# BAPATLA ENGINEERING COLLEGE B A P A T L A

# M.Sc. CHEMISTRY

### (PREVIOUS: 2015-16)

**SYLLABUS** 

### Acharya Nagarjuna University Syllabus for M.Sc., Chemistry

### **SEMESTER – I**

### PAPER - I, GENERAL CHEMISTRY 60Hrs.(4Hrs./Week)

### UNIT I

**Treatment of analytical data** : Classification of errors - Determinate and indeterminate errors - Minimisation of errors - Accuracy and precision - Distribution of random errors - Gaussian distribution - Measures of central tendency - Measures of precision - Standard deviation - Standard error of mean - student's t test - Confidence interval of mean - Testing for significance - Comparison of two means – F test- Criteria of rejection of an observation - propagation of errors - Significant figures and computationrules - Control charts - Regression analysis - Linear least squares analysis.

### **UNIT-II**

### **Titrimetric Analysis:**

Classification of reactions in titrimetric analysis- Primary and secondary standards-Neutralisation titrations-Theory of neutralisation indicators-Mixed indicators- Neutralisation curves-Displcement titrations-Precipitation titrations-Indicators for precipitation titrations-Volhard method-Mohr method-Theory of adsorption indicators-Oxidation redution titrations-Change of electrode potentials during titration of Fe(II) with Ce (IV)-Detection of end point in redox titrations-Complexometric titrations- Metal ion indicators-Applications of EDTA titrations-Titration of cyanide with silver ion.

### **UNIT -III**

**Visible spectro photometry and potentiometry** - Beer-Lambert's law - Deviations from Beers law - Instrumentation - Applications - Photometric titrations - Spectrophotometric determination of pK value of an indicator - Simultaneous spectrophotometric determinations -Advantages of potentiometric methods - Reference electrode - Standard hydrogen electrode . Calomel electrode - Indicator electrodes: Metal-metal ion electrodes - Inert electrodes -Membrane electrodes - theory of glass membrane potential - Direct potentiometry , potentiometric titrations - Applications.

### UNIT-IV

**Programming in FORTRAN 77** - Flow charts-Constants and variables - Arithmetic expressions -Arithmetic statement - Replacement statement - Input and output statements - Format specifications - Termination statement - Branching statement - IF statement - Arithmetic and logical IF statement - GOTO statement - Subscripted variable and DIMENSION Statement - DATA Statement. Control statements - DO statement - Rules for DO statements - Functions and subroutines – common statement Flow charts and computer programs for

- i) Summing of power series  $1+x+x^2+x^3+...x^n$
- ii) Rate constant of First order reaction or Beer's law by linear least square method.
- iii) Hydrogen ion concentration of a strong acid/Quadratic euqation.
- iv) Solution for Vander Waals equation or Hydrogen ion concentration of a monoprotic weak acid.

v) Standard deviation and variance of univariant data.

### **REFERENCES:**

- 1. Vogel's text book of quantitative analysis. Addition Wesley Longmann Inc.
- 2. Quantitative analysis R.A Day and A.L.Underwood. Prentice Hall Pvt.Ltd.

3. Principles of computer programming (Fortran 77 IBM PC)V.Rajaraman, Prentice Hall.

4. An introduction to Digital computers.V.Rajaraman and T.Radhakrishnan

5. Fundamentals of Analytical Chemistry - Skoog and West.

6. Basics of computers for Chemists, P.C.Jurs.

### PAPER – II, INORGANIC CHEMISTRY 60Hrs.( 4Hrs./Week)

### UNIT I

**Introduction to Exact Quantum Mechanical Results :** Schrodinger equation , Importance of wave function ,Operators , derivation of wave equation using operator concept . Discussion

of solutions of Shrodingers equation to some model systems viz. particle in one dimensional box

(applications), three dimensional box, Rigid rotator system and the Hydrogen atom.

**Approximate Methods** - Variation theorem, linear variation principle perturbation theory, (first order and non degenerate). Application of variation method to the Hydrogen atom.

**Angular momentum -** Eigen functions and Eigen values of angular momentum, Addition of angular moment.

### UNIT II

**Chemistry of non- transition elements** - Inter halogen compounds, Halogen oxides and oxyfluorides . Noble gas compounds with special reference to clathrates. Spectral and Magnetic properties of Lanthanides and Actinides .Analytical applications of Lanthanides and Actinides.

Structure and bonding -  $p\pi$  -  $d\pi$  bonding - Evidences (in non-transition metal compounds). Concept of Hybridization, Bent's rule, energetics of Hybridisation, concept of Resonance, Non-valence cohesive forces, Hydrogen bonding -Symmetric and unsymmetric, VSEPR theory, Walsh diagrams for linear(Be H2) and bent (H2O) molecules. Molecular Orbital theory, Symmetry of Molecular orbitals, Molecular orbitals in triatomic (Be H2) molecules and ions (NO2 -) and energy level diagrams. Some simple reactions of covalently bonded molecules.

### UNIT III

**Metal** –ligand bonding - Crystal Field Theory of bonding in transition metal complexes – Splitting of d-orbitals in Trigonal bipyramidal and Square pyramidal fields .Tetragonal distortions - Jahn Teller effect . Applications and limitations of CFT . Experimental evidences for covalence in complexes .Moleccular Orbital Theory of bonding for Octahedral , tetrahedral and square planar complexes . $\pi$ - bonding and MOT - Effect of  $\pi$  - donor and  $\pi$  - acceptor ligands on  $\Delta o$ . Experimental evidence for  $\pi$  - bonding in complexes.

### UNIT IV

**Metal – ligand Equilibria in solutions** - Step wise and over all formation constants .Trends in stepwise constants (statistical effect and statistical ratio). Determination of formation constants by Spectrophotometric method (Job's) and pH metric method (Bjerrum's). Stability orrelations - Irwing – William's series. Hard and soft acidsand bases – Acid-base strength and HSAB, Electronegetivity and HSAB. Macrocyclic complexes - Crown ethers and Cryptates. Preparation and structures of Isopoly and Heteropoly acids and their salts.

### **Reference Books**

1. Inorganic Chemistry Huheey, Harper and Row.

2. Physical methods in inorganic chemistry, R.S. Drago. Affliated East-West Pvt. Ltd.

- 3. Concise inorganic chemistry, J. D. Lee, ELBS.
- 4. Modern Inorganic Chemistry, W. L. Jolly, McGrawHill.
- 5. Inorganic Chemistry, K. F. Purcell and J. C. Kotz Holt Saunders international.

6. Concepts and methods of inorganic chemistry , B. E. Douglas and D.H.M.C. Daniel, oxford

Press.

- 7. Introductory quantum mechanics, A. K. Chandra
- 8. Quantum Chemistry ,R. K. Prasad.
- 9. Inorganic Chemistry , Atkins, ELBS
- 10. Advanced Inorganic Chemistry ,Cotton and Wilkinson, Wiley Eastern
- 11. Quantum Chemistry ,R. K. Prasad.
- 12. Text book of Coordination chemistry, K.SomaSekhar rao and K.N.K. Vani, Kalyani Publishers .

### PAPER – III, ORGANIC CHEMISTRY; 60Hrs.( 4Hrs./Week)

### UNIT-I

a) Nature of Bonding in Organic Molecules: Localised and Delocalized covalent bonds,

Delocalised chemical bonding conjugation, cross conjugation, hyper conjugation, tautomerism.

b) Aromaticity: Concept of aromaticity, Aromaticity of five membered, six membered rings and

fused systems.- Non benzonoid aromatic compounds:-cyclopropenyl cation, cyclobutadienyl dication, cyclopentadienyl anion-tropyllium cation and cyclo octatetraenyl dianion. - Metallocenes, Ferrocene, Azulenes, Fulvenes, Annulenes, Fullerenes. - Homo aromaticity, Anti aromaticity and pseudo  $(\Box)$  aromaticity.

