

S. V. K. P & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)
PENUGONDA, W. G. DIST., A. P.

(Accredited by NAAC with 'A' Grade and College with Potential for Excellence)

M.Sc. Organic Chemistry



SYLLUBUS AND MODEL QUESTION PAPERS

(W.e.f. 2019-20 admitted batch)

S. V. K. P. & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)
FIRST SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2019-20 Admitted batch)

(19OCHT11) Paper-I: GENERAL CHEMISTRY – I

UNIT-I

Basic Quantum Chemistry-I- Wave equation-interpretation of wave function-properties of wave function-normalization and orthogonalisation, Postulates of quantum mechanics; Operators- linear and non-linear- commutators of operators – Eigen functions and eigen values - Hermitian operator- Eigen values and Eigen functions of Hermitian operator; Unitary operator - setting up of operators to observables; position, linear momentum, energy and angular momentum – Eigen values of angular momentum operator.

UNIT-II

Basic Quantum Chemistry-II- Wave mechanics of simple systems with constant potential energy, particle in one-dimensional box- factors influencing color transition- dipole moment integral, Symmetry arguments in deriving the selection rules, the concept of tunneling- particle in three -dimensional box. Calculations using wave functions of the particle in a box- Rigid rotor, Wave mechanics of rigid rotator - Wave mechanics of systems with variable potential energy-simple harmonic oscillator- solution of wave equation- selection rules.

UNIT-III

Fundamentals of Molecular Spectroscopy-I: Microwave and IR- Spectroscopy- Rotational spectra of diatomic molecules- Rigid rotor-Selection rules- Calculations of bond length- Isotopic effect in rotational spectra - Second order stark effect and its applications. Infrared spectra of diatomic molecules- harmonic and anharmonic oscillators - Selection rules - Overtones- Combination bands - Calculation of force constant, anharmonicity constant and zero point energy. Fermi resonance, simultaneous vibrational-rotational spectra of diatomic molecules.

UNIT-IV

Fundamentals of Molecular Spectroscopy-II: Raman and Electronic Spectra - Classical and quantum mechanical explanations - Vibrational Raman spectra - Rotational fine structure of Raman spectra of diatomic molecules - Electronic spectra of diatomic molecules - Vibrational Coarse structure - intensities of spectral lines - Franck-Condon principle - applications, Rotational Fine structure - band head and band shading. Charge transfer spectra.

References/ Text books

1. Fundamentals of Molecular spectroscopy: by C. N. Banwell
2. Molecular spectroscopy: by B. K. Sharma
3. Molecular spectroscopy: by Aruldas
4. Introductory quantum mechanics: by A. K. Chandra
5. Quantum chemistry: by R. K. Prasad

Ch. K. Prasad



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(19OCHT12) Paper- II: INORGANIC CHEMISTRY-I

UNIT-I

Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in π -bonding. Application of MO theory to Tetrahedral $[\text{CoCl}_4]^{2-}$, Square planar $[\text{PtCl}_4]^{2-}$ and Octahedral complexes $[\text{CoF}_6]^{3-}$, $[\text{Co}(\text{NH}_3)_6]^{3+}$. Classification of ligands based on π -bonding using MO theory. Walsh diagram for H_2O molecule.

UNIT-II

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes. Electron counting in boranes – Wades rules (Polyhedral skeletal electron pair theory).

Heterocyclic inorganic ring systems: Boron–Nitrogen ($\text{H}_3\text{B}_3\text{N}_3\text{H}_3$), Phosphorus–Nitrogen ($\text{N}_3\text{P}_3\text{Cl}_6$) and Sulphur–Nitrogen (S_4N_4 , $(\text{SN})_8$) cyclic compounds.

Cage Compounds: Phosphorous oxides and Phosphorous sulphides.

Isopoly and heteropoly anions.

UNIT-III

Coordination compounds: Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series – Jahn – Teller effect, nephelauxetic effect – ligand field theory.

Term symbols – Russell – Sanders coupling – derivation of term symbols for various configurations. Spectroscopic ground states.

