course Outcome:

- Knowing the polymers and its types
- Significant knowledge in the mechanism of polymerization
- Acquire ideas about various polymerization techniques
- Understanding the application of polymer in day to-day life
- Acquire ideas about molecular weight determination of polymers
- Gain considerable knowledge in properties of polymers
- Gain knowledge about preparation and uses of individual polymers.
- Expertise on processing technique in polymers
- Get idea about the physical properties of polymers
- Understanding the way of techniques involved in the degradation of polymers

Unit-I **(15Hrs)**

Classification of polymers and chemistry of polymerization

Classification of polymers – linear polymers – non- linear or branched polymers, cross – linked polymers, homo chain, hetero chain, homo polymer –co – polymer and graft polymer

Chemistry of polymerization: types of polymerization – mechanism – chain, growth, free radical, ionic, co-ordination, ring opening, metathetical, group transfer, poly addition and polycondensation polymerizations.

Unit-II **(15Hrs)**

Individual polymer

Individual polymers: Monomers required general methods of preparation, repeat units and uses of the following polymers and resins – polyethylene, polystyrene, polyacrylonitrile,

polymethylacrylate, PVC, Polytetrafluoroethylene, polyisoprenes, polybutadienes and poly chloroprene, polyethylene, polycarbonates, polyimides, polyamides (Kevlar), polyurethanes, polyethyleneglycol, phenol-formaldehyde, melamine – formaldehyde and epoxy resins – silicone polymers.

Unit-III **(15Hrs)**

Properties of polymers

Intrinsic properties – processing properties – article properties – basic idea of isomerism of polymers – configuration of polymer chain – geometrical structure – syndiotactic, isotactic and atactic polymers.

Glass transition temperature: Definition – factors affecting transition temperature – relationships between glass transition temperature and (a) molecular weight (b) melting point and (c) Plasticiser – 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 **(15Hrs)**

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 photo degradation – photo stabilizers – oxidative degradation – antioxidants - hydrolytic degradation.

Uses of polymers in electronics and biomedicine.

Unit-V **(15Hrs)**

Polymer processing:

Polymer processing: Plastics (thermo and thermosetting), electronic fibres, compounding, plasticizers, colorants, flame retardants.

Compression and injection mouldings – film extrusion and calendaring – die casting and interfacial polycondensation – reinforcing.

Reference:

1. V.R.Gowariker, N.V.Viswanathan and Jayadev, "Polymer Science", Wiely Eastern Ltd., New Delhi, 1986.
2. G. Odian, "Principles of polymerization" 2nd edition, John Wiley and sons, New York, 1981.
3. D.W.Van Krevelen and P.J. Hotfyrager, "Properties of polymers", Elsevier, New York, 1976.
4. B.K.Sharma, "Polymer chemistry", Goel publishing house, Meerut, 1989.
5. P.J. Flory, "Principles of polymers chemistry", Cornell University press, Ithaca, 1953.
6. F.M. Billmeyer, Text book of polymer science, 3rd edition, John Wiley and Sons, New York, 1984.
7. Harry R. Allocok, F.W. Lampe and J.E. Mark, " Contemporary polymer chemistry" , 3rd edition, pearson. Prentice Hall, Delhi,2005.

Sri Kaliswari College (Autonomous), Sivakasi
Choice based credit system – curricular pattern
P. G Programme - M.Sc Chemistry - 2015-2017
MAJOR PRATICALS
I YEAR – I SEMESTER.

Core IV -Organic Preparation, Qualitative and Quantitative Analysis – 15PCHC1P
Duration: 15 Hrs **Credit: 5**

Course Outcome:

- Learn the importance of Quantitative and qualitative organic analysis
- Knowing the confirmation of the sample through the functional group and its derivative
- Get an idea about the hydrocarbon, nitrogen, carbonyl compounds and its analysis
- Enhancing the skill for the estimation through iodometric analysis, Bertrand's method
- Develop the synthetic knowledge in the derivative preparation
- Report the sample in a systematic way of proceedings
- Knowing the concept involved in the multistep synthesis
- Preparation of disubstituted and trisubstituted organic compound
- Role of electrophilic and nucleophilic substitution reagent in the synthetic reaction
- Applying the knowledge of directive influencing effect in the organic compound preparation
- Learn how to convert the monosubstituted compound into di and tri substituted compound

1. Qualitative Analysis

Separation and analysis of two component mixture. Identification of the components and preparation of solid derivatives.

2. Quantitative 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

3. Organic preparation

e) P- Nitro aniline from acetanilide

f) P- Bromoaniline from acetanilide

g) m-Nitrobenzoic acid from methyl benzoate

h) Benzanilide from benzophenone

i) sym-Tribromobenzene from aniline

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015-201
Semester – II

Core paper – V : Reaction Mechanism And Natural Products – 15PCHC21

Duration :60 Hrs **Credits: 4**

Aim and Objectives

- To understand the mechanism of molecular rearrangement.
- To understand the mechanism of aromatic electrophilic and nucleophilic substitution reactions. Study the type of vitamins and Terpenoids.
- To learn the chemistry of heterocyclic compounds.

Course Outcome:

- Understanding the concepts of various types of rearrangement reactions involved in organic chemistry
- Enhance the ideas of rearrangement reactions into C-C, C-O, C-N migration reactions
- To increase the knowledge on electrophilic and nucleophilic addition reactions and its stereo chemical aspects
- Deepen the ideas of elimination reactions and its stereo chemical aspects into various types of elimination reactions
- Gain knowledge about aromatic electrophilic and nucleophilic reaction with various examples
- Deepen the ideas of orientation in aromatic electrophilic and nucleophilic reactions
- Get ideas of the classification of terpenes and structural elucidation of specific terpenoids
- Understand the structure and synthesis of various vitamins
- Knowing the preparation and properties of various heterocyclic compounds
- Enhance the knowledge on the biosynthesis of heterocyclic compounds

Unit I **(12 Hrs)**

Molecular rearrangements

Mechanism of the rearrangement reactions – Wagner-Meerwin, Pinacol-Pinacolone, Demjanov, Beckmann, Hofmann, Curtius, Wolff, Baeyer-Villeger, Stephen, Sommelet-Hauser, Favorski, Benzil-benzilic acid, Claisen, Cope, Fries, Dienone-phenol, Di-pi methane, hydroxamine-p-amino phenol and Benzidine.

Unit II **(12 Hrs)**

Addition to multiple bonds and Elimination

Electrophilic, nucleophilic addition to conjugated systems- stereochemical factors in reactions like addition of hydrogen, halogens, hydrogen halides and hypohalous acids, hydroboration and hydroxylation - epoxidation .Elimination–elimination E1, E2 and E1cB Mechanisms – stereochemistry of elimination – pyrolytic cis elimination –Bredt's rule.

Unit III **(12 Hrs)**

Aromatic nucleophilic and electrophilic substitution

Aromatic electrophilc substitution – orientation – reactivity - mechanism of nitration, halogenation, Friedal – Craft's reaction and sulphonation. Partial rate factors ortho/para ratio - Quantitative treatment of reactivity of the electrophile (the selectivity relationship). Aromatic nucleophilic substitution reactions - S_NAr, S_N^1 and benzyne mechanisms.

Unit IV **(12 Hrs)**

Terpenes and Vitamins

Classification of terpenes - structure, stereochemistry and synthesis of α-pinene, camphor, zingiberene and squalene.

Structure and synthesis of Vitamins A_1, B_1, B_2, B_3, C, E and H.

Unit V **(12 Hrs)**

Heterocyclic compounds

Anthocyanins: – preparation, properties and structure of Flavylium chloride- Cyanidine chloride - Flavones: Synthesis of Flavone, Flavonol – Isoflavone - Synthesis and properties of Quercetin - Biosynthesis of Flavonoids.

Reference:

1. E.L.Eliel, S.H Wilen & L.N Mandar, Stereochemisstry of Carbon compounds, John Wiley & Sons, 2003.
2. I.L Finar, Organic chelistry, Vol.II, 5th edn. ELBS, 1975.
3. D.Nasipuri, Stereochemistry of organic compounds, Principles and applications, New age International (P) Ltd., 2nd edn, 1994.
4. P.S Kalsi, Stereochemistry, Conformation and mechanism, new age International (P) Ltd., 4th edn., 1997.
5. Jerry March, advanced Organic Chemistry, John Wiley & Sons, 4^{th} edn.,2000.
6. F.A Carey and R.J Sundberg, Advanced organic chemistry, part B, 4th edn., Plenum Publishers 2001.