### UNIT – II

### **REACTIVE INTERMEDIATES AND HETEROCYCLIC COMPOUNDS:**

a) **Reactive Intermediates**:- Generation, Structure, Stability and reactivity of Carbocations, Carbanions, free radicals, Carbenes, nitrenes and Benzyne.

b) **Heterocyclic Chemistry**:- Synthesis and Ractions of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis.

c) Heterocyclic compounds more than one hetero atom: - Pyrazole, Imidazole, Oxazole Iso-Oxazole, Thiazole, isothiazole, synthesis and properties.

### UNIT - III

### **STEREOCHEMISTRY**:

a) Concept of Chirality: Recognition of symmetry elements and chiral structures (one and more than one chiral centers); D-L and R – S nomenciature, diastereoisomerism; Interconversion of Fischer, Newman and Sawhorse projections. Threo and Erythro isomers, methods of resolution, stereospecific and stereoselective synthesis. Asymmetric synthesis. - Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes). b) Geometrical isomerism – E, Z- nomenclature – physical and chemical methods of determining the configuration of geometrical isomers.

c) Stereochemistry of compounds containing nitrogen, sulphur and phosphorous.

### $\mathbf{UNIT} - \mathbf{IV}$

### **CONFORMATIONAL ANALYSIS:**

a) Conformation of acyclic molecules – alkanes and substituted alkanes –compounds having intramolecular hydrogen bonding, conformations around C-C and carbon hetero atom bonds

### having C - O & C - N.

b) Conformations of monocyclic compounds – cyclohexane- chair, boat and twist boat cyclo hexanes, energy profile diagram – Mono and di- substituted cyclohexanes – conformations and physical properties. Effect of conformation on reactivity in mono and disubstituted cyclohexane derivatives.

c) Elementary treatment of fused and bridged ring systems – Decalines and Bornanes. Conformation of sugars, steric strain due to unavoidable crowding.

### **Reference Books**

1. Advanced organic chemistry – reaction, mechanism and structure, Jerry March, John Wiley.

2. Advanced organic chemistry, F.A.Carey and R.J.Sundberg, Plenum.

- 3. A guide book to Mechanism in organic chemistry, Peter Sykes, Longman.
- 4. Organic chemistry, I.L.Finar, Vol. I & II, Fifth ed. ELBS, 1975.
- 5. Organic chemistry, Hendrickson, Cram and Hammond (Mc Graw Hill).
- 6. Stereo Chemistry of carbon compounds E.L. Eliel.
- 7. Modern organic Reactions, H.O. House, Benjamin.
- 8. An introduction to chemistry of Heterocyclic compounds, R.M.Acheson.
- 9. Structure and mechanism in organic chemistry, C.K.Ingold, Cornell University Press.
- 10. Principles of organic synthesis, R.O.C.Norman and J.M.Coxon, Blakie Academic & Professional.
- 11. Reaction Mechanism in Oganic Cemistry, S.M.Mukherji and S.P.Singh, Macmillan.
- 12. Basic Principles of Organic Chemistry by J. B. Roberts and M. Caserio.
- 13. Stereochemistry of Organic compounds, P. S. Kalsi, New Age International.

### PAPER – IV, PHYSICAL CHEMISTRY 60Hrs.( 4Hrs./Week)

### UNIT-I

### **Thermodynamics - I**

Classical thermodynamics - Brief review of first and second laws of thermodynamics -Entropy change in reversible and irreversible processes - Entropy of mixing of ideal gases -Entropy and disorder – Free energy functions - Gibbs-Helmoboltz euqation - Maxwell partial relations - Conditions of equilibrium and spontaneity - Free energy changes in chemical reactions: Van't Hoff reaction isotherm - Van't Hoff equation - Classiuss Clapeyron equation - partial molar quantities - Chemical potential - Gibbs- Duhem equation - partial molar volume - determination of partial molar quantities - Fugacity - Determination of fugacity -Thermodynamic derivation of Raoult's law.

### UNIT – II

**Surface phenomena and phase equilibria** - Surface tension - capillary action - pressure difference - across curved surface (young - Laplace equation) - Vapour pressure of small droplets (Kelvin equation) - Gibbs-Adsorption equation - BET equation - Estimation of surface area - catalytic activity of surfaces – ESCA , X- ray flouresence and Augar electron spectroscopy.

Surface active agents - classification of surface active agents - Micellisation - critical Micelle

concentration (CMC) - factors affecting the CMC of surfactants, microemulsions - reverse micelles - Hydrophobic interaction.

### UNIT - III

**Electrochemistry** – **I** - Electrochemical cells - Measureement of EMF - Nernst equation – Equilibrium constant from EMF Data - pH and EMF data - concentation cells with and without transference – Liquid junction potential and its determination - Activity and activity coefficients - Determination by EMF Method - Determination of solubility product from EMF measurements. Debye Huckel limiting law and its verification. Effect of dilution on equivalent conductance of electrolytes - Anamolous behaviour of strong electrolytes.Debye Huckel-Onsagar equation - verification and limitations - Bjerrum treatment of electrolytes conductometric titrations.

### UNIT - IV

**Chemical kinetics**- Methods of deriving rate laws - complex reactions - Rate expressions for opposing, parallel and consecutive reactions involving unimolecular steps. Theories of reaction rates - collision theory - Steric factor - Activated complex theory - Thermodynamic aspects – Unimolecular reactions - Lindemann's theory - Lindemann-Hinshelwood theory. Reactions in solutions - Influence of solvent - Primary and secondary salt effects - Elementary account of linear free energy relationships - Hammet - Taft equation - Chain reactions - Rate laws of H2-Br2, photochemical reaction of H2 - Cl2 Decomposition of acetaldehyde and ethane - Rice-Hertzfeld mechanism.

### **REFERENCES:**

- 1. Physical Chemistry P.W.Atkins, ELBS
- 2. Chemical Kinetics K.J.Laidler, McGraw Hill Pub.
- 3. Text Book of Physical Chemistry. Samuel Glasstone, Mcmillan Pub.
- 4. Physical Chemistry, G.W.Castellan. Narosa Publishing House
- 5. Thermodynamic for Chemists. Samuel Glasstone
- 6. Electrochemistry, Samuel Glasstone, Affiliated East West
- 7. Physical Chemistty, W.J.Moore, Prentice Hall
- 8. Atomic structure and chemical bond. Manas chanda. Tata McGraw Hill Company Limited.