UNIT-IV

Electronic spectra of transition metal complexes: Types of electronic transitions – d-d transitions - Selection rules, break down of selection rules – Orgel and Tanabe-Sugano diagrams for d^1 – d^9 octahedral and tetrahedral transition metal complexes of 3d series – Calculation of Dq, B and β parameters. Charge transfer spectra.

Magnetic properties of transition and inner transition metal complexes – spin and orbital moments – quenching of orbital momentum by crystal fields in complexes.

Reference books& Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International Edition, 1983.
3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press pvt. Ltd., New Delhi.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999).
5. Inorganic Chemistry 5th Edition by Gary L. Miessler et al, Pearson Publications.

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(19OCHT13) Paper –III: ORGANIC CHEMISTRY -I

UNIT – I

Nature of bonding in organic molecules and Aromaticity

15 Hrs

(A) *Electronic Effects and Reactive intermediates*:- Inductive effect, Mesomeric effect (Resonance), Hyperconjugation, Steric effect, Tautomerism, acidity and basicity of organic molecules Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes

(B) *Criteria of Aromaticity*:- The Energy, Structural and Electronic Criteria for Aromaticity, Relationship among the Energetic, Structural, and Electronic Criteria of Aromaticity. Huckle's rule and MO Theory, aromaticity in benzenoid non-benzenoid compounds, Aromaticity in Charged and Fused-Ring Systems, Hetero-aromatic Systems, Annulenes: Cyclobutadiene, Benzene, 1,3,5,7-Cyclooctatetraene, [10] Annulenes- [12], [14], [16] and [18] annulenes, azulenes, fulvenes, fullerenes, ferrocene, anti-aromaticity and homo-aromaticity.

UNIT – II

Stereo Chemistry & Molecular representation of organic molecules

20Hrs

(A) *Molecular Symmetry and Chirality*:- Symmetry elements, Definition and classification of Stereoisomers, Enantiomer, Diastereomer, Invertomer, Homomer, Epimer, Anomer, Configuration and Conformation Configurational nomenclature: D,L and R, S nomenclature, Molecules with a single chiral center: Tetra and Tri coordinate chiral center, Molecules with two or more chiral centers; constitutionally unsymmetrical and symmetrical molecules.

(B) *Geometrical Isomerism and Conformations of Cyclic Systems*:- Cis-trans, E, Z- and Syn& anti nomenclature, Methods of determining configuration of Geometrical isomers using physical, spectral and chemical methods, Stability, Cis-trans inter conversion. Conformations of cyclobutane, cyclopentane, cyclohexane, mono and disubstituted cyclohexanes.

(C) *Stereoisomerism in molecules without chiral Center* -Axial chirality Allenes, Alkylidene cycloalkanes, spiranes, nomenclature. *Atropisomerism*: Biphenyl derivatives, nomenclature. *Planar chirality*: Ansa compounds, paracyclophanes, trans-cyclooctene and Helicity.

UNIT – III

Heterocyclic compounds

15 Hrs

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size, number and nature of hetero atoms. Chemistry of heterocyclic compounds, synthesis and reactivity of the following systems: Quinoline, Isoquinoline, Indole, Pyrazole, Imidazole, Oxazole, Isoxazole, Pyridazine, pyrimidine and Pyrazine.

UNIT - IV

Chemistry of some typical natural products (Alkaloids and Terpenoids)

10 Hrs

A study of the following compounds involving their isolation, structure elucidation, synthesis and biogenesis of

Alkaloids: Atropine, Nicotine, and Quinine.

Terpenoids: α - Terpineol, α -Pinene and Camphor.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6th Ed. (John Wiley & Sons)
2. Organic Chemistry, Paula Yurkanis Bruice, 4th Ed. (Printice Hall)
3. Organic chemistry-Clayden J. (Oxford)
4. Organic Chemistry, Wade, L.G. Jr. 5th Ed. (Pearson)
5. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2nd Ed. (Pearson)
6. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.)
7. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Ed., (Longman).
8. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2nd Ed. (New Age International).
9. Organic Chemistry, R. T. Morrison and R. N. Boyd (Prentice-Hall)
10. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
11. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International).
12. Organic Chemistry Structure and Reactivity, EgeSeyhan, 3rd Ed. (AITBS)
13. Heterocyclic Chemistry, J.A.Joule, K. Kils and G. F. Smith, Chapman and Hall
14. Heterocyclic Chemistry, T.L.Gilchrist, Longman Scientific Technical
15. Heterocyclic Chemistry, Raj.K. Bansal.
16. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.