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015-17
Semester – II

Core VI : Bio-Inorganic and coordination compound – 15PCHC22
Duration -75 hrs **Credits: 5**

Aim and Objectives :

- To understand the basic concepts of co-ordination chemistry.
- To know the reaction mechanism of coordination compounds.
- To understand the concepts of bio- inorganic chemistry.

Course Outcome:

- Understanding the basic ideas of coordination compounds, nomenclature of coordination compounds and its isomerism
- Knowing the various theories and its effects explaining the stability and geometry of coordination compounds
- Ain knowledge about various types of reactions and its mechanism involved in coordination chemistry
- Deepening the ideas of the concepts of coordination chemistry into electron transfer reactions, photochemical reactions
- Deliberating the concepts of structure and work function of various bio inorganic compounds
- Gain proficiency on electron transfer, respiration, photosynthesis in biological process by bio inorganic compounds
- Expertise the knowledge on co-enzymes and trace elements in biological systems
- Boost the ideas of ion pumps in biological systems
- Gain knowledge on metal toxicity and detoxification
- Realise the ideas of chemotherapy, chelation therapy and anticancer drugs

Unit I **(15 Hrs)**

Coordination Compounds

IUPAC Nomenclature of coordination compounds - isomerism in coordination compounds - ORD & CD - Types of ligands - monodentate, ambidentate and macro cyclic ligands - Stability constant - Factors affecting stability constant in solution. VB - CFT - MO theories - Splitting of d-orbitals in octahedral, tetrahedral, square planar and tetragonal

geometries - CFSE calculation in terms of Dq - Factors affecting crystal field splitting - Spectrochemical series - Nephelauxetic effect - Jahn-Teller effect.

Unit II **(15 Hrs)**

Reaction mechanism of coordination compounds

Substitution reactions of octahedral complexes - labile - inert complexes - mechanism of acid hydrolysis, base hydrolysis and anation reactions. Substitution reactions of square planar complexes - Factors affecting reactivity of square planar complexes - The trans-effect and its applications - Electron transfer reactions - complementary and non - complementary reactions - outer sphere and inner sphere electron transfer mechanisms - Synthesis of coordination complexes using electron transfer and substitution reactions. Photochemistry - photoredox and substitution reaction occurring in Co (III) and Cr (III) complexes - photochemistry of ruthenium polypyridyls.

Unit III **(15 Hrs)**

Bio – inorganic Chemistry – I

Porphyrin ring system - metalloporphyrins - hemoglobin and myoglobin - structure and work functions - synthetic oxygen carriers - cytochromes - structure and work functions in respiration - chlorophyll - structure - photosynthetic sequence - iron-sulphur protein (non-heme iron protein) - Copper containing proteins - classification - blue copper proteins - Structure of blue copper electron transferases - copper proteins as oxidases - cytochromeCoxidase - mechanistic studies of C oxidase - Hemocyanin - Copper enzymes - Azurin, Plastocyanin.

Unit IV **(15 Hrs)**

Bio – inorganic Chemistry – II

CarboxypeptidaseA: structure, function - carbonic anhydrase - inhibition and poisoning - corin ring system - vitamin B_{12} and B_{12} coenzymes - in-vivo and in-vitro nitrogen fixation - essential and trace elements in biological systems - Structure and function of Biological membranes, molecular mechanism of ion transport across the membrane - sodium and potassium ion pumps.

Unit V **(15 Hrs)**

Inorganic Medicinal Chemistry

Metals in medicine. Metal toxicity and homeostasis. Metal deficiency and diseases. Toxic effects of metals. Effect of deficiency and excess of essential metal ions. Toxicity due to non essential elements and speciation. Detoxification, mechanism. Role of lithium and aluminium in biological systems. Chelation therapy and chemotherapy. Anticancer drugs and vanadium based diabetic drugs.

Reference:

1. W.E. Addition, Stuctural Principles of Inorganic Chemistry, Wiley, 1981.
2. A.F. Wells, Stuctural Inorganic Chemistry, 4th Edition, Oxford, New York, 1975.
3. F.A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry" ,5th Edn, John Wiley & sons, Singapore, 1998.
4. K.F. Purcell and J.C.Koltz, An Introduction to Inorganic Chemistry. W.B.Saunders Company, Philadelphia, 1980.
5. James E.Huheey, Ellen A.Keitler and Richard L.Keitler, Inorganic Chemistry, 4th Edn. Harper Collins College Publishers, New York, 1993.
6. I. Bretini et al.Bioinorganic Chemistry, Viva Books Private Ltd, Chennai,1998.
7. F. Basalo and R.G. Pearson, Mechanism of Inorganic reaction, 2nd Edn., Wiley, new York, 1967.

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Semester – II

Core – VII : Quantum, Phase rule and Chemical Equilibria – 15PCHC23
Duration -60 hrs **Credits:4**

Aim and Objectives:

- To know the concepts of Quantum mechanics.
- To study the applications of Quantum mechanics.
- To know the concepts of Phase and Chemical Equilibria.

Course Outcome:

- To understand the basic concepts of quantum chemistry such as operators, uncertainty principle
- To know the ideas of postulates of quantum mechanics, eigen function, orthonormal set
- To apply the concepts of quantum mechanics into particle in a box, ring, rigid rotator
- To gain knowledge on the quantum mechanical concepts by hydrogen atom problem, shapes of various atomic orbitals
- To know the need of approximation method in quantum mechanics and its application to many electron systems
- To deepen the ideas of perturbation theory and its application to many electron system, VB theory and MO theory
- To introduce the concept of phase equilibria and its application to various one component and two component system
- To enhance the ideas of phase equilibria into three component system
- To know the concepts of chemical equilibrium and various relations involved in chemical equilibrium
- To understand concept of thermodynamic derivation of equilibrium constant and Le-chatelier's principle

Unit-I **(12 Hrs)**

Introduction to Quantum mechanics:

Particle and Wave nature of electron – de Broglie's concept of matter waves-derivation of de Broglie equation - Davison-Germer experiment – photoelectric effect – Compton Effect – Heisenberg's uncertainty principle – Operators - Linear operators – Methods of getting the following quantum mechanical operators - position, linear momentum, kinetic

energy, potential energy, total energy and angular momentum Postulates of quantum mechanics – Hermitian operator – properties of Hermitian operator(two theorem only)- proving the quantum mechanical operators of position, linear momentum, kinetic energy, potential energy, total energy are Hermitian - Commutator algebra – evaluation of following commutators [x,d/dx], [y,d/dx] and [d/dx,d^2/dx^2] - Postulates of quantum mechanics - Eigen function and Eigen value (Problems based on Eigen value equation) - significance of ψ and ψ^2 - Orthogonality and normalization of wave functions - Orthonormal set

Unit II **(12 Hrs)**

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 (Rectangular and cubic box) – Degeneracy – distortion – Particle moving in a ring – Rigid rotator – Spherical harmonics – Hydrogen atom problem – Radial wave function – radial probability distribution - Shapes of various atomic orbitals.

Unit III **(12 Hrs)**

Approximation methods in Quantum mechanics

Need for approximation methods - Schrodinger equation for He atom and other many electron system - time independent perturbation theory - First order correction term for energy and wave function (derivation required) - Application to hydrogen atom - Variation theorem - Application to hydrogen and He atom- Hartee-Fock Self Consistent Field (HFSCF) method of many electron system and its application to He atom –Slater determinants – Born-Oppenheimer approximation – VB and MO theories (theory only & applications not included).

Unit IV **(12 Hrs)**

Phase equilibria

Introduction - Derivation of Gibb's phase rule – one component system - sulphur system - two component system - types of two component system - Solid - liquid systems of two components – Lead - Silver system - KI - water system - Type II A solid - liquid equilibrium -

Zinc - magnesium system - Ferric Chloride - water system - three component system - Formation of one pair of partially miscible liquids - Formation of two pairs of partially miscible liquids - Formation of three pair of partially miscible liquids - Two salt and water – no chemical combination – Double salt formed – one salt forms a hydrate.