### M.Sc. CHEMISTRY PEVIOUS PRACTICALS (I SEMESTER)

### **INORGANIC CHEMISTRY (PRACTICAL-I)**

Quantitative Analysis:

- A. Volumetric Analysis:
  - 1. Acid-Base Titrations:
    - a. Determination of a mixture of carbonate and hydroxide- Analysis f commercial caustic soda
- B. Red-Ox Titrations:
  - Determination of Ferrous ammonium sulphate (Fe<sup>+2</sup> ions)by titrating against KMnO<sub>4</sub>
  - 2. Determination of Ferous ammonium sulphate (Fe<sup>+2</sup> ions) by titrating against  $K_2Cr_2O_7$
- C. Complexometric Titrations:
  - 1. Determination of  $Mg^{+2}$  ions by titrating against EDTA
  - 2. Determination of Hardness of water
  - 3. Determination of Ni<sup>+2</sup> ions by titrating against EDTA
- D. Miscellaneous Titrimetric Determinatiobns
  - 1. Determination of  $Zn^{+2}$  ions by titrating against  $K_4[Fe(CN)_6]$

Gravimetric Analysis

- 1. Determination of Ni as Nickel dimethyl glyoxime
- 2. Determination of Zn as Zinc Ammonium phosphate
- 3. Determination of Cu as cuprous thiocyanate

### **ORGANIC CHEMISTRY (PRCTICAL-II)**

Preparation and purification of organic compounds involving 1 & 2 steps. (minimum of 5 each compounds)

Single step

- 1. Asprin
- 2. Iodoform
- 3. m-dinitrobenzene
- 4. p-bromo Acetanilide
- 5. Acetnilide

Two step

- 1. P-nitro acetanilide from aniline
- 2. Phthalamide from Phthalic acid
- 3. 2,4-dinitro phenyl hydrazine from chlorobenzene'

- 4. M-nitro phenol from m-dinitrobenzene
- 5. M-dinitribenzene from benzene

### PHYSICAL CHEMISTRY (PRACTICAL III)

- 1. Distribution coefficient of Benzoic acid between benzene and water
- 2. Determination of equilibrium constant of  $KI_3 KI + I_2$  by partition coefficient method and determination of unknown concentration of potassium iodide
- 3. Determination of rate constant of oxidation of iodide ion with persulphate ion.
- 4. Determination of rate constant of sodium formate and iodine
- 5. Relative strengths of acids by studying hydrolysis of ethyl acetate/methylacetate
- 6. Determination of critical solution temperature of phenol-water systemand study of the effect of electrolyte on the miscibility of phenol-water system
- 7. Adsorption of acetic acid on charcoal
- 8. Determination of the formula of cuprammonium cation.

### SEMESTER-II

#### PAPER – I, GENERAL CHEMISTRY 60Hrs.(4Hrs./Week)

#### UNIT-1

**Symmetry and Group theory in Chemistry** - Symmetry elements, symmetry operation, definition of group, suib group, relation between order of a finite group and its sub group. Point symmetry group. Schonfiles symbols, representation of groups by Matrices (representation for the Cn, Cnv, Cnh, Dn etc. groups to be worked out, explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use. Application of group theory in IR and Raman spectroscopy.

### UNIT – II

Motion of molecules-Degrees of freedom –Energy associates with the degrees of freedom Type of spectra **Microwave spectroscopy.** Classification molecules, rigid rotator model, effect of isotopic substitution on the transition frequency Intensities non-rigid rotator-Microwave spectra of polyatomic molecules.

### Infared spectroscopy

Harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths, anhoremonicity Morse potential energy diagram. Vibration – rotation spectroscopy. PQR braches, Born – oppenheimer approximation, Break down Born – openheimer approximation, selection rules, normal modes of vibration group frequencies, overtones, hot bands, application of IR spectra to polyatomic molecules.

### UNIT – III

### Raman spectroscopy.

Classical and quantum theories of Raman effects, pure rotational, vibrational and Vibrational – rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent antistrakes Raman Spectroscopy (CARS) – Application.

**Visible and ultraviolet spectroscopy:** - Electronic Spectra of diatomic molecules, vibrational structure of an electronic transition, classification of bands, rotational fine structure of electronic vibrational transition. Electronic Spectra of Polyatomic Molecules – Instrumentation – applications.

### $\mathbf{UNIT} - \mathbf{IV}$

### Nuclear Magnetic Resonance Spectroscopy: -

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its

measurements, factors influencing chemical shift, desheilding, spin - spin interactions, factors

influencing, coupling constant J. Classification (ABX, AMX, ABC, A2, B2 etc.) Basic ideas about instrument NMR studies of nuclei other than proton -13C, 19F, 31P. Use of NMR in medical diagnostics.

#### Electron spin resonance spectroscopy. : -

Basic principles, zero field splitting and kranners's degeneracy, factors affecting the 'g' value. Istropic and anisotropic hyperfine coupling constants, spin hamiltenia, Spin densities measurement techniques - applications.

### **SUGGESTED BOOKS:**

1.Fundamentals of Molecular spectroscopy: by C.N.Banwell

2.Introductory Group Theory for Chemists - George Davidson

3.Group theory for chemistry – A.K.Bhattacharya

4. Molecular spectroscopy by B.K. Sharma

5. Vibrational Spectroscopy by D.N.Sathyanarayana New Age Int. Pub.

6. Spectroscopy by Aruldas.

7. Chemical Analysis by H.A.Laitinan and W.E.Harris, McGraw Hill.

### PAPER-II INORGANIC CHEMISTRY 60 Hrs (4 Hrs/WEEK)

### UNIT I

### Non metal cages and metal clusters:

**Nonmetal cages**, structure and bonding in phosphorous- oxygen and phosphorous -sulphur cages; structure and bonding in higher boranes with (special reference to B12 icosahedra). Carboranes , metalloboranes, metallo carboranes.

**Metal clusters:** Classification- LNCs and HNCs ,Isoelectronic and Iso lobal relation ships , electron counting rules: Wade's and Lauher's rules. M-M multiple bonding; preparation, structrure and bonding in dinuclear [Re2Cl8] 2- ion, trinuclear [Re3Cl9] , tetra nuclear W4OR16, hexa nuclear [Mo6Cl8]4+ and [Nb6Cl12]2+ poly atomic Zintle ions and Chevrel phases. Applications of clusters

Metal  $\pi$ - complexes: preparation, structrure and bonding in Nitrosyl ,Dinitrogen and Dioxygen

complexes.

### UNIT II

Organometallic complexes of transition metals: Classification and electron counting rules.

Metallocenes with four, five, six, seven and eight  $(\Box 4 - \Box 8)$  membered rings, synthesis, structure and bonding of Ferrocene. Cyclopenta dienyl, Arene, Cyclohepta triene and Tropylium complexes of transition metals. Reactions of organometallic compounds oxidative addition reductive elimination, insertion and elimination. Applications of organometallic compounds- Catalytic hydrogenation, Hydro formylation Zeigler- Nutta catalyst for polymerization of olefins.

**Bio chemical aspects of iron and cobalt:** Binding, storage and transport of dioxygen by Hemoglobin and Myoglobin. Vitamin B12 and its importance.

### UNIT III

### **Reaction mechanism of transition metal complexes:**

Kinetics of octahedral substitution, acid hydrolysis, base hydrolysis -conjugate base(CB) mechanism. Direct and indirect evidences in favour of CB mechanism. Anation reactions. Reactions without metalligand bond cleavage. Factors affecting the substitution reactions in octahedral complexes. Trans effect on substitution reactions in square planar complexes. Mechanism of redox reactions, outer sphere mechanism, cross reactions and Marcus –Hush equation, inner sphere mechanism, complementary and non – complementary reactions.

**Photo reactions:** Introduction, Adamsons rules, photo redox reactions, photo isomerisation, photo anation and photo aquation reactions. Photo chemical decomposition of water, photo reactions of Fe(II) and Fe(III).

### **UNIT IV**

Electronic spectra of transition metal complexes Electronic configurations

and Spectroscopic terms . Selection rules , Slator - Condon parameters , Racah parameters , Term separation energies for dn configurations Correlation diagrams and Orgel diagrams . Tanabe- Sugano diagrams for d1 to d9 configurations . Calculations of Dq ,B and  $\beta$ parameters. Charge transfer spectra.