REFERENCE BOOKS:

1. Chemistry of Natural Products, K.W. Bentley
2. Stereochemistry of carbon compounds by E.Eliel, John Wiley & Sons, Inc.
3. Stereochemistry to Organic Compounds, D. Nasipuri, 2nd Ed. (New Age International).
4. Chemistry of Natural products by R.S. KalsiKalyani Publishers. 1983.

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(19OCHT14) Paper – IV: PHYSICAL CHEMISTRY-I

UNIT-I

Thermodynamics-I: Concepts of partial molar properties – partial molar volume and its significance; Determination of partial molar volume: Graphical method, intercept method and apparent molar volume method. Partial molar free energy, chemical potential, Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance. Phase equilibrium - Derivation of phase rule from the concept of chemical potential. *Ideal solutions* - Thermodynamic properties of ideal solutions mixing quantities; Vapour pressure-Raoult's law; Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Non-ideal systems -Concept of fugacity, fugacity coefficient. Determination of fugacity; Non ideal solutions. Activities and activity coefficients; Standard state conventions for non ideal solutions; Determination of activity coefficients from vapour pressure measurements. Activity coefficients of non-volatile solutes using Gibbs-Duhem equation. Chemical equilibrium-effect of temperature on equilibrium constant - Van't-Hoff equation

UNIT-II

Micelles and Macro molecules: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization - phase separation and mass action models, Micellar solubilization, micro emulsion, reverse micelles.

Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of free radical polymerization. Molecular mass- Number and mass average molecular weight, molecular weight determination-End group analysis, Osmometry, viscometry, ultracentrifugation and light scattering methods.

UNIT-III

Chemical Kinetics: Theories of reaction rates- Collision theory- Limitations, Transition state theory, Thermodynamic formulation of transition state theory. Effect of ionic strength - Debye Huckel theory - Primary and secondary salt effects; Effect of dielectric constant, effect of substituent, Hammett equation-limitations, Taft equation; Prediction of rate constants- Consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation). Specific and general acid-base catalysis; Skrabal diagram; Fast reactions, different methods of studying fast reactions- flow methods. Continuous flow method and stopped flow method - relaxation methods: temperature jump and pressure jump methods.

UNIT-IV

Photochemistry: Electronic transitions in molecules, Franck-Condon principle. Electronically excited molecules - singlet and triplet states, spin-orbit interaction. Quantum yield and its determination; Actinometry - ferrioxalate and uranyl oxalate actinometers. Derivation of fluorescence and phosphorescence quantum yields. Quenching effect- Stern-Volmer equation. Photochemical equilibrium - delayed fluorescence: E-type and P-type delayed fluorescence. Photochemical primary processes, types of photochemical reactions - photodissociation, addition and isomerisation reactions with examples.

Books:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Physical Chemistry by G.W. Castellon, Narosha Publishing House
3. Physical Chemistry by W.J. Moore, Prentice Hall
4. Thermodynamics for Chemists, Samuel Glasstone
5. Chemical Kinetics by K.J. Laidler, McGraw Hill Pub.
6. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
7. Polymer Chemistry by Billmayer
8. Introduction to Polymer Science, V.R. Gowriker, N.V. Viswanadhan and J. Sreedhar., Wiley Easter.
9. Micells, Theoretical and applied aspects, V. Morol, Plenum publishers.

