K.V.R GOVERNMENT COLLEGE FOR WOMEN (A), KURNOOL II YEAR SYLLABUS

SEMESTER - III

Course III (ORGANICCHEMISTRY& SPECTROSCOPY) 60hrs (4 h / w)

ORGANIC CHEMISTRY 34h

UNIT – I

1. Chemistry of Halogenated Hydrocarbons: 6h

Alkylhalides: Methods of preparation and properties, nucleophilic substitution reactions– SN1, SN2 and SN I mechanisms with stereo chemical aspects and effect of solvent etc.; nucleophilic substitution vs.elimination, Williamson's synthesis. Arylhalides: Preparation (including preparation from diazonium salts) and properties, nucleophilic aromatic substitution; SN Ar, Benzyne mechanism. Relative reactivity ofalkyl, allyl, benzyl, vinyl and arylhalids towards nucleophilic substitution reactions.

2. Alcohols & Phenols 6h

Alcohols: preparation, properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt Blanc Reduction; Oxidation of diols by periodic acid and lead tetra acetate, Pinacol- Pinacolone rearrangement;

Phenols : Preparation and properties ;Acidity and factors effecting it, Ring substitution reactions, Reimer-Tiemann and Kolbe's-Schmidt Reactions, Fries and Claisen rearrangements with mechanism;

UNIT-II

Carbonyl Compounds 10h

Structure, reactivity, preparation and properties; Nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives

Mechanisms of Aldol and Benzoin condensation, Claisan-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann haloform reaction and Baeyer Villiger oxidation, α - substitution reactions, oxidations and reductions (Clemmensen, wolf –kishner, with LiAlH4 &NaBH4).

Addition reactions of α , β -unsaturated carbonyl compounds: Michael addition. Active methylene compounds: Keto- Enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl aceto acetate.

UNIT-III

Carboxylic Acids and their Derivatives 12h

General methods of preparation, physical properties and reactions of mono carboxylic acids, effect of

Substituent on acidic strength. Typical reactions of di carboxylic acids, hydroxyl acids and unsaturated acids.

Preparation and reactions of acid chlorides, anhydrides, esters and amides; Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Reformatsky reactions and Curtius rearrangement

Reactions involving H, OH and COOH groups- salt formation, anhydride formation, acid chloride formation, amide formation and esterification (mechanism). Degradation of carboxylic acids by Huns-Diecker reaction,

de-carboxylation by Schimdt reaction, Arndt- Eistert synthesis, halogenations by Hell- Volhard- Zelinsky reaction

SPECTROSCOPY 26 h

UNIT-IV

Molecular Spectroscopy: 18h

Interaction of electro-magnetic radiation with molecules and various types of spectra;

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear tri-atomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, Harmonic and an harmonic oscillator, Morse potential curve, vibrational degrees of freedom for polyatomic molecules, modes of vibration. Selection rules for vibrational transitions, Fundamental frequencies, overtones and hot bands.

Electronic spectroscopy: Energy levels of molecular orbitals (σ , π , n). Selection rules for electronic spectra. Types of electronic transitions in molecules, effect of conjugation. Concept of chromophore. Batho-chromic and hypso-chromic shifts. Beer-Lambert's law and its limitations.

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of nuclear magnetic resonance, equivalent and non-equivalent protons, position of signals. Chemical shift, NMR splitting of signals - spin-spin coupling, coupling constants. Applications of NMR with suitable examples - ethyl bromide, ethanol, acetaldehyde, 1,1,2-tribromo ethane, ethyl acetate, toluene and acetophenone.

UNIT-V 8h

Application of Spectroscopy to Simple Organic Molecule

Application of visible, ultraviolet and Infrared spectroscopy in organic molecules. Application of electronic spectroscopy and Woodward rules for calculating λ max of conjugated dienes and α , β – unsaturated compounds.