Magnetic properties of transition complexes Types of magnetism, factors affecting paramagnetism, anomalous magnetic moments - Orbital and spin contribution, spin - orbit coupling and magnetic moments. Chiroptical properties, Cotton effect and Faraday effect.

### **References:**

1. Inorganic Chemistry, Huheey. Harper and Row.

- 2. Concise inorganic chemistry ,J. D. Lee, ELBS.
- 3. Inorganic chemistry ,K.F. Purcell and J.C. Kotz, Holt Saunders international
- 4. Organometallic chemistry ,R.C. Mehrotra and A. Singh. New Age International.
- 5. Advanced Inorganic Chemistry, Cotton and Wilkinson, Wiley Eastern
- 6. Inorganic reaction mechanism, Basolo and Pearson, Wiley Eastern
- 7. Bioinorganic Chemistry K. Hussan Reddy

8. Biological Aspects of inorganic chemistry, A. W. Addiso, W. R. Cullen, D. Dorphin and G. J.

james. Weliey Interscience.

9. Photochemistry of coordination compounds, V.Balzaniand V.Carassiti. Academic Press

10. Text book of Coordination chemistry by K.SomaSekhar rao and K.N.K. vani, Kalyani Publishers .

### PAPER – III, ORGANIC CHEMISTRY; 60Hrs. (4Hrs./Week)

### UNIT-I

### SYNTHETIC METHODS AND NAMED REACTIONS

### a) General Methods for synthesis:

Additions: Addition to carbon – carbon multiple bonds, HX, X2, HOX, stereo chemistry of formation and reaction of epoxides, syn and anti hydroxylation, addition. hydrogenation(catalytic and Non catalytic), sythetic reactions of CO and CN and Cram's rule.

### b) Familiar Name Reactions and Mechanisms:

Perkin. Dieckmann and Benzoin. cannizaro. Stobbe condensations; Hofmann, Schmidt, Lossen, Curtius, Clasien, Backmann and Fries rearrangements; Reformatsky, Favoursky, Mannich reaction, Baeyer Villiger reaction and Chichibabin reaction, Michael addition, Oppenaur oxidation, Clemmensen, Wolff-Kishner, Meerwein-Ponndorf-Veriev and Birch reductions.

### **UNIT-II**

### a) Aliphatic Nucleophilic substitutions:

The SN2, SN1, mixed SN1 and SN2 and SNi reactions : Mechanism, effect of structure, nucleophile, leaving group. The neighbouring group mechanism, neighbouring group participation by  $\Box$  and  $\Box$  bonds, anchimeric assistance.

### b) Aromatic Nucleophilic substitution:

The SNAr, SN1 mechanisms and benzyne mechanism. Reactivity- effect of substrate structure.

leaving group and attacking nucleophile. The Von-Ritcher, Sommelet – Hauser and Smiles rearrangements.

### UNIT –III

### Eliminations and protecting agents :

a) Types of elimination (E1,E1CB,E2) reactions, mechanisms, stereochemistry and orientation,

Hofmann and Saytzeff's rules, Syn elimination versus anti elimination. Competitions between

elimination and substitution.

b) Dehydration, dehydrogenation, decarboxylative elimination, pyrolytic elimination, molecular rearrangement during elimination.

c) Theory and importance of functional group protection in organic synthesis:- Protecting agents for the protection of functional groups Hydroxyl group, Amino group, Carbonyl group and Carboxylic acid group

### UNIT – IV

### CHEMISTRY OF NATURAL PRODUCTS:

a) Alkaloids: General methods of identification of alkaloids, Structure and synthesis of Atropine,

Berberine and Yohimbine.

b) Lower Terpinoids: General methods of identification of terpnoids, Isoprene rule, biogenetic

isoprene rule and classification of terpenes. Structural elucidation and synthesis of  $\Box$ -terpeniol, $\alpha$ -pinene and camphor.

c) Quinones: Identification of quinones, Lapachol. Chrysophenol and Physcion.

### **Books suggested**:

- 1. Advanced organic chemistry reaction, mechanism and structure, Jerry March, John Wiley.
- 2. Advanced organic chemistry, F.A.Carey and R.J.Sundberg, Plenum.
- 3. A guide book to Mechanism in organic chemistry, Peter Sykes, Longman.
- 4. Organic chemistry, I.L.Finar, Vol. I & II, Fifth ed. ELBS, 1975.
- 5. Organic chemistry, Hendrickson, Cram and Hammond (Mc Graw Hill).
- 6. Stereo Chemistry of carbon compounds E.L. Eliel.
- 7. Modern organic Reactions, H.O.House, Benjamin.
- 8. An introduction to chemistry of Heterocyclic compounds, R.M.Acheson.
- 9. Structure and mechanism in organic chemistry, C.K.Ingold, Cornell University Press.
- 10.Principles of organic synthesis, R.O.C.Norman and J.M.Coxon, Blakie Academic & Professional.
- 11.Reaction Mechanism in organic chemistry, S.M.Mukherji and S.P.Singh, Macmillan.
- 12. Nturally occurring quinines R. H. Johnson Vol. I & II, Academic Press, London.

### PAPER – IV, PHYSICAL CHEMISTRY 60Hrs.( 4Hrs./Week)

### UNIT – I:

**Thermodynamics II : Third law and Statistical thermodynamics**-Nernst Heat theorem -Third law of thermodynamics - Its limitations - Determination of absolute entropy - concept of districution - Thermodynamic probability and most probable distribution - Ensembleensemble averaging - Maxwell-Boltzmann distribution law - Partition function - Fermi-Dirac statistics - Bose Einstein statistics - Entropy and probability - Boltzmann-Plank equation calculation of thermodynamic properties in terms of partition function - Application of partition function - Chemical equilibrium and partition function - Translational, rotational and electronic partition function - Entropy of Monoatomic gases (Sackur - Tetrode equation). **UNIT –II** 

**Polymer chemistry:** Classification of polymers - Free radical , ionic and Zeigler -Natta Polymerisation - kinetics of free radical polymerisation - Techniques of polymerisation - Glass transition temperature - Factors influencing the glass transition temperature - Number average and Weight average, Molecular weights –molecular weights determination - End group analysis - Osmometry - Light scattering and ultra centrifugation methods.

### UNIT – III:

**Electro Chemistry-II** :Electrode potentials - Double layer at the interface - rate of charge transfer - Decomposition potential - Over potential - - Tafel plots - Derivation of Butler-Volmer equation for one electron transfer - electro chemical potential.

**Electro catalysis** - - Fuel cells-Theory of polarography - Diffusion current - Ilkovic equation – Equation for half- wave potential –Applications of polarography - Amperometric titrations - Corrosion - Forms of corrosion - prevention methods.

### UNIT – IV

**Chemical kinetics and photo chemistry -** Branching Chain Reactions - Hydrogen-oxygen reaction - lower and upper explosion limits - Fast reactions - Study of kinetics by flow methods -

Relaxation methods - Flash photolysis - Mechanism of homogeneous catalysis - Acid base catalysis - protolytic and prototropic mechanism - Enzyme catalysis - Michelis-Menten kinetics.