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LABORATORY WORK (6 hrs/week)

(19OCHP15) Practical-1: INORGANIC CHEMISTRY-I LAB

I. Inorganic Synthesis: Preparation of

- (i) Tetraamminecopper(II) sulphate
- (ii) Potassium tris-oxalato ferrate(III) trihydrate
- (iii) Tris-thiourea copper(II) sulphate

II. Semi micro qualitative analysis of six radical mixtures

(One interfering anion and one less familiar cation for each mixture)

Anions: CO_3^{2-} , S^{2-} , SO_3^{2-} , Cl^- , Br^- , I^- , NO_3^- , SO_4^{2-} , CH_3COO^- ,
 $\text{C}_2\text{O}_4^{2-}$, $\text{C}_4\text{H}_4\text{O}_6^{2-}$, PO_4^{3-} , CrO_4^{2-} , AsO_4^{3-} , F^- , BO_3^{3-}

Cations: Ammonium (NH_4^+)
1st group: Hg, Ag, Pb, Tl, W
2nd group: Hg, Pb, Bi, Cu, Cd, As, Sb, Sn, Mo
3rd group: Fe, Al, Cr, Ce, Th, Ti, Zr, V, U, Be
4th group: Zn, Mn, Co, Ni
5th group: Ca, Ba, Sr
6th group: Mg, Li

Reference books:

Vogel's textbook of semimicro qualitative analysis, 5th Edition by G. Svehla.

(19OCHP16) Practical-2: ORGANIC CHEMISTRY-I LAB

Preparation, recrystallization, and determination of melting point & yield of the following compounds:

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|-----------------------------------|-----------------------------|--------------------------------|
| (i) Aspirin, | (ii) Nerolin, | (iii) Chalcone, |
| (iv) <i>p</i> -Nitro acetanilide, | (v) 2,4,6- Tribromoaniline, | (vi) <i>m</i> -Dinitrobenzene, |
| (vii) Phthalimide, | (viii) Diels-Alder adduct. | |

Books Suggested

1. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J. Thomas, 4th & 6th Ed. (Pearson Education Asia).
2. Vogel's Text Book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, 5th Ed. (Longman Scientific & Technical)

(19OCHP17) Practical-3: PHYSICAL CHEMISTRY-I LAB

1. Determination of critical solution temperature of phenol-water system.
2. Effect of added electrolyte on the CST of phenol-water system.
3. Conductometric titration of Strong acid versus Strong base
4. Conductometric titration of Weak acid versus Strong base
5. Determination of cell constant
6. Dissociation constant of weak acid (CH_3COOH) by conductometric method
7. Adsorption of acetic acid on animal charcoal
8. Acid-catalyzed hydrolysis of methyl acetate

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SECOND SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS
(With effect from 2019-20 Admitted batch)

(19OCHT21) Paper- I: GENERAL CHEMISTRY-II

UNIT-I

Basic Quantum Chemistry-III- Hydrogen atom - solution of $R(r)$, $\Phi(\phi)$ and $O(\theta)$ equations. Probability density in orbitals- shapes of orbitals - Perturbation theory - Time independent perturbation theory (only first order perturbation is to be dealt with) - application to ground state energy of Helium atom - Variation principle - applications - calculation of zero-point energy of harmonic oscillator - many electron atom - Hartree-Fock self-consistent field method (qualitative treatment only).

UNIT-II

Molecular symmetry and Group Theory in chemistry: Basic concepts of symmetry and Group theory - Symmetry elements, symmetry operations and point groups- Schoenflies symbols - Classification of molecules into point groups - Axioms of Group theory - Group multiplication tables for C_{2v} and C_{3v} point groups - Matrix representations for symmetry operations - Similarity transformations and classes - Representations: reducible and irreducible representations, Mulliken symbols, Orthogonality theorem and its implications, Character table and its anatomy (need not to derive Character table).

UNIT-III

Treatment of analytical data: Accuracy and precision - Classification of errors - Determination of Indeterminate errors - Minimization of errors - Absolute and Relative errors, propagation of errors - Distribution of Indeterminate 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 - Significant figures and computation rules.

UNIT- IV

Introduction to computer programming- FORTRAN 77: Basic structures and functioning of computer with P.C. as an illustrative example - Main memory - Secondary storage memory - input/output devices - computer languages - operating systems - principles of algorithms and flow charts - constants and variables - Arithmetic expressions - Arithmetic statements - Replacement statement - IF statement- logical IF and BLOCK IF statements - GOTO statements - subscripted variable and DIMENSION statement. DO statement - Rules for DO statement - Functions and subroutines - Development of FORTRAN statements for simple formulae in chemistry such as Vander Waals equation - pH of a solution- First order rate equation- Beer's law.