Unit V

Chemical equilibria **(12 Hrs)**

Reversible reactions - irreversible reactions chemical equilibrium - characteristics of chemical equilibrium - experimental proof for dynamical equilibrium - limitations of the equation for chemical equilibrium - law of mass action - relation between Kp and Kc - equilibrium constant - Factors influencing equilibrium constant - De Donders concept of degree of advancement of a reaction - Derivation of law of mass action - experimental verification of law of mass action - Thermodynamic derivation of law of mass action - Derivation of law of mass action from chemical potential - vant Hoff's reaction isotherm - free energy change method – Le-Chatelier's principle – Applications of Le-Chatelier's principle.

Reference:

1. Introductory Quantum Chemistry by A. K. Chandra, TataMcgrawhill.
2. Quantum Chemistry by IRA – N. Levine, Printice hall,2003.
3. Quantum Chemistry by Donald A McQuarrie,Viva books private limited,2005.
4. Quantum chemistry by R.K. Prasad , Second edition,2003
5. Advanced physical chemistry by Gurdeep Raj – Thirty Ninth edition (2014)
6. Advanced Physical Chemistry by Bajpai. D.N, S.Chand and company private limited.2010
7. Principles of physical chemistry by Puri, Sharma, Pathania – 45th edition (2011-2012)

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Semester – II

Optional/Elective-III : Instrumentation Techniques with Cheminformatics – 15PCHO21
Duration :75 hrs **Credit-5**

Aim and Objectives

- To study the basics of error analysis and chromatography.
- To learn the basic principle of Spectrophotometric methods and Radiochemical methods.
- To understand the concept of Programming and Applications of C Language in Chemistry.
- To know the Principles of Cheminformatics and Molecular modeling.

Course Outcome:

- Apply the knowledge of accuracy and precision in the analysis
- Known about the Separation of compounds through various chromatographic techniques
- Learn the Principles of AAS and flame photometry method in metal ion concentration analysis
- Developed skill towards the Laser technology and its application in the analytical and Medicinal field, Molecular weight determination through Turbidimetry
- Know the Various substance physical characteristic through TGA, DSC
- Knowing the redox character of the compound through the potential study of Cyclic voltammeter and Coulometry
- Framing of programme through C-language for Concentration of the solution
- Syntax and Structural format of C-langauage in the chemistry Basic laws
- QSAR application and drug design through cheminformatics studies
- Learn about the Molecular Docking Software and its importance in the pharma industry

Unit –I **(15Hrs)**

Error Analysis and Chromatography

Error Analysis-Accuracy and Precision, Determinate and Indeterminate errors, Significant figures, Ways of expressing accuracy – Absolute and relative error, Standard deviation, Propagation of errors, The confidence limit, Tests of significance – The F test and The Student's t-test, Rejection of a result – The Q test, Linear least squares to plot the data, Correlation coefficient, Statistics of sampling.

Chromatography -Principles, Adsorption, Partition, ion-exchange and size exclusion chromatography, HPLC, Paper and Gas Chromatography.

Unit –II **(15Hrs)**

Spectrophotometric methods and Radiochemical methods

Principles and applications of photometry, Flame emission spectrometry, Atomic absorption spectrophotometry – Principles, Instrumentation (Block diagram), Fluorimetry, Turbidimetry, Nephelometry and photometric titrations. Applications of Lasers.

Unit – III **(15Hrs)**

Electro analytical methods and Thermal methods

Electroanalytical methods - Coulometry and coulometric titrations, Cyclic Voltametry.

Thermal methods-Principles of TGA, DTA and DSC - Applications to simple salts - Oxysalts, Carbonates and complex salts, Thermometric titrations

Unit –IV **(15Hrs)**

Programming and Applications of C Language in Chemistry

Programming in C Language-Introduction, Character set in C, Style of C Language – Identifiers and Key words – Constants, Variables and Data types, Operators in C.

Applications of C Language in Chemistry-Writing the Program using the various features of C language - Determination of Normality, Molarity and Molality of solutions, Determination of half life of a radioactive nucleus – Determination of Concentration using Beer – Lamberts Law – RMS velocity – pH – ionic strength.

Unit –V **(15Hrs)**

Principles of Cheminformatics and Molecular modeling

Cheminformatics : Definition - Elements of cheminformatics and drug design. 3D data base searching. - Data base search- chemical data bank, CCDC, PDB- 3D pharmacophore, Structure based drug design-De Nova drug design.

Introduction to molecular modeling; Coordination system –Cartiesian coordinates. Potential energy surfaces (definition only) Empirical force field models-molecular mechanics, energy calculations. (Bond strength, bond angles, bihedral angle, on bonded interactions) Energy minimizations-.Molecular modeling studies on SB205553 and analogues.

Reference:

1. Analytical Chemistry by G.D.Chiristian.
2. Analytical Chemistry by U.N.Dash
3. Instrumental methods of analysis by Willard merit Dean
4. Fundamentals of analytical chemistry by Skoog. West&Holler.
5. Programming in ANSI C by E.Balagurusamy
6. Computers in Chemistry by K.V.Raman
7. Molecular Modeling -Andrew R.Leach

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Optional/Elective-IV : Introduction to nano science – 15PCHO22
Duration -75Hrs **Credits-5**
Aim and Objectives

- To study the basic principles of nano chemistry.
- To understand the preparation, properties and applications of nano material.

Course Outcome:

- Understand the basic concepts Nano chemistry.
- Gain knowledge about crystal structure and its types
- Get an idea of various special properties of nano materials
- Make deeper knowledge about various methods for synthesis of nano particles.
- Knowing the instrumentation techniques of characterization of nano materials.
- Deepening the knowledge of application of nano particles in the various fields.
- Enhance the ideas about UV-Visible and Photoluminescence and IR spectroscopy.
- Perceptive the knowledge of optical and magnetic properties on nano particles.
- Know the concepts hall effect and electronic properties.
- Discerning the knowledge about biological application of nanomateials

Unit-I

Introduction **(15Hrs)**

Forms of matter – crystal structures – Electronic properties of atoms amd solids – surface energy tension – defining nano dimensional materials – 0D, 1D and 2D nanostructures – size dependence of properties – special properties resulting fron nano dimensionality – potential uses of nano materials.

Unit-II **(15Hrs)**

Synthesis of nano materials

General approaches – Nucleation process – size of the crystal – Influence of nucleation rate on the size of the crystal – chemical methods – sol- gel techniques – control of grain size Co – precipitation – hydrolysis –sonochemical method – colloidal precipitation – Bottom up and Top down approaches – Kinetically confined synthesis of nano particles.

Unit-III **(15Hrs)**

Principle and instrumentation

Spectrometry, XRD, EXAFS, XPS, SEM, AFM – application of nanomaterial characterization.

Unit- IV **(15Hrs)**

Optical properties of nano material

UV-Visible, IR absorption- Photoluminescence and stimulated emission – non linear optical mixing – photoconductivity.

Magnetic properties

Concepts on dia, Para and Ferro magnetism- Exchange correlation – exchange interaction.

Electrical properties

Electrical conductivity- Hall effect – charge carrier density – Activation energy – electronic properties – field emission properties.

Unit-V **(15Hrs)**

Biological nano material

Sizes of building blocks – proteins – DNA double nanowire – Enzymes – Protein synthesis – Micelles and Vesicles - Biomimetic nanostructures – Worm micelles and Vesicles from block copolymers.

Reference:

1. Charles P. Poole Jr. and Franck owens, Introduction to nano technology.
2. T. Pradeep, Understanding nanoscience and nanotechnology
3. Vincent Rotell, nanoparticles: Building blocks for Nanotechnology, 2004.

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Semester – II

Core VIII- Inorganic Qualitative and Quantitative Analysis and Preparations : 15PCHC2P

Duration : 15 Hrs **Credit: 5**

Course Outcome:

- Mastering the techniques involved in the qualitative analysis
- Get an idea about the analysis involving mixture of familiar and less familiar cations
- Learn the importance of group separation for the analysis of cation
- Knowing the role of common ion effect and solubility product in the separation of cations
- Impact of the effect of acid and base addition in excess or deficient in the analysis
- Gaining the way of reporting the mixture in the ordered form
- Enrich the skill to identify the cation by the systematic procedure
- Know how to synthesis inorganic complex and its condition to maintain the stability of it
- Separation of mixture of metal ion through gravimetric and volumetric estimation
- Importance of complexing agent and the role of buffer solution in the precipitation of metal ion and also in the estimation

1. **Semimicro qualitative analysis:**

Analysis of mixture containing one familiar and one less familiar from the following:

W, Pb, Se, Mo, Cu, Bi, Cd, Ce, Th, Zr, V, Mn, Ni, Co, Zn, Ca, Ba, Sr, Li and Mg. (Insoluble and Interfering anions may be avoided)

2. Estimation of one metal in the presence of another by EDTA (demonstration only)

3. **Inorganic Preparations**: Preparation of atleast 6 inorganic complexes.