**Photochemical reactions** - Quantum yield and its determination - Actinometry - Reactions with low and high quantum yields - Photo sensitisation - Exciplexes and Excimers - Photochemical equilibrium - Chemieluminescence-Kinetics of collisional quenching-Stern - Volmer equation - Photo Galvanic cells

### **REFERENCE BOOKS:**

1. Physical chemistry, G.K. Vemulapalli (Prentice Hall of India).

- 2. Physical chemistry, P.W.Atkins. ELBS
- 3. Chemical kinetics K.J.Laidler, McGraw Hill Pub.
- 4. Text book of Physical Chemistry, Samuel Glasstone, Macmillan pub.
- 5. Statistical Thermodynamics M.C.Gupta.
- 6. Polymer Sceince, Gowriker, Viswanadham, Sreedhar
- 7. Elements of Nuclear Science, H.J.Arniker, Wiley Eastern Limited.
- 8. Quantitative Analysis, A.I. Vogel, Addison Wesley Longmann Inc.
- 9. Physical Chemistry-G.W.Castellan, Narosa Publishing House, Prentice Hall

10. Physical Chemistry, W.J.Moore, Prentice Hall

11. Polymer Chemistry - Billmayer

12. Fundamentals of Physical Chemistry, K K

### M.Sc., Chemistry Previous Practicals (II Semester)

### **Inorganic Chemistry (Practical-I):**

Qualitative Analysis:

Semimicro qualitative analysis of an inorganic mixture containing three catations (one less familiar cation) and three anions (one interfering anion)

Less familiar cations: Tl, Mo, Th, Zr, V and U. Interfering anions: Oxalate, tartrate, phosphate and chromate.

Chromatography: Separation of cation and anion by Paper Chromatography (at least one experiment)

### **Organic Chemistry (Practical-II):**

Qualitative Analysis of organic compounds.

Phenols, Carbonyl compounds (Aldehydes & Ketones), Acids, Nitro compounds, Amines, Amides and carbohydrataes.(2 compounds are to be given for analysis with preparation of one solid derivative for each).

### **Physical Chemistry (Practical-III):**

Potentiometric determinations of

- 1. Fe(II) with Ce(IV)
- 2. Fe(II) with  $K_2Cr_2O_7$
- 3.  $V^{5+}$  &MnO<sub>4</sub> with Fe(II)

Conductometric titrations of

- 1. Strong acid (HCl) with strong base (NaOH)
- 2. Weak acid (AcOH) with strong base (NaOH)
- 3. Mixture of strong &weak acids with strong base.

p<sup>H</sup> metric titrations of

- 1. Strong acid with strong base
- 2. Mixture of carbonate and bicarbonate with HCl

### Colorimetry:

- 1. Verification of Beers Law with 1.  $K_2Cr_2O_7$
- 2. Colorimetric determination of Fe (III) with thiocyanate.

# BAPATLA ENGINEERING COLLEGE B A P A T L A

## M.Sc. CHEMISTRY

(Specialization: ORGANIC)

(FINAL: 2015-16)

### **SYLLABUS**

### Acharya Nagarjuna University Syllabus for M.Sc., Chemistry

### SEMESITER III

### PAPER – I : ORGANIC SPECTROSCOPY –I. (C3.1(O)-10)

### UNIT –I

(a) Ultraviolet spectroscopy : Mechanics of measurement – Energy transitions – Simple chromophores – UV absorption of Alkenes – polyenes unsaturated cyclic systems – Carbonyl compounds  $\alpha$ , $\beta$ - unsaturated carbonyl systems - Woodward – Fieser rules – aromatic systems – solvent effects – geometrical isomerism – acid and base effects – typical examples – calculation of  $\lambda$ max values using WF-rules.

(b) Optical rotatory dispersion: Theory of optical rotatory dispersion – Cotton effect – The octant rule – application in structural studies.

### UNIT –II

(c) Infrared spectroscopy : Mechanics of measurement – Fundamental modes of vibrations – Stretching and bending vibrations – hydrogen bonding – finger print region and its importance – Typical group frequencies for – CH, -OH, -NH, -CC, -CO and aromatic systems - Application in structural determination – Examples – simple problems.

### UNIT –III

(a) NMR spectroscopy: Magnetic properties of Nuclei theory of Nuclear Resonance Fourier transformation and its importance in NMR spectrometry. The chemical shift its importance and measurement calculation of chemical shift integration and J values from the spectral data problems related to calculation of chemical shift integration and J values Factors effecting chemical shift such as electro negativity and anisotropy – Shielding and deshielding mechanisms in acetylene carbonyl and Benzene anisotropy – spin-spin Interactions related to first order and higher order spectra – AB - A2 - AB2. ABX - ABC - AMX interactions – temperature dependence spectra – double irradiation and its importance in the interpretation of Proton Spectra – Hydrogen bonding – Geometrical and optical isomerism interpretation of NMR spectrum of a given compound leading to identification –typical examples of PMR spectroscopy.

### UNIT-IV

(a) Problems involving individual spectral methods – UV, IR and PMR

(b) Problems involving combined any two of UV, IR and PMR

(c) Problems involving all the three of UV, IR and PMR.

### **TEXT BOOKS:**

1. Spectrometric identification of organic compounds by R.N. Silverstein & G.C. Bassier (John Willey)

2. Spectroscopic methods in Organic Chemistry by Williams and Fleming (Mcgraw Hill)

3. "Organic Photochemistry" by R.O.Kan (Mc Graw Hill)

4. "Advanced organic Chemistry Reaction Mechanisms and Structure" by J March (McGraw Hill & Kogshusha)

5. "Carbon-13 NMR Spectroscopy" by J.B.Stothers.

### PAPER-II: ORGANIC SYNTHESIS, MECHANISMS AND NANO CHEMISTRY (C3.2(O)-10)

### **UNIT-I:**

### i) Methods for determining Reaction mechanisms by kinetic and non-kinetic studies.

Kinetics of reaction, Energy profile diagram, Intermediate versus transition state, Reaction rate and rate limiting step. Identification of products, testing possible intermediates, trapping of intermediates, Cross over experiments, Isotopic labeling.

### ii) Free radicals and their reactions

Introduction, formation, detection and stability of radicals. Some radical reactions, Addition of halogens, Hydrogen halides. Substitution reactions-Halogenation, Aromatic substitution, Sandmayer reaction, Autooxidation, Decomposition of dialkyl and diacyl peroxides.

### **UNIT-II:**

**Oxidations** Introduction: Different Oxidative processes. Hydrocarbon: alkenes, aromatic rings saturated C-H groups (activated and unactivated), Alcohols, diols, aldehydes, Ketones, Carboxylic acids, Amines, hydrazines, sulphides. Oxidations with ruthenium tetroxide iodobenzene diaccetate and Tl(III) nitrate, Lead tetra acetate, SeO2, MnO2 Ag2CO3, oppenauer oxidation, peracids. Oxidation of C=C perhydroxylation using KMnO4, OsO4, peracids.

### UNIT –III:

**Reductions:** Introduction: Reductive process Hydrocarbons: Alkanes, alkenes, alkynes, and aromatic rings

Carbonyl compounds – aldehydes, ketones, acids and their derivatives. Nitro, nitroso, azo and oxime group Hydrogenolysis. Catalytic hydrogenations, Reduction by dissolving metals, Reduction with metal and acid. Reduction with metal in liquid ammonia (Birch reduction). Reduction by hydride transfer reagents Aluminium alkexide, LiAlH4, NaBH4, Diisobutyl aluminium hydrides – Sodium cyano borohydride ,tryalkyl borohydirdes – Reduction with diimide.

### **UNIT-IV:**

**Nanochemistry :** Introduction, carbon nanotubes: structure of single and multi wall carbon nanotubes, synthesis-solid and gaseous carbon source-based production techniques, synthesis with controlled orientation. Growth mechanism of carbon nanotubes-catalyst free growth, catalyst activated growth, properties-general, adsorption, electronic & optical, Mechanical and reactivity. Applications.