Flowcharts and computer programs for

- a) Rate Constant of First order reaction or Beer's law by linear least square method.
- b) Hydrogen ion concentration of a strong acid solution Quadratic equation.
- c) Solution for Vander Waals equation or Hydrogen ion concentration of a monoprotic weak acid
- d) Standard deviation and Variance of univariant data

References/ Text books:

1. Introductory Quantum chemistry: by A.K.Chandra
2. Group theory for Chemistry: by A.K.Bhattacharya
3. Introductory Group theory for chemists : by George Davidson
4. Vogel's text book of quantitative analysis: by Vogel
5. Fundamentals of Analytical chemistry: by Skog and West
6. Principles of computer programming(FORTRAN 77 IBM PC): by V.Rajaraman
7. Basics of computers for chemists: by P.C.Jurs

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(19OCHT22) Paper- II: INORGANIC CHEMISTRY-II

UNIT-I

Metal cluster compounds - definition - evidences for existence of M-M bonds - conditions favorable for formation of M-M bonds - preparation, structure and bonding of the following metal cluster compounds.

$\text{Re}_2\text{Cl}_8^{2-}$, $\text{Mo}_2\text{Cl}_8^{4-}$, $\text{Re}_2(\text{RCOO})_4\text{X}_2$, $\text{Mo}_2(\text{RCOO})_4(\text{H}_2\text{O})_2$, $\text{Cr}_2(\text{RCOO})_4(\text{H}_2\text{O})_2$, $\text{Cu}_2(\text{RCOO})_4(\text{H}_2\text{O})_2$, $\text{Cr}_2\text{Cl}_9^{3-}$, $\text{Mo}_2\text{Cl}_9^{3-}$, $\text{W}_2\text{Cl}_9^{3-}$, Re_3Cl_9 , $\text{Re}_3\text{Cl}_{12}^{3-}$, $\text{Mo}_6\text{Cl}_8^{4+}$, $\text{Nb}_6\text{X}_{12}^{2+}$ and $\text{Ta}_6\text{X}_{12}^{2+}$.

Polyatomic clusters - Zintl ions, Chevrel phases.

UNIT-II

Organometallic compounds - 16 and 18 electron rules. Isoelectronic relationship - Synthesis, structure, bonding and reactions of carbon monoxide, dinitrogen and nitric oxide complexes. Isolobal relationship - H, Cl, CH₃, Mn(CO)₅, S, CH₃, Fe(CO)₄, P, CH, Co(CO)₃. Synthesis, structure, bonding and reactions of metallocenes with special reference to ferrocene. Catalysis by Organometallic compounds - Homogeneous Catalysis - Alkene hydrogenation - Wilkinson's catalyst, Hydroformylation.

UNIT-III

Metal Ligand equilibria in solution: Stepwise and overall formation constants and their interaction - trends in stepwise constants - factors affecting the stability of metal complexes - Pearson's theory of hard and soft acids and bases (HSAB), chelate effect and its thermodynamic origin, determination of stability constants of complexes - spectrophotometric method and pH-metric method. Reactivity of metal complexes - inert and labile complexes. Explanation of lability on the basis of VBT & CFT.

Bio-Inorganic Chemistry: Metalloporphyrins with special reference to Haemoglobin & Myoglobin. Biological role of alkali and alkaline earth metal ions with special reference to Ca^{2+} . Biological and abiological Nitrogen Fixation.

UNIT-IV

Inorganic Reaction Mechanisms: Substitution reactions of metal complexes - D, Id, Ia and A mechanisms - Ligand replacement reactions of octahedral complexes - Acid hydrolysis - factors affecting acid hydrolysis - Anation and Base hydrolysis of Cobalt(III) complexes. Ligand displacement reactions of square planar complexes of platinum (II). Factors affecting square planar substitution - trans effect (theories).

Electron transfer reactions of complexes - concept of complementary and non-complementary reactions with examples. Inner and outer sphere mechanisms.