4. **Quantitative Analysis**:

Separation and Estimation of mixture by volumetric and gravimetric methods.

Cu,Ni; Cu,Zn; Fe,Ni; Fe,Cu.

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

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Semester – III

Core IX: ORGANIC SPECTROSCOPY, REAGENTS AND SYNTHETIC METHOD

Duration:60Hrs **Credits: 4**

Aim and Objectives :

- To understand the basic concepts and application of UV, IR, ORD, PMR, ^{13}C NMR and mass spectroscopy of organic compounds.
- To understand the role of reagents in organic synthesis.
- To understand the synthetic planning of organic compounds.

Course Outcome:

- Know the basic concepts, principles involved in UV spectroscopy, IR spectroscopy and ORD spectrum
- Deepen the ideas of the spectroscopic principle into its application to identify the organic compounds
- Gain knowledge on the basic principles, concepts of resonance spectroscopy such as 1H NMR and 13C NMR
- Enhance the ideas of the application of 1H and 13C NMR to organic compounds
- Understand the principles of mass spectrometry and various peaks observed in organic compounds
- Boost the ideas of fragmentation of various organic compounds using mass spectrum
- Understand the various types of mechanism, application and stereochemical aspects of oxidation and reduction reactions
- Know the various concepts of the reagents involved in organic synthesis
- Know the concepts of retro synthesis and total synthesis
- Deepen the idea of functional group inter conversion

Unit I **(12 Hrs)**

Spectroscopy I

UV spectroscopy: Principle- absorption spectra of conjugated dienes - α,β-unsaturated carbonyl compounds - Woodward-Fieser rules.

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

ORD – Octant rule - α-haloketone rule - applications.

Unit II **(12 Hrs)**

Spectroscopy II

^{1}H NMR Spectroscopy:

^{1}H NMR Spectroscopy: Basic Principle - number of signals - chemical shift- factors influencing the chemical shift - spin-spin coupling- coupling constant and factors influencing the coupling constant, Simplification of spectra: Shift reagent, Deuterium substitution and Spin decoupling.

^{13}C NMR Spectroscopy: Basic principle – Comparison with ^{1}H NMR - Noise decoupling- Off-resonance decoupling- factors influencing the ^{13}C chemical shift – Additivity relationship – Calculation of chemical shifts for aliphatic hydrocarbons upto five carbon atoms (data must be given)

Unit III **(12 Hrs)**

Mass spectrometry

Mass spectrometry: Principle- type of ions- base peak-molecular ion peak - isotopic peaks- nitrogen rule – determination of molecular formula from isotopic peak - general rules for fragmentation pattern – McLafferty rearrangement- Retro Diels- Alder reaction – ortho effect. Fragmentation pattern of simple compounds of hydrocarbons, amines, alcohols, ketones, acids and phenols.

Unit IV **(12 Hrs)**

Reagents

Mechanism, application and stereochemistry aspects of the following oxidation – reduction reactions: oxidation reactions involving CrO_3, SeO_2, OsO_4, lead tetraacetate, periodic acid, N-bromosuccinimide – Oppenauer oxidation.

Catalytic hydrogenation – reactions involving $LiAlH_4$, DIBAL and sodium borohydride – Birch reduction – hydroboration – selectivity in oxidation and reduction.

Reagents in organic synthesis – Gilman's reagent – Lithium diisopropylamide – DCC - 1,3-dithiane – Woodward and Prevost hydroxylation, DDQ.

Unit V **(12 Hrs)**

Synthetic Methods:

Planning of synthesis – relay approach and convergent approach to the total synthesis Retrosynthetic analysis of simple organic compounds like arildone, cinflumide and venlafaxine.

Functional group interconversions – uses of activating and blocking groups in synthesis regioselective, diastereoselective and enantioselective reactions. Umpolung synthesis- Robinson annelation.

Reference:

1. John R.Dyer, Application of absorption Spectroscopy, Prentice-Hall.
2. William Kemp, Organic 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, I & II, ELBS, 1975.
5. R. E. Ireland, Organic Synthesis, Prentice – Hall of India Pvt. Ltd., 1975.
6. R.T. Morrison and R.N. Boyd, Organic Chemistry, Prentice – Hall of India, 6th edn., 2001.

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Semester – III

Core X : Physical methods in inorganic chemistry - 15PPCHC32
Duration -60Hrs **Credits: 4**

Aim and Objectives

- To understand the basic principle of Electronic spectra.
- To learn the application of spectroscopy in inorganic chemistry.
- To study the concepts of metal – metal bond in complexes

Course Outcome:

- Understand the concepts of electronic transition using electronic spectra and selection rule involved in metal complexes
- Enhance the ideas of magnetic properties of complexes and its determination in coordination compounds
- Deepen the ideas of analysis of coordination complexes using IR and Raman spectroscopy
- Understand the concepts of Mossbauer spectroscopy and its application in the study of iron and tin complexes
- Know the application of 31P, 19F and 15N NMR spectroscopy to inorganic metal complexes
- Understand the principle of ESR spectroscopy and its application in transition metal complexes
- Develop the principles and application of NQR spectroscopy
- Gain the knowledge on photoelectron spectroscopy, Auger spectroscopy and its applications
- Understand the concepts of metal metal bonds in various poly nuclear complexes
- Deepen the ideas of polyatomic zintl ions, metal carbonyls and metal clusters

Unit I **(12 Hrs)**

Electronic spectra and magnetic properties

Electronic spectra of transition metal complexes: Term symbols for d^n system – d-d transition – charge transfer transition – selection rules – mechanism of breakdown of selection rules – bandwidths and shapes – Jahn-Teller effect – Tanabe-Sugano diagram – evaluation of 10Dq and β for octahedral and tetrahedral complexes of d^3, d^6, d^7 and d^8 configurations

Magnetic properties of complexes-paramagnetic and diamagnetic complexes, molar susceptibility, Gouy's method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism(TDP) - Temperature Independent Paramagnetism(TIP). Spin state crossover, Antiferromagnetism - inter and intra molecular interaction. Application of magnetic measurements in the determination of structure of transition metal complexes.

Unit II **(12 Hrs)**

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 – geometrical and linkage isomerism – detection of inter and intramolecular hydrogen bonding – stretching mode analysis of metal carbonyls.

Mossbauer spectroscopy: 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.

Unit III **(12 Hrs)**

Application of spectroscopy to the study of Inorganic compounds II

NMR Spectroscopy: ^{31}P, ^{19}F and ^{15}N – NMR – introduction – application in structural problem – evaluation of rate constants – monitoring the course of reaction – NMR of fluorine molecules – NMR of paramagnetic molecules – contact shift and shift reagents.

ESR Spectroscopy: Principles – presentation of the spectrum – hyperfine splitting – evaluation of g and A tensors – factor affecting the magnitude of g - values – zero field splitting – Kramer's degeneracy – ESR of d^3 octahedral complexes – anisotropy and hyperfine splitting constant. Application of ESR in the study of transition metal complexes – Jahn-Teller distortion studies in Cu (II) complexes – evaluation of spin-orbit coupling.

Unit IV **(12 Hrs)**

Application of spectroscopy to the study of Inorganic compounds III

NQR Spectroscopy – principles and application.

Photoelectron Spectroscopy: Theory – XPS – UV – PES – instrumentation evaluation of Ionization potential – Chemical identification of elements – Koopmann's theorem – chemical

shift – UPS – XPES of N_2, O_2 and HCl – evaluation of vibrational constants from UPS – spin – orbit coupling – Auger spectroscopy – principle and its application.