### **SUGGESTED BOOKS:**

1.Mechanism and structure in Organic Chemistry " E.S.Gould Henry - Holt and Co, Newyork

2. Advances in Organic Reaction mechanism and structure J. March (McGrew Hill)

3. Aguide Book to Mechanism in Organic Chemistry" by P.Sykes

4.Synthetic approaches in organic chemistry by R.K.Bansal(Narosa Publications)

- 5. Some modern methods of synthesis by Carruthers (Cambridge).
- 6. G.A.Ozin, A.C. Arsenault Nano chemistry, RSC.

7. Diwan, Bharadwaj, Nanocomposites, Pentagon.

8. V.S.Muralidharan A.Subramania, Nanoscience and Technology, Ane Books.

### PAPER – III : ALKALOIDS AND PHENOTHIAZINES (C3.3(O)-10)

### UNIT-I

Alkaloids: (1) Definition, nomenclature and physiological action – occurrence – isolation – general

methods of structural elucidation – degradation – classification based on nitrogen

heterocyclic ring –role of alkaloids in plants. (2) Cinchona alkaloids : Cinchonine ,quinine, stereochemistry of cinchonine and quinine (3) Isoquinoline alkaloids: Aporphines: Glaucine and dicentrine phthalide isoquinolines: Hydrastine and narcotine Protoberberines: Berberine and canadine Benzylisoquinoline: Coclawrine.

### UNIT-II

### Isoquinoline & Morphine group Alkaloids:

(1) Ipecac alkaloids: Emetine, Stereochemistry of emetine.(2) Morphine alkaloids: Morphine Thebaine Codeine – Stereochemistry of morphine alkaloids – some rearrangements of morphine alkaloids

(3) Biogenesis of alkaloids

### UNIT-III

(1) Indole alkaloids: Reserpine, strychnine, brucine, physostigmine, lysergic acid, isolysergic acid, erogotamine and Ibogamine (2) Structure, stereochemistry, synthesis and biosynthesis of Ephedrine, Conine and nicotine.

### UNIT-IV

Phenothiazines: (1) Classification, general methods of synthesis of phenothiazines – pharmacological properties of phenothaizines (2) Dimethylamine series:Promazine and promethazine (3) Piperazine series:Prochlorperazine and trifluoperazine (4) Piperdine sereies: Thioriazine and mesoridiane

### **TEXT BOOKS:**

1. Alkaloids by K.W.Bentley Vols I & II.

2. Text Book of Organic Chemistry I.L. Finar Vol. II

3.An introduction of alkaloids by G.A.Swain,

### **Books for further Study:**

1. Chemistry and physiology of alkaloids by Manske Vol.I & II, VII

- 2. Medicinal Chemistry by A. Burger
- 3. Isoquinoline Alkaloids by M.Shamma
- 4. Heterocylclic Chemistry by JA Joule etal, Chapman Hall

5. An introduction to heterocyclic compounds by RM Acheson, John - Wiley

6. Non-Antibiotics – A new class of unrecognized antimicrobics by AN Chakraborthy etal,

National Institute of Science Communication, (CSIR), New Delhi, India, 1988

7. Principles of Medicinal Chemistry by William O.Foye, Lea & Febiger, Philadelphia/London,

1989

### PAPER-IV: CHEMISTRY OF NATURAL PRODUCTS (C3.4(O)-10)

### UNIT-I

Terpenoids: Classification, sources, isolation, synthesis and stereochemistry with special reference to zingiberene, santonin, eudesmol, abietic acid., Biosynthesis of terpenoids Flavnoids: Classification, sources, isolation, chemistry and synthesis with special reference to quercetin and kampferol

### UNIT-II

Steroid Hormones: Chemistry & synthesis of equilenine,oestrone,progestrone,androsterone, testosterone, cartisone. Non steroid hormones: Chemistry & synthesis of thyroxin, epinephrine and oxytocin

### UNIT-III

Fat Soluble Vitamins:Chemistry,Synthesis & biosynthesis of vitamin A1,vitamin  $E(\alpha,\beta,\gamma,\delta-$ tocopherols) and vitamin K Water soluble Vitamins:Chemistry,Synthesis and biosynthesis of B1 and C

Chemistry of biomolecules a)Enzymes : classification , kinetics and mechanism of enzyme action

b) Coenzymes and cofactors: NAD FAD folic acid citric acid cycle. c) Prostaglandins with special reference to PGE and PGF

### **UNIT-IV**

Naturally occuring insecticides: Introduction, general properties, sources, isolation, synthesis and stereochemistry of Pyrethrin I and II; Jasmolin I & II; Jasmolone and Cinerelone. Strucutre activity relation ship(SAR) studies and bio synthesis of pyrethrins Rotenoids – Chemistry and synthesis of rotenone Isobutylamines: Chemistry and synthesis anacyclin, spilanthol Minor insecticides of plant origin: pachyrrhizin and custard-apple.

### **TEXT BOOKS:,**

1. The Chemistry of Natural Products Vol.II Mono and Sesqui-Terpenes" by P.De Mayo (John Wiley Inc)

- 2. The Higher Terpenoids Vol.III by P.De mayo.,
- 3. Steroids by Fieser and Fieser.;
- 4. The Vitamins by S.F.Dykes.,
- 5. The Natural Pigments by K.W.Bentley;
- 6. Biological Chemistry by Holum,
- 7. Organic Chemistry Vol.II by I.L.Finar,

8. Naturally occuring insecticides by M.Jacobson and D.G.Crosby, Marcel- Decker Inc, New York

9. General Organic and Biochemistry by F.A.Bettelheim and Jerry March, Saunders College, Publishing ,

### **Further Study:**

1.The terpenoids by Simonsen;

2. The steroids by Shoppee,

3. Chemistry of Carbon compounds by Rodd.

# Course: M.Sc. Specialization: ORGANIC CHEMISTRY <u>Practical Syllabus</u> (Semester: III; Batch: 2014-15) PRACTICAL-I: Multistage Organic Synthesis (3 & 4 stage) (Any five experiments must be carryout) Max. Marks: 70 (60Prac. + 10Rec.)

Expt-1: Synthesis of paracetomol from benzene

Step 1: Benzene to Nitrobenzene (Nitration)

Step 2: Nitrobenzene to N-phenyl hydroxylamine (reduction)

Step 3: N-phenyl hydroxyl amine to *p*-aminophenol (Rearrangement)

Step 4: *p*-amino phenol to *p*-hydroxy acetanilide/paracetomol(acetylation)

Expt-2: Synthesis of *o*-chlorobenzoic acid from phthalic acid

Step 1: Phthalic acid to phthalic anhydride (Dehydration)

Step 2: Phthalic anhydride – phthalic amide (Amide formation)

Step 3: Phthalmide- Anthranilic acid (Hoffman's Bromamide reaction)

Step 4: Anthranilic acid -ortho-chloro benzoic acid

Expt-3: Synthesis of sulpha drug from aniline

Step 1: Aniline to acetanilide

Step 2: Acetanilide to *p*-acetamide benzene sulphonyl chloride (sulphonation)

Step 3: p-acetamide benzenesulphonylchloride to p-acetamide benzenesulphonamide

(s-amination)

Step 4: p-acetamide benzene sulphonamide to p-amino

benzenesulphonamide(hydrolysis)

Expt-4: *m*-Chloro-nitrobenzene from nitrobenzene

Step 1: Nitro benzene to *m*-dinitro benzene (nitration)

Step 2: *m*-dinitrobenzene to *m*-nitro aniline (partial reduction)

Step 3: *m*-nitro aniline to *m*-nitrodiazoniumchloride (diazotization)