Infrared radiation and types of molecular vibrations, functional group and finger print region. IR spectra of alkanes, alkenes and simple alcohols (inter and intra-molecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on >C=O stretching absorptions).

List of Reference Books

- 1. A Text Book of Organic Chemistry by Bahl and Arunbahl
- 2. A Text Book of Organic chemistry by I L FinarVol I
- 3. Organic chemistry by Bruice
- 4. Organic chemistry by Clayden
- 5. Spectroscopy by William Kemp
- 6. Spectroscopy by Pavia

- 7. Organic Spectroscopy by J. R. Dyer
- 8. Elementary organic spectroscopy by Y.R. Sharma
- 9. Spectroscopy by P.S.Kalsi
- 10.Spectrometric Identification of Organic Compounds by Robert M Silverstein, Francis X Webster
- 11.Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- 12.Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. Practical Organic Chemistry, 5th Ed. Pearson (2012)
- 13.Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).

LABORATORY COURSE -III 30hrs (2 h / w)

Practical Course-III Organic preparations and IR Spectral Analysis

(At the end of Semester- III)

Organic preparations: 40M

i. Acetylation of one of the following compounds:

amines (aniline, o-, m-, p toluidines and o-, m-, p-anisidine) and phenols (βnaphthol, vanillin, salicylic acid) by any one method:

a. Using conventional method.

ii. Using green approach

iii. Benzolyation of one of the following amines

(aniline, o-, m-, p- toluidines and o-, m-, p-anisidine)

iv. Nitration of any one of the following:

a. Acetanilide/nitrobenzene by conventional method

b. Salicylic acid by green approach (using ceric ammonium nitrate).

IR Spectral Analysis 10M

IR Spectral Analysis of the following functional groups with examples

- a) Hydroxyl groups
- b) Carbonyl groups
- c) Amino groups
- d) Aromatic groups

SEMESTER - IV

Course IV (INORGANIC, ORGANIC AND PHYSICAL CHEMISTRY) 60hrs (4 h / w)

UNIT - I

Organometallic Compounds 8h

Definition and classification of organometallic compounds on the basis of bond type, Concept of hapticity of organic ligands. Metal carbonyls: 18electron rule, electron count of mono nuclear, poly nuclear and substituted metal carbonyls of 3d series. General methods of preparation of mono and binuclear carbonyls of 3d series. P-acceptor behavior of carbon monoxide. Synergic effects (VB approach) - (MO diagram of CO can be referred to for synergic effect to IR frequencies).

UNIT – II

Carbohydrates 8h

Occurrence, classification and their biological importance, Mono saccharides: Constitution and absolute configuration of glucose and fructose, epimers and anomers, mutarotation, determination of ring size of glucose and fructose, Haworth projections and conformational structures; Interconversions of aldoses and ketoses; Killiani- Fischer synthesis and Ruff degradation; Disaccharides– Elementary treatment of maltose, lactose and sucrose. Polysaccharides– Elementary treatment of starch.

UNIT- III

Amino acids and proteins 6h

Introduction: Definition of Amino acids, classification of Amino acids into alpha, beta, and gamma amino acids. Natural and essential amino acids - definition and examples, classification of alpha amino acids into acidic, basic and neutral amino acids with examples. Methods of synthesis: General methods of synthesis of alpha amino acids (specific examples - Glycine, Alanine, valine and leucine) by following methods: a) from halogenated carboxylic acid b) Gabriel Phthalimide synthesis c) strecker's synthesis.

Physical properties: Zwitter ion structure - salt like character - solubility, melting points, amphoteric character, definition of isoelectric point.

Chemical properties: General reactions due to amino and carboxyl groups - lactams from gamma and delta amino acids by heating- peptide bond (amide linkage). Structure and nomenclature of peptides and proteins.

Heterocyclic Compounds 7h

Introduction and definition: Simple five membered ring compounds with one hetero atom Ex. Furan. Thiophene and pyrrole - Aromatic character – Preparation from 1, 4, -dicarbonyl compounds, Paul-Knorr synthesis. Properties: Acidic character of pyrrole - electrophillic substitution at 2 or 5 position, Halogenation, Nitration and Sulphonation under mild conditions - Diels Alder reaction in furan.