Unit V **(12 Hrs)**

Metal-metal bonds and metal clusters

Metal-metal bonds: Factors affecting the formation of metal-metal bond. Dinuclear compounds of Re, Cu and Cr, metal-metal multiple bonding in $(Re_2X_8)^{2-}$, Trinuclear clusters, tetranuclear clusters, hexanuclear clusters. Polyatomic zintl anion and cations. Metal carbonyl clusters. Anionic and hydrido clusters. LNCCs and HNCCs. Hetero atoms in metal clusters: Carbide and nitride containing clusters. Electron counting schemes for HNCC

Reference:

1. F.Basalo and R.G.Pearson, Mechanism of Inorganic Reaction, 2nd Edn., Wiley, New York, 1967.
2. Adamson, Concept of Inorganic Photochemistry, Wiley, New York, 1975.
3. S.F.A.Kettle, Cordination Chemistry- Spectrum Academic Publishers Oxford, 1996.
4. R.S. Drago, Physical Methods In Chemistry, Saunders Golden Sunburst Series, W.B.Saunders Company, London, 1997.
5. K.F. Purcell and J.C.Koltz, An Introduction to Inorganic Chemistry. W.B.Saunders Company, Philadelphia, 1980.
6. P.W. Atkins, D.K. Shriver and C.H. Langfood, Inorganic Chemistry, Oxford ELBS. U.K, 1990.

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Semester – III

Core XI : Group Theory and Spectroscopy – 15PCHC63

Duration -75 Hrs **Credits: 5**

Aim and Objective:

- To understand the basic concepts and application of spectroscopy
- To know the basic principles and applications of group theory.

Course Outcome:

- Gain the knowledge on various symmetry elements, symmetry operation involved in molecules and its classification by point group assignment
- Develop the concepts of matrix algebra to symmetry elements, reducible representations, Great orthogonality theorm into the construction of character table
- Deepen the basic ideas of group theory for the application of finding normal modes of vibrations, symmetry selection rule for IR, Raman and electronic spectroscopy
- Enhance the knowledge on froup theory using quantum mechanics to find hybridization, HMO calculation for simple molecules
- Develop the theoretical knowledge on rotational spectroscopy
- Gain knowledge on the theoretical aspects of vibrational spectroscopy and the principle involved
- Enhance the ideas of vibrational, rotational concepts with Raman spectroscopy and laser Raman spectra
- Understand the principles involved in NQR spectroscopy
- Gain knowledge on various NMR instrumentation techniques
- Know the principles and concepts involved in ESR spectroscopy

Unit I **(15 Hrs)**

Group Theory

Molecular symmetry elements and symmetry operations - group – definition and properties of a group –Types of groups - Abelian and non-abelian groups- classes and sub groups- groups multiplication table – C_{2v} -Point groups – classification of molecules into point groups - C_{2v}, C_{3v}, C_{2h}, D_{2h} , D_{4h}, D_{6h} T_d and O_h.- Vector and matrix algebra -matrix representation

of symmetry operations(E, C_n, σ, S_n and i)- reducible and irreducible representations – Great orthogonality theorem – Characters – Construction of character tables – C_{2v}, C_{3v} and C_{2h} – Direct product concept.

Unit – II **(15 Hrs)**

Application of Group Theory to spectroscopy and Molecular Problems

Symmetry of normal modes of vibrations, applications of group theory to normal modes of vibrations and to normal mode analysis of simple molecules like water, ammonia and Trans 1,2-dichloro ethylene) – Symmetry properties of integrals – application for spectral selection rules of vibration spectra – IR and Raman active fundamentals – Symmetry of molecular orbitals and symmetry selection rule for electronic transitions in simple molecules like ethylene and formaldehyde. Group theory and quantum mechanics – Wave functions as the basis of irreducible representation – group theory applied to hybridization in simple molecules like BF_3 and$[PtCl_4]^{2-}$ – HMO theory – HMO calculations and delocalization energy for cyclopropenyl and butadiene systems.

Unit – III **(15 Hrs)**

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 – Information 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- concepts of group frequencies – coupling interaction – Fermi resonance – Fourier transform infrared spectroscopy.

Unit – IV **(15 Hrs)**

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 electrical field, nuclear quadrupole resonance, nuclear quadrupole coupling in atoms and molecules – identification of ionic character and hybridization.

Unit-V **(15 Hrs)**

Spin resonance spectroscopy:

Magnetic properties of nuclei-Resonance – condition –NMR instrumentation – Relaxation processes – Bloch equations –chemical shift – spin-spin coupling, relaxation times, line shape and line width experimental technique, Double resonance technique, ENDOR, Over Hauser 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- Zero field splitting in ESR and Krammer's degeneracy.

Reference:

1. F.A.Cotton-Chemical application of group theory-wiley eastern Ltd-1971.
2. V.Ramakrishnan and M.S.Gopinathan-Group theory in Chemistry-Vishal -1988
3. Molecular Spectroscopy by Banwell & Drago,Affiliated east-west press pvt limited . East west edition.

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Semester – III

Non Major Elective-I: Industrial chemistry – 15PCHN31
Duration -75 hrs **Credits-5**
Aim and Objectives

- To study the basic principles of chemical technology.
- To learn the manufacturing processes in small scale and large scale industry.

Course Outcome:

- Understand the basic concepts of chemical technology
- Desgining and modeling of chemical industry
- Gain knowledge about the petroleum product
- Induce the knowledge to idea about the chemical corrosion and its preventive measures
- Get an idea of various pollutants involved in water pollution and its prevention methods
- Boosting the basic idea related to water pollution and the treatment of sea water into soft water
- Knowing the manufacturing process involved in matches and fireworks
- Learning the knowledge about the cement and ceramic in large scale industry
- Enrich the chemical knowledge towards the framing of small scale industry like cosmetics, soap and detergents
- Initiate the process involved to design a chemical industry and its various aspects

Unit-I **(15Hrs)**

Principles of chemical technology

Introduction – basic principles of chemical technology – importance of chemical technology – classification of technological processes – designing and modeling of chemical plants – unit process and unit operations.

Basic requirements of industrial reactors – choice and selectivity of reactors - basic principles of homogenous and heterogeneous processes and reactors with examples.

Unit-II **(15 Hrs)**

Raw materials and energy for chemical industry

Raw materials – characterization of raw materials and their resources – methods of raw material concentration – integral utilization of raw materials.

Energy for chemical industry -power and fuels – classification of fuels –coal –fuel gases and liquid fuels –petroleum – cracking –chemical corrosion – types of corrosion and preventive measures.

Unit-III **(15 Hrs)**

Water pollution and its control

Water in chemical industry –soft and hard water –softening of water – basic principles of water pollution – water pollutants – pollution parameters – industrial pollution control – waste water treatment methods –Water (prevention and control of pollution) act.

Unit-IV **(15 Hrs)**

Small scale chemical industries

Electro-thermal and electro-chemical industries – electroplating – surface coating industries – oils, fats and waxes –soaps and detergents – cosmetics.

Match industries and fireworks – Manufacture of some industrially important chemicals like potassium chlorate, potassium nitrate, barium nitrate and red phosphorus – metal powders.

Unit-V **(15 Hrs)**

Large scale industries

Manufacturing process- raw materials – composition and uses of products in Portland cement – ceramics – plastics film industries – commercial aspects of starting an industry.

Reference:

1. B.K.Sharma, Industrial chemistry, Goel publishing, 2002.
2. The art, science and technique of fire works by Dr. Takeo Shimizu. of engineering, Director of Koa fireworks co Tokyo, 1981.
3. The Principles of fire works by K.N. Ghosh, second edition. 1988.
4. Text Book of Inorganic analysis By P.L.Sony Mohan katya. Sultan Chand & Sons- New Delhi 2004.

5. Engineering Chemistry by Jain and Jain – Dhanpat Rai publishing company, New Delhi – 14th edition 2004.

Sri Kaliswari College (Autonomous), Sivakasi
Choice based credit system
P. G Programme - M.Sc Chemistry - 2015- 2017
Semester- III

Non-Major Elective – II : Environmental Science – 15PCHN32
Duration: 75 Hrs **Credits: 5**

Aim and Objective

- To study the sources and effects of pollution.
- To learn the remedial measures of pollution.