Step 4: *m*-nitrodiazoniumchloride to *m*-Chloro-nitrobenzene (sandmayers reaction)

Expt-5: Synthesis of *p*-bromo benzanilide from benzophenone

Step 1: Benzophenone to benzopenone oxime (Addition)

Step 2: Benzophenone oxime to benzanilide (Beckman's rearrangement)

Step 3: Benzanilide to *p*-bromobenzanilide) (bromination)

### Expt-6: Synthesis of Methyl orange from aniline

Step 1: Aniline to sulphonic acid (sulphonation)

Step 2: sulphonic acid to Diazonium chloride (diazotization)

Step 3: Diazonium chloride to methyl orange (coupling reaction)

Expt-7: Synthesis of Acridone from Anthranilic acid

Step 1: Anthraninile acid to o-chlorobenzoic acid (Diazotosation followed by sand mayer's reaction)

Step 2: o-chlorobenzoic acid to N-phenyl anthranilic acid (Substitution)

Step 3: N-phenyl anthranilic acid to acridone (Cyclisation)

### All the students must submit the TLC for all the stages of preparation and a photo copy must be pasted in records.

### **REFERENCES:**

- 1. Practical Organic Chemistry A.I. Vogel (Longmans)
- 2. Text Book of practical organic Chemistry F.G.Mann & B.C. Sanders.
- 3. A Manual of Practical Organic Chemistry Day Sitaramam & Govindachari
- 4. Organic Experiments L.F.Fieser.
- 5. Practical Organic Chemistry H.T.Openshaw
- 6. Systematic Identification of Organic Compounds, P.L.Shriner, R.C.Fuson & D.Y.Curtin.
- 7. Identification of Organic Compounds N.D.Cheronis & J.B.Entrilkin
- 8. Advanced Organic Synthesis by R.S.Monson Academic Press

#### Note: For University Practical Examination: Duration: 9 hours

### **PRACTICAL – II :: Estimations**

(All experiments must be carryout) Max. Marks: 70 (15 QA+45Prac.+10Rec.)

Part I: One theory question either relating to spectral characterization or any or as wish by the examiner.	y practical 15M
Part II: The following Estimations/Isolations	45M
Expt. 1: Estimation of hydroxyl group by acetylation or pthalation method	
Expt. 2: Estimation of phenol (bromination method)	
Expt. 3: Estimation of aniline (Bromination method)	
<b>Expt. 4:</b> Estimation of carbonyl groups (Hydrazone formation method)	

**Expt. 5:** Estimation of sugars –glucose and sucrose by using Fehlings solution

Expt. 6: Determination of iodine value of oil or fat

Expt. 7: Determination of saponification value of oil or fat

Expt. 8: Estimation of vitamin 'C' in lime juice.

Expt. 9: Isolation of caffeine from tea/coffee sample.

Record: 10M

For University Practical Examination: Duration: 9 hours

### **SEMESITER IV**

### PAPER – I: ORGANIC SPECTROSCOPY –II (C4.1(O)-10)

### UNIT-I

(a) CMR spectroscopy – noise decoupled and offresonance spectra of simple Compounds – typical examples: of CMR spectroscopy – simple problems

### UNIT-II

(a) Mass spectrometry : Introduction – determination of Molecular weight and formulae – Behavior of organic compounds in Mass spectrometer – fragmentation of typical organic compounds – stability of fragments – rearrangements – metastable peaks – Mass spectra of representative compounds and related problems.

### **UNIT-III**

(a) 2D NMR spectroscopy – Definitions and importance of COSY DEPT HOMCOR HETCOR INADEQUATE INDOR INEPT NOESY HOM2DJ HET2DJ DQFCOSY – COSY of menthol DEPT of ethanol – study of simple organic compounds.

### **UNIT-IV**

(a) Spectral characters and Structural elucidation of the following natural and synthetic compounds involving all the spectral data 1) 4',8-disubsituted Flavone 2) 4,4'-disubsituted chalcone 3) apigenin 4)Kaempferol 5)lawsone 6) nicotine 7) Di-subsituted phenanthrene 8) Di-substituted nalphthalene 9) camphor 10) Zingiberene 11) Equilenine 12) Progesterone

### **TEXT BOOKS:**

1.Spectrometric identification of organic compounds by R.N.Silverstein & G.C.Bassier (John Willey)

2.Spectroscopic methods in Organic Chemistry by Williams and Fleming (McGraw Hill). 3.Organic photochemistry by R.O.Kan (Mc Graw Hill)

4.Advanced organic Chemistry Reaction Mechanisms and Structure by J March ( Mc Graw Hill & Kogshusha)

5.Carbon-13 NMR Spectroscopy by J.B. Stothers.

### PAPER – II: ORGANIC SYNTHESIS, MECHANISMS AND GREEN CHEMISTRY (C4.2(O)-10)

### **UNIT-I:**

### Formation of C-C single & double bonds and Diels–Aider & related reactions

Formation of C-C single bonds – enamines and related reactions – Formation of C-C double bonds – witting reaction of Phosphorus ylides – stereoselective synthesis of tri and tetra substituted alkenes. Diels–Aider and related reactions –diene-dienophile, intra molecular Diels –Alder reactions, Stereochemistry and mechanism Retro Diels – Alder reaction –1,3-dipolar reactions.

### UNIT-II:

### Synthetic applications of organoboranes and Organic synthesis by Disconnection approach.

Synthetic applications of organoboranes –protonolysis, oxidation, carbonylation Reaction of alkenylborane – enantioselective synthesis of secondary alcohols from alkenes – organolithium compounds. An introduction of synthesis and synthetic equivalents,

disconnection approach, functional group interconversions. One group, two group disconnections in simple molecules. Alcohols, Olefins, aryl ketones,  $\alpha$ , $\beta$ -Unsaturated compounds – 1,3 dicarbonyl compounds.

### UNIT-III:

### Green Chemistry and Photochemistry

**Green Chemistry**: Introduction, Principles, examples of green reactions-synthesis of Ibuprofen, Clean Fischer-Indole synthesis comparison of the above with conventional methods. Introduction toMicrowave organic synthesis, Applications: solvents (water and organic solvents), solvent free reactions (solid state reactions), multistep V/s single pot synthesis.

**Photochemistry:** Photochemistry of olefins–conjugated olefins–Aromatic compounds– isomerisation–additions. Photochemistry of carbonyl compounds – Norrish type I and II reactions – Paterno – Buchi Reaction. Photo reduction, Photochemical rearrangements – Photo Fries rearrangement, Di- $\pi$ -methane rearrangement.

### **UNIT-IV:**

**Pericyclic reactionss**: Definition, classification, MO theory, Electronic configuration in ground and first excited states of aliphatic conjugated polyene system(upto 4 double bonds).

**Electrocyclic Reactions**: Mechanism, stereochemistry, PMO, FMO, correlation diagram, Woodward Hoffman rules.

**Cycloaddition Reactions**: FMO and correlation diagram methods-(2+2) and (4+2) cycloaddition reactions, stereochemistry. Woodward Hoffman rules.

**Sigmatropic Rearrangement**: classification, Mechanism by FMO method, Woodward Hoffman rules. Cope, claisen and Aza-cope rearrangements. Fluxional molecules.