Pyridine – Structure - Basicity - Aromaticity- Comparison with pyrrole- one method of preparation and properties - Reactivity towards Nucleophilic substitution reaction.

UNIT- IV

Nitrogen Containing Functional Groups

Preparation, properties and important reactions of nitro compounds, amines and diazonium salts.

1. Nitro hydrocarbons 3h

Nomenclature and classification-nitro hydrocarbons, structure -Tautomerism of nitroalkanes leading to aci and keto form, Preparation of Nitroalkanes, reactivity -halogenation, reaction with HONO (Nitrous acid), Nef reaction and Mannich reaction leading to Micheal addition and reduction.

2. Amines: 11h

Introduction, classification, chirality in amines (pyramidal inversion), importance and generalmethodsofpreparation.

Properties : Physical properties, Basicity of amines: Effect of substituent, solvent and steric effects. Distinction between Primary, secondary and tertiary amines using Hinsberg's method and nitrous acid. Discussion of the following reactions with emphasis on the mechanistic pathway: Gabriel Phthalimide synthesis, Hoffmann- Bromamide reaction, Carbylamine reaction, Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction and Cope elimination.

Diazonium Salts: Preparation and synthetic applications of diazonium salts including preparation of arene haloarenes, phenols, cyano and nitro compounds. Coupling reactions of diazonium salts (preparation of azo dyes).

UNIT- V

Photochemistry 5h

Difference between thermal and photochemical processes, Laws of photochemistry- Grothus-Draper's law and Stark-Einstein's law of photochemical equivalence, Quantum yield-Photochemical reaction mechanism- hydrogen- chlorine and hydrogen- bromine reaction. Qualitative description of fluorescence, phosphorescence, Jablonski diagram, Photo sensitized reactions- energy transfer processes (simple example).

Thermodynamics 12 h

The first law of thermodynamics-statement, definition of internal energy and enthalpy, Heat capacities and their relationship, Joule-Thomson effect- coefficient, Calculation of work for the expansion of perfect gas under isothermal and adiabatic conditions for reversible processes, State function. Temperature dependence of enthalpy of formation- Kirchoff s equation, Second law of thermodynamics Different Statements of the law, Carnot cycle and its efficiency, Carnot theorem, Concept of entropy, entropy as a state function, entropy changes in reversible and irreversible processes. Entropy changes in spontaneous and equilibrium processes. Third law of thermodynamics, Nernst heat theorem, Spontaneous and non- spontaneous processes, Helmholtz and Gibbs energies-Criteria for spontaneity.

List of Reference Books

- 1. Concise coordination chemistry by Gopalan and Ramalingam
- 2. Coordination Chemistry by Basalo and Johnson
- 3. Organic Chemistry by G.Mareloudan, Purdue Univ
- 4. Text book of physical chemistry by S Glasstone
- 5. Concise Inorganic Chemistry by J.D.Lee
- 6. Advanced Inorganic Chemistry Vol-I by Satyaprakash, Tuli, Basu and Madan
- 7. A Text Book of Organic Chemistry by Bahl and Arunbahl
- 8. A Text Book of Organic chemistry by I L FinarVol I
- 9. A Text Book of Organic chemistry by I L FinarVol II
- 10. Advanced physical chemistry by Gurudeep Raj

LABORATORY COURSE -IV 30hrs(2 h / w)

Practical Course-IVOrganic Qualitative analysis 50 M

(At the end of Semester- IV)

Organic Qualitative analysis 50 M

Analysis of an organic compound through systematic qualitative procedure for functional group identification including the determination of melting point and boiling point with suitable derivatives. Alcohols, Phenols, Aldehydes, Ketones, Carboxylic acids, Aromatic primary amines, amides and simple sugars