Course Outcome:

- Create the awareness about the environment studies to make pollutant free environment
- Impact of various natural cycles in the environment and its current issue about them
- Demerits of Green house gases, Ozone layer depletion and the steps taken to reduce them
- Awareness on current global issues and its threatening matter in the future
- Know the water pollutant and the role of microorganism in the merit and the demerit way in the water pollution
- Idea towards the government project in the desalination process of sea water to rectify the scarcity of water
- Realization of deforestation effect and disposal of solid waste into the land
- Effect of soil erosion and its impact to the microorganism in the soil and idea about its remedial measure
- More appreciation of various organization involved in the remeditation of social issues
- Create awareness about the various act involved in the protection of environment

Unit – I **(15hrs)**

Introduction to environmental studies

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 – Effects and control of pollutions: air pollution – water pollution – soil pollution – radioactive pollution – thermal pollution – noise pollution – marine pollution - remedial measures.

Unit – II **(15hrs)**

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 monoxide - effects and control - photo chemical smog - effects and control – fly ash - effects and control – green house gases, global warming - effects and control – ozone layer depletion – chlorofluorocarbons - effects and control.

Unit – III **(15hrs)**

Water pollution

Introduction – types of water - 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 – sewage and industrial waste water treatment – desalination – reverse osmosis.

Unit – IV **(15hrs)**

Soil pollution

Introduction – sources and types of soil pollution – indicators of soil pollution – plants as indicators of pollution – soil sediments as pollutant – soil erosion – control measures of soil pollution – treatment of solid wastes – thermal method – land filling – composting –land protection –remedial measures for soil pollution.

Unit – V **(15hrs)**

Social issues and the environment

From unsustainable to sustainable development – urban problems related to energy – water conservation, rain water harvesting, watershed management – resettlement and rehabilitation of people; its problems and concerns – role of non-governmental organization-environmental ethics: Issues and possible solutions – nuclear accidents and holocaust –

wasteland reclamation – consumerism and waste products – environment protection act – Air (Prevention and Control of Pollution) act – Water (Prevention and control of Pollution) act – Wildlife protection act – Forest conservation act – central and state pollution control boards- Public awareness.

Reference:

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.
4. N.Manivasakam, physic – chemical Examination of water, sewage and industrial effluents, Pragati prakashan publication, Meerut,1985.
5. Engineering Chemistry by Jain and Jain –Dhanpat Rai publishing company,New Delhi – 14^{th} edition 2004.

Sri Kaliswari College (Autonomous), Sivakasi
Choice based credit system – curricular pattern
P. G Programme M.Sc Chemistry - 2015-2017
Semester III

Core XII : Physical Chemistry Practical – 15PCHC3P

Duration: 15 Hrs **Credit: 5**

Course Outcome:

- Knowing the importance of the various physical properties by practical
- Pursuing the role of potentiometric method to study pH of the buffer solution
- Ability to know the solubility product of sparingly soluble salt through potentiometric method
- Enrich the concept of precipitation titration of halide mixture *via* potentiometry
- Finding the strength of the mixture of acid through conductometric method
- Rate of the reaction study through kinetic method
- Impact of the conductivity and potentiometry methods to study the electrical properties of the ionic substance, acids and bases
- Interpretation of the potentiometric curve through first order derivative and second order derivative
- Applying Frendlich and Langmuir Adsorption theory practically to study monolayer adsorption occur by acid solution on the surface of charcoal
- Knowing the dissociation of weak acid through potentiometric and conductometric method

1. Conductometric Experiments

(i) Double displacement and 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

(iii) Determination of dissociation constant of weak acids.

II. Adsorption Experiments

Adsorption of oxalic acid / Acetic acid on charcoal.

III. Kinetic Experiments

(i) Kinetics of alkaline 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 solubility product of sparingly soluble salts.

V. Titrations using pH meter

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

VI. Experiments based on UV – Visible and Infrared Spectrophotometers.

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Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015-17
Semester – IV

Core XIII: Photochemistry And Natural Products – 15PCHC41

Duration: 60 Hrs **Credits: 4**

Aim and Objectives

- To study the structure of carbohydrates, proteins and nucleic acids.
- To understand the photochemical and free radical reactions.
- To know the feasibility of pericyclic reactions by molecular orbital approach.
- To understand the structure and application of alkaloids, steroids, antibiotics and prostoglandins.

Course outcome:

- Know the structure of various disaccharides, polysaccharides and its determination
- Understand the concepts of peptides, proteins, enzymes and biosynthesis of aminoacids
- Enhance the idea of types of electrocyclic reactions using frontier, Huckel, molecular orbital theory and gain the knowledge on various photochemical reactions
- Deepen the ideas of free radical formation, stability and various free radicals mediated organic reactions
- Gain the knowledge on the general structural determination of alkaloid
- Enhance the ideas of structural elucidation to specific alkaloid
- Know the classification, and structural elucidation of steroids
- Understand the structure and properties of sex harmones
- Knowing the definition, structure and synthesis of antibiotics
- Understand the concept og prostaglandins

Unit I **(12 Hrs)**

Carbohydrates, Proteins and Nucleic Acids

Carbohydrates: Disaccharides-Structure elucidation of Sucrose, Maltose, and Lactose. Polysaccharides: General methods for determining 1,2- 1,4- and 1,6- linkages in polysaccharides (Smith Degradation): End Group Analysis - A brief study of starch and cellulose.

Proteins and Nucleic Acids: Classification of Proteins – Structure of Peptides – Chemistry of glutathione and oxytoxcin – an elementary treatment of enzymes, coenzymes and nucleic acids – Biosynthesis of Aminoacids – Protein synthesis – RNA and DNA.

Unit II **(12 Hrs)**

Photochemistry

Electrocyclic reactions – cycloaddition reactions and sigmatropic rearrangements application of Correlation diagram approach, Frontier molecular orbital approach, Huckel-Mobius concept and Perturbation Molecular orbital approach to the above reactions.

Photochemical reactions of ketones – Photosensitization – Norrish I and Norrish II type reactions – Paterno-Buchi reactions – Photo oxidation – Photo reduction - Photochemistry of arenes

Free radicals: Formation, detection and stability of short and long lived free radicals – Free radical reactions: halogenation, addition, oxidation, reduction and rearrangement reactions – Barton, Sandmeyer, Gomberg, Bachmann, Ullmann, Pschorr and Hundsdiecker reactions.

Unit III **(12 Hrs)**

Alkaloids

General methods of structural determination - Hofmann, Emde and Von Braun degrations. Structure elucidation of quinine, papaverine, atropine, morphine, reserpine and Piperine.

Unit IV **(12 Hrs)**

Steroids

Classification- configurational aspects of A/B cis and A/B trans steroids- structural elucidation of cholesterol, (synthesis not necessary) erogsterol and Vitamin D_2.
Male sex hormones - androsterone and testosterone. Female sex hormones - oestrone, equilenin and progesterone. Basic idea about adrenocortical hormones - Conversion of cholesterol to hormones

Unit V **(12 Hrs)**

Antibiotics and Prostaglandins

Antibiotics: Definition, classification of antibiotics, structure, stereochemistry and synthesis of penicillin, chloroamphenicol and Terramycin.

Prostaglandins: General study of prostaglandins- Chemistry of PGE_1 and $PGF_1\alpha$.

Reference:

1. A.L.Lehninger, Biochemistry, Nath Publications.
2. C.H.Depuy and O.L.Chapman, Molecular Reaction and Photochemistry, Prentice Hall, 1972.
3. S.M.Mukherji and S.P.Singh, Reaction Mechanism in Organic Chemistry, McMilan Indian Ltd., 1978.
4. R.B.Woodward and R.Hoffmann, 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. I and II, 5^{th} edn., ELBS, 1975.