### **SUGGESTED BOOKS:**

- 1. Some Modern methods of synthesis By Caruthers (Cambridge)
- 2. Organic synthesis by Robert & Ireland (Printce Hall of India)
- 3. Designing Organic Synthesis B staurt Warron, John Wiley & Sons
- 4. "Pericyclic reactions a mechanistic study" S.M.Mukheji
- 5. Synthetic approaches in Organic Chemistry "R.K.Bansal Narosa Publications
- 6. Advances in Organic Chemistry Reaction mechanism and structure" by J. March (Mc Graw Hill)
- 7. 'Organic Photo chemistry and Pericyclic reactions' M.G.Arora Anmol Publications Pvt. Ltd.
- 8. Fundamentals of photochemistry by K.K.Rohatgi–Mukharjee Now Age international publishers.
- 9. Anastas, P.T.; Warner, J. C., *Green Chemistry, Theory and Practice,* Oxford University Press, Oxford, 2000. ISBN: 0 19 850698 8 (Paperback).

10. Green chemistry, V.K.Ahluwalia, Ane books.

11. P.T. Anastas and J.C. Warner Green chemistry, Oxford.

### PAPER – III: ANITIBIOTICS AND DRUGS (C4.3(O)-10)

### UNIT-I

Antibiotics: (I) Cell wall biosynthesis, inhibitors,  $\beta$ -lactam rings, antibiotics inhibiting protein synthesis, synthesis of penicillin-G, penicillin-V, ampicillin, amoxicillin, chloramphenicol and cephalosporin (II) Streptomycin, tetracyclins, terramycin, aureomycin, gramidin.

### UNIT-II

Drugs and Medicinal chemistry: (I) Chemotherapy : Methodology for structure – activity relationship determination. (II) Drugs: Structure synthesis & Activity of the following : Anticancer Agents: Taxol, Vinblastine, Vincristine, Campothecin

### UNIT-III

Chemotherapy of Brain: Introduction – neurotransmitters CNS stimulants : Strychnine (CNS activity only ) Picrotoxin nikethemide caffeine Nicotine CNS depressants General anesthetics, mode of action of Sedatives & Hypnotics.

### **UNIT-IV**

(I) Antimalarials: Paludrin – quinacrin – chloroquin – camoquin – pamaquin – sontoquine.
(II) Antiamoebic agents : Chiniofon – Resotren – Iodochlorohydroxyquin. (III) Sulpha drugs: Sulphanilamide – Dihydrocurprine – Prontosil (IV) Antiseptics: Diphenyl – Chlorophene-2,4,4-trichloro-2'-hydroxydiphenyl ether – aminocerine hydrochloride. (V) Antifungal agents: 1,8 dihyrosxyanthranol – griseofulvin.

### **TEXT BOOKS:**

- 1. Introduction to Medicinal Chemistry Wiley VCH
- 2. Text Book of Organic Medicinal and Pharmaceutical Chemistry, Wilson and Gisvild, (ed Robert F. Dorge)
- 3. An introduction to drug design by SS Pandeya
- 4. Buger's Medicinal Chemistry and drug discovery Vol.I by (Ed) ME Wolff John Wiley by A. Burger
- 5. The Organic Chemistry of drug design and drug action by RB Silverman, Academic press
- 6. Principles of Medicinal Chemistry by William O. Foye, Lea & Febiger, Philadelphia/London,1989.

### PAPER- IV: TECHNIQUES FOR MODERN INDUSTRIAL APPLICATIONS. (C4.4(O)-10)

### UNIT-I

### **Classical Methods of purification**

**1. Recrystallization**: Basic principles, choice of solvent, seeding, filtration and centrifugation and drying. Industrial applications. Concepts of fractional crystallization.

**2. Distillation: Basic principles**. Distillation types- continuous distillation, batch distillation, fractional distillation, vacuum distillation and steam distillation. Industrial applications.

**3.** Solvent extraction: Basic priciples. Different types of extraction. Selection of solvents. Avoiding emulsion formation. Basic concepts on Soxhlet extraction. Industrial applications.

### UNIT-II:

### Adsorption and Partition Chromatography

**1. Introduction to chromatography.** Different types of Chromatography. Adsorption chromatography-adsorbents, solvents, solutes, apparatus. Column Chromatography-stationary phase, Mobile phase, packing of column, advantages and disadvantages.

**2. Thin Layer chromatography:** Basic Principles. Common stationary phases, Methods of preparing TLC plates, Selection of mobile phase, Development of TLC plates, Visualization methods, Rf value. Application of TLC in monitoring organic reactions. identification and quantitative analysis.

**3. Paper chromatography:** Basic Principles. Ascending and descending types. Selection of mobile phase, Development of chromatograms, Visualization methods. Application of paper chromatography in the identification of sugars and amino acids. One and two dimensional paper chromatography.

### UNIT-III:

**Gas chromatography:** Basic Principles. Different types of GC techniques. Selection of columns and carrier gases. Instrumentation. detectors; RT values. Applications in the separation, identification and quantitative analysis of organic compounds.

**High Performance liquid chromatography(HPLC):** Basic Principles. Normal and reversed Phases. Selection of column and mobile phase. Instrumentation. detectors; RT values. Applications in the separation, identification and quantitative estimation of organic compounds. Concepts on HPLC method development.

### **UNIT-IV:**

### Ion Exchange Chromatography and Electrophoresis

**1. Ion exchange chromatography**: Basic Principles. Preparation of cross linked polystyrene resins. Different types of cation and anoin exchange resins. Application in the purification of carboxylic acids and amines.

**2.** Electrophoresis: Basic Principles. Capillary electrophoresis. Instrumentation, applications, zone-electrophoresis, gel-electrophoresis.

### **SUGGESTED BOOKS:**

1. Principles of Instrumental Analysis by D. A. Skoog, F. J. Holler and T. A. Nieman, Harcourt College Pub.

2. Separation Techniques by M. N. Sastri, Himalaya Publishing House (HPH), Mumbai.

3. Bio Physical Chemistry by A. Upadhyay, K. Upadhyay and N. Nath, (HPH), Mumbai.

4. A Hand Book of Instrumental Techniques for Analytical Chemistry- Ed-F. A. Settle, Prearson Edn, Delhi.

5. Introduction to Organic Laboratory Techniques-D. L. Pavia, G. M. Lampman, G. S. Kriz and R. G. Engel, Saunders College Pub (NY).

6. Instrumental methods of Chemical Analysis by B. K. Sharma, Goel Publish House, Meerut.

7. Instrumental methods of Chemical Analysis by H. Kaur, Pragati Prakasan, Meerut. 8. Protein

### Course: M.Sc.; Specialization: ORGANIC CHEMISTRY <u>Practical Syllabus</u> (Semester: IV; Batch: 2014-15) PRACTICAL-I: Analysis of Binary Organic Mixture

(Any five experiments must be carryout) Max. Marks: 70 (15QA+45Prac.+10Rec.)

Part I: One theory question either relating to spectral characterization or any practical or as wish by the examiner. 15M

Part II: Two component organic mixture analysis

(The student must be given training in at least eight mixtures with different functional groups)

[Note: For University examinations the student has to submit at least two derivatives for each individual component].

**NOTE:** For University Practical Examination: Duration: 9 hours.

Course: M.Sc.; Specialization: ORGANIC CHEMISTRY

Practical Syllabus (Semester: IV; Batch: 2014-15)

PRACTICAL-II: Project Work/Home Paper

Max. Marks: 100

**Project Work / Internship is compulsory for the University students.** 

Selection of Home Paper/Project Work is optional for affiliated college students.

• The students opted for Home Paper must be assigned a latest topic and the students have to submit a dissertation (50-60 pages) covering all the latest literature on the topic assigned. The candidate will be assessed at the time of the conduct of final practical examination of the semester taking into consideration of dissertation and viva-voce on the topic chosen for home paper.