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and R.G. Wilkinson, IV Edition, John, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III edition, Harper International Edition, 1983.
3. Organometallic Chemistry-A unified approach by A. Singh and R.C. Mehrotra, Wiley Eastern Ltd.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999)
5. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press Pvt. Ltd., New Delhi.
6. Mechanisms of Inorganic reactions in solution by D.Benson, McGraw Hill, London, 1968.
7. Inorganic chemistry by K.F. Purcell and J.C. Kotz, W.B. Saunders company, New York, 1977.
8. Elements of Bioinorganic Chemistry by G.N. Mukherjee and Arabinda Das, U.N. Dhur & sons Pvt. Ltd, Calcutta.

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(19OCHT23) Paper-III: ORGANIC CHEMISTRY-II

UNIT-I

Reaction Mechanism

15Hrs

(A) Aliphatic Nucleophilic Substitution and Nucleophilic Aromatic substitution: Stereochemistry of S_N1 and S_N2 mechanisms, Neighboring Group Participation (Anchimeric assistance), NGP by O, S, N. Aromatic Nucleophilic substitution: $SN2(Ar)$ (Addition - Elimination), $SN1(Ar)$ and benzyne mechanisms (Elimination - Addition); evidence for the structure of benzyne. Von Richter Sommelet-Hauser and Smiles rearrangements.

(B) Elimination Reactions: Type of elimination reactions, mechanisms, Stereochemistry and Orientation, Hofmann and Saytzeff rules, Syn elimination versus anti-elimination, competition between elimination and substitution, dehydration, dehydrogenation, dehalogenation, decarboxylative eliminations and pyrolytic eliminations

UNIT-II

Addition Reactions

15 Hrs

(A) Addition to Carbon - Carbon Multiple Bonds: Mechanistic and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, region and chemo selectivity, orientation and reactivity, Hydrogenation of double and triple bonds, hydrogenation of aromatic rings, Hydroboration.

(B) Addition to Carbon-Hetero Multiple Bonds: Steric course of addition reactions to $C=O$ and $C=N$, Aldol, Cannizzaro, Perkin, Knoevenagel, Claisen-Schmidt, Claisen, Dieckman, Benzoin and Stobbe condensations, Reformatsky reaction, Tollen's reaction, Prins reaction: Wittig, Grignard, Mannich, and Michael reaction, Hydrolysis of Carbon-Nitrogen bond, Isocyanates and isothioyanates.

UNIT-III

Molecular Rearrangements

15 Hrs

Types of molecular rearrangements, migratory aptitude:

Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerwein, Tiffeneau - Demjanov, Dienone

Phenol, Arndt-Eistert synthesis:

Rearrangements to electron deficient nitrogen: Beckmann, Hofmann, Curtius, Schmidt and Lossen rearrangements;

Rearrangements to electron deficient oxygen: Baeyer-villiger, Hydro peroxide rearrangement and Dakin rearrangements;

Neber rearrangement, Benzil-Benzilic acid and Favorskii rearrangements

UNIT-IV

Spectroscopy and Protecting Groups

15 Hrs

- A. Basic principles and importance of UV, IR, NMR and Mass.
- B. Protection of carbonyl, Hydroxyl, carboxylic and Amine groups

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Books Suggested:

1. Advanced Organic Chemistry: Reactions, Mechanism and structure, Jerry March, 6th Ed. (John Wiley & Sons)
2. Modern Organic Reactions, H. O. House (Benjamin)
3. Structure and Mechanism in Organic Chemistry C. K. Ingold (Cornell University Press)
4. Organic Chemistry, Paula Yurkanis Bruice, 4th Ed. (Printice Hall)
5. Organic chemistry-Clayden J. (Oxford)
6. Organic Chemistry, Wade, L. G. Jr. 5th Ed. (Pearson)
7. Organic Chemistry, Salmons, P.W. & Others, 8th Ed. (John Wiley & Sons)
8. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2nd Ed. (Pearson)
9. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.)
10. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Ed., (Longman)
11. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2nd Ed. (New Age International)
12. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley). 13. Stereochemistry to Organic Compounds, Nasipuri, 2nd Ed. (New Age International)
14. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International). Organic Chemistry Structure and Reactivity, Ege