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015-17
Semester – IV
Core XIV: Nuclear Chemistry, Lanthanide, actinides and Organometallic Chemistry
Duration -60hrs **Credits: 4**

Aim and Objectives:

- To understand the basic principle and applications of nuclear chemistry.
- To learn the properties and applications of Lanthanides and Actinides.
- To study the structure and properties of organometallic compounds.
- To understand the structure and bonding in Inorganic Chains , Rings and Cages
- To understand the basic concepts of nucleus and theory governs the nuclear size, shape, configuration

Course Outcome:

- Know the radioactive series and the equilibrium in nuclear chemistry
- Deepen the ideas of nuclear reaction by nuclear fission, fusion reactions and its applications
- Gaining the knowledge of the application of radioactive isotopes in various fields
- Know the chemistry of inner transition elements and its position in the periodic table
- Deepen the ideas of oxidation state, spectral and magnetic properties of inner transition elements
- Enhance the ideas of various organometallic compounds, their stability, metal carbonyls
- Understand the concepts of π acceptor, metal alkyls, multicentre bond in organometallic compounds
- Knowing the preparation, properties and structure of sandwich complexes
- Enhance the ideas of the applications of organometallic compounds in catalysis

Unit I **(12 Hrs)**

Structure of Nucleus and Radioactivity Decay

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

Radioactive decay: Group displacement law – decay series – rate of disintegration – half life – average life – units of radioactivity – secular and transient equlibria – theories of alpha

decay, beta decay, gamma emission, positron decay, nuclear isomerism, internal conversion and electron capture – Auger effect.

Unit II **(12 Hrs)**

Nuclear Fission and Fusion and Application of Radio Active Isotopes

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

Application of radioactive isotopes: Characteristics of tracer isotopes – chemical investigation – age determination – medical field – agriculture – industry – analytical application – isotope dilution analysis – neutron activation analysis – biological effects of radiation – waste disposal management.

Unit III **(12 Hrs)**

Actinides and Lanthanides

Chemistry of Lanthanides and actinides – Lanthanide – Occurrence, extraction from ores – separation 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 lanthanide ions – separation of Pu from fission products - electronic configuration – oxidation state – Comparison of lanthanides and actinides – Position in the periodic table.

Unit IV **(12 Hrs)**

Organometallic chemistry I

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition) of mono and binuclear carbonyls of 3d series. Structures of mononuclear and

binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. π-acceptor behaviour of CO (MO diagram of CO to be discussed), synergic effect and use of IR data to explain extent of back bonding.

Metal Alkyls: Important structural features of methyllithium (tetramer) and trialkylaluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethane

Unit V **(12 Hrs)**

Application of organometallic compound in industry

Synthesis, properties, structure and bonding in 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 catalyst) – Tolman catalytic loops – hydroformylation (oxo process) – acetic acid from ethanol – oxidation of alkenes to aldehydes and ketone (Wacker process) – catalyst involved in the synthesis of gas-olefin polymerization (Ziegler – Natta) – Cyclo oligomerisation of acetylenes (Reppe's or Wilke's catalysts) – olefin isomerisation using Ni catalyst.

Reference:

1. S.Glasstone, Source book on Atomic energy, 3rd Edn., Van Nostrand Reinhold Company, New York, 1967
2. G. Friedlander, J.W.Kennedy, 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, 3 rd Edn., Wiley Eastern Ltd., New Delhi, 1987
4. U.N. Dash, Nuclear Chemistry, Sultan Chand and sons, New Delhi,1991
5. James E.Huheey, Ellen A.Keitler and Richard L.Keitler, Inorganic Chemistry, 4th Edn. Harper Collins College Publishers, New York, 1993.
6. K.F.Purcell and J.C.Koltz, An Introduction to Inorganic Chemistry. W.B.Saunders Company, Philadelphia, 1980.
7. P.W. Atkins, D.K. Shriver and C.H. Langfood, Inorganic Chemistry, Oxford ELBS.

U.K, 1990.

Sri Kaliswari College (Autonomous), Sivakasi
Choice Based Credit System
P.G Programme -M.Sc Chemistry - 2015-17)
Semester – IV

Core XV : Chemical Kinetics and Surface chemistry – 15PCHC43
Duration :60 Hrs **Credits: 4**

Aim and Objectives

- To understand the concepts of catalysis and chemical kinetics.
- To understand the principles of surface chemistry and bio physical chemistry.
- To study the basics of phase rule.

Course Outcome:

- Enhance the concept of activation energy and activated complex by collision theory
- Gain the knowledge on collision theory and absolute reaction rate theory
- Develop the concept of molecularity and its classification
- Deepen the basic ideas of molecularity by the study of various theories
- Enhance the knowledge on mechanism and kinetics of chin reaction and the application of steady state treatment
- Develop the theoretical knowledge on primary and secondary salt effect and kinetics of fast reaction by different techniques
- Gain proficiency in the theoretical aspects of homogeneous and heterogeneous catalysis
- Enhance the ideas of enzyme catalysis and acid-base catalysis
- Understand the characteristics and terms involved in adsorption
- Gain knowledge on various adsorption isotherms, B.E.T equation and applications of adsorption in everyday life

Unit-I **(12 Hrs)**

Chemical Kinetics I

Effect of temperature on reaction rate – simple collision theory – Arrhenius equation- Activated energy and chemical reaction - characteristics of an activated complex - Mathematical treatment of classical collision theory – Modified collision theory - ARRT – Statistical – Mechanical derivation of the rate equation – Wyne – Jone and Erying equation- comparison of collision theory and Absolute reaction rate theory.

Unit-II **(12 Hrs)**

Chemical Kinetics II

Unimolecular reactions – Elementary unimolecular reactions – Unimolecular reactions in free radical mechanism -Theories of unimolecular reactions – Perrin theory – Lindemann's theory – mathematical formutation of Lindemann's theory – Criticism of Lindemann's theory – Hinshelwood's theory- RRK theory – RRKM theory – Slater's treatment – Trimolecular reactions -Trauz's theory – Bodenstein's theory.

Unit-III **(12 Hrs)**

Chemical Kinetics III

Chain reactions -distinguishing features of chain reactions – mechanism of chain reactions – Detection and estimation of atoms and radicals in chain reactions – kinetics of chain reactions – Steady state treatment – Examples -decomposition of ozone – reaction between Hydrogen and Bromine – salt effect - primary and secondary salt effect – Kinetics of fast reactions – flow methods – Flash photolysis – shock tube- pulse radiolysis – chemical relaxation method.

Unit-IV **(12 Hrs)**

Catalysis

Types of catalysis – Homogeneous – Heterogeneous catalysis -characteristics of catalysis – theory of Homogeneous catalysis – theory of heterogeneous catalysis – Kinetics of heterogenous reactions -Effect of temperature on heterogenous reactions – absolute rate theory in heterogenous reactions – classification of catalysis – characteristics of enzyme catalysis – Factors affecting the rate of an enzyme reaction. Michaelis and Menten's equation- Acid base catalysis- types of acid base catalysis -kinetics of acid- base catalysis -Hammett and Bronsted equation.

Unit-V **(12 Hrs)**

Adsorption

Introduction – characteristic of adsorption – sorption and occlusion – measurement of adsorption volumetric method – Gravimetric method – various adsorption isotherm – Freundlish's adsorption isotherum - Langumuir adsorption isotherm – B.E.T equation – Determination of surface area – Harkins and Jura method – Benton and white method – B.E.T. method – point B-method – From permeability method – Applications of adsorption.

Reference:

1. Chemical Kinetics By Laidler
2. Advanced physical chemistry by Gurdeep Raj – Thirty Ninth edition (2014)
3. Advanced Physical Chemistry by Bajpai. D.N, S.Chand and company private limited.2010
4. Principles of physical chemistry by Puri, Sharma, Pathania – 45th edition (2011-2012)

Sri Kaliswari College (Autonomous) - Sivakasi
Choice based credit system
PG Programme - M.Sc (Chemistry) - 2015-2017
Semester – IV

Optional/Elective-V: Concepts of Green Chemistry – 15PCHO41
Duration :75 Hrs **Credit-5**
Aim and Objectives

- To study the basic principle of green chemistry.
- To understand the concepts of green synthesis.

Course Outcome:

- Understanding the requirement of global needs to reduce the pollution created by the various chemical industry
- New method of way and technology for the Greener environment and the basic principle of green chemistry
- Awareness about the atom economy of the reaction and its improvement for the higher efficiency of the reaction
- Enrichment of Modern technology like microwave, sonochemistry, one pot synthesis, water medium and the solvent free medium
- Role of Greener solvents, catalyst and its importance in the synthetic chemistry
- Techniques to know the Reduction of multistep synthetic process into one pot synthesis with minimium amount of waste disposal\
- Realise the current movement of resources like renewable source, alternative feedstock in organic synthesis
- Intiation towards the supporting catalyst of polymer, ionic liquid, phase transfer catalyst in the synthesis
- Preference to the solvent free reaction, smart technology for the less consumption of various factors in the chemical industry
- Role of biodegradable waste in the synthesis of the raw material which is the building block for the synthesis
- Milestone for the synthesis of organic compounds using novel technical methods

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Unit I **(15Hrs)**

Introduction to green chemistry

Anasta's twelve Principles of Green Chemistry – atom economy – atom economy reactions- Planning a Green synthesis in a laboratory – choice of starting materials, choice of reagents, choice of catalysts, choice of solvents-Synthesis involving basic principles of green

chemistry - synthesis of adipic acid, methyl methacrylate, paracetamol, Ibuprofen, Nicotinic acid.

Unit II **(15Hrs)**

Sonochemistry

Basic concepts - importance of sonochemistry - Generation of ultrasound - magnetostrictio method & piezoelectric method - sonochemical yield - applications of acoustic cavitation.

Ultrasound assisted reactions – esterification, reduction, coupling reactions. Strecker synthesis, Reformatsky reaction, substitution reaction, Cannizzaro reaction, Barbier reaction, oxidation and saponification.

Unit III **(15Hrs)**

Green Catalysts

Acid Catalysis- Oxidation Catalysis-Basic catalysis- Polymer supported Catalysis- Polystyrene-aluminum chloride-Polymeric super acid Catalysis- Polystyrene-metalloporphyrins- Polymer supported photosensitizers- Polymer supported Phase Transfer Catalysis- TiO_2 Photocatalyst in Green Chemistry – biocatalysts.

Unit IV **(15Hrs)**

Alternative Feedstocks and Solvents

Renewable feedstock- introduction- carbohydrate as a feedstock – lignin as a feedstock- advantages and disadvantages of biomass as a chemical feedstock – biomass versus petrochemical refining.

Ionic Liquids- introduction-properties- types- synthesis-synthetic applications-Friedelcrafts reaction,Diels – Alder reaction,Knoevenagel condensaion,Heck reaction, Michael addition reaction-CO_2 as supercritical fluid-advantages-Reactions in $ScCO_2$

Unit V **(15Hrs)**

Solvent Free Organic Synthesis

Solvent free microwave assisted organic synthesis – microwave activation, microwave heating, advantages of microwave exposure and specific effects of microwaves- advantages of microwave heating over conventional heating-differences between microwave heating and conventional heating Organic synthesis under microwaves – benefits, limitations, equipments. Reactions on solid supports, phase transfer catalysis, solvent free esters saponification, reactions without support or catalyst, examples – microwave assisted reactions in water – oxidation of

toluene to benzoic acid, microwave assisted reactions in organic solvent Diels Alder reaction-Neat reactions.

Reference:

1. K.R. Desai, Green Chemistry (Microwave synthesis), Himalaya Publishing House, Mumbai,2005
2. N. R. Sanghi and M.M.Srinivasta, Green Chemistry (Environmental Friendly Alternatives), Narosa Publishing House, New Delhi,2003
3. T.J. Mason and d. Peters, Practial Sonochemistry-Power Ultrasound and Applications, 2nd edition, Howard Publishing, England 2002
4. Kenneth . Klabunde, Nanoscale Materials in Chemistry, John Wiley & Sons, Inc. 2002
5. Rashmi Sanghi, M. M. Srivastava, Green Chemistry, Environment Friendly Alternatives, Narosa Publishing House, 2007
6. V. Kumar, An Introduction to Green Chemistry, Vishal Publishing CO. Jalandhar, 2007.
7. V.K. Ahuluwalia, M. Kidwai, New Trends In Green Chemistry, 2nd Edn,Anamaya Publishers, New Delhi.

Sri Kaliswari College (Autonomous) - Sivakasi
Choice based credit system
PG Programme - M.Sc (Chemistry) - 2015-2017
Semester – IV

Optional/Elective-VI: Supramolecular chemistry – 15PCHO42
Duration -75 Hrs **Credit-5**
Aim and Objectives

- To understand the basic concepts of supramolecular chemistry.
- To Know the structure of supramolecules.
- To s tudy the synthesis and properties and applications of supramolecules

Course Outcome:

- Understand the various nonbonding interaction involved in supramolecular chemistry
- Knowing the basic ideas of Host-Guest interaction
- Learn the structure and the synthesis of dendrimers and cryptands
- Deepen the concept of dendrimers and cryptands into its applications
- Get the idea of types of cyclodextrins and its role in chemistry
- Enhance the knowledge of application in the pharma and chemical industry
- Know the chemistry of fullrenes and its application
- Understand the synthesis, properties involved in Cucurbitnrils
- Enrich the knowledge on the crown ether compound as phase transfer catalyst and other applications
- Learn the synthesis, application of calixarenes

Unit-I **(15Hrs)**
Introduction

Definition, self-assembly, top-down approach, bottom up approach, host-guest chemistry, lock and key principle, nature of supramolecular interaction, electrostatic, hydrogen bonding, Π-Π stacking interaction, cation- Π interaction ,van der Waals forces hydrophobic effect, stability, templating effect, examples.

Unit-II **(15Hrs)**
Dendrimers and cryptands

Dendrimers- structure, synthesis, properties and applications, cryptands-structure, properties and applications. Synthetic molecular receptors for different substrates.

Unit-III **(15Hrs)**

Cyclodextrins and cyclophanes

Types, properties, structure, synthesis, uses, receptor theory for Cyclodextrins, Cyclophanes, Catenanes and Rotaxanes.

Unit-IV **(15Hrs)**

Fullerenes and Cucurbitnrils

Fullerenes: structure, synthesis, properties, and applications. Cucurbitnrils: structure, synthesis and applications.

Unit-V **(15Hrs)**

Crown ethers and Calixarenes

Structure, synthesis, properties, applications and Receptor theory of Calixarenes and crown ethers.

Reference:

1. Ajay kumar bhagi, G.R.Chatwal, Bioinorganuic and supramolecular chemistry, Himalaya publishing house, 2003.
2. Asim k.Das, Fundamental concepts of inorganic chemistry, Volume 3, CBS publishers and distributors, 2011.

Sri Kaliswari College (Autonomous) - Sivakasi
Choice based credit system
PG Programme - M.Sc (Chemistry) - 2015-2017
Semester – IV

Core XVI : Project / Review of recent aspects of Chemistry

Duration: 15 Hrs **Credit:4**

Course Outcome:

- Gain fundamental knowledge in research.
- Develop skill in innovative thinking towards research.
- Improve fundamental analytical skill
- Get thorough idea about literature survey.
- Expertise the knowledge about published research works.
- Uunderstand the way of thesis writing.
- Explore the presentation skill of research work.
- Eenhance the interdisciplinary research work
- Realise the characterization of newly synthesized compounds in synthetic field of organic and inorganic chemistry
- Enhance the proficiency in the characterization of a compound using instrumentation techniques such as UV-Visible, IR, NMR etc

Project work:

1. Each leaner can select for his / her research project in any one of the areas of chemistry in consultation with his / her guide and the head of the department.
2. The project report should be submitted to the principal through the head of the department of chemistry one week prior to the commencement of the summative examination. If a candidate fails to submit his/her project report on the date presented above, he / she may be permitted to submit the same 4 days prior to the date of viva-voce examination with a fine as prescribed by the college..
3. Each learner shall submit 2 copies of his / her project report for valuation.
4. The project report shall contain at least 25 pages excluding bibliography and appendices.
5. The project report shall be valued for a total of 100 marks out of which the external examiner and guide share 30 and 18 marks respectively. The sum of marks awarded by

both the examiners shall be considered to be the final mark. For the pass in the project the learner shall secure a minimum of 24 marks. If the leaner fails to get the minimum pass mark in the project report he/ she shall be permitted to resubmit his / her project report once again within a period of 6 months after the publication of the result.

6. For those candidates who have passed in the evaluation of the project there will a viva-voce examination of the above. The viva-voce carried a minimum of 20 marks and it will be conducted jointly by the guide and the external examiner. The learner should secure a minimum of 10 marks for a pass in the viva-voce examination failing which he / she would be required to reappear for the same after a month but within a period of 3 months for which he/ she will have to pay a fee as prescribed by the college.
7. Further for a pass in this paper as a whole, a leaner should secure atleast 50 marks in project report and viva – voce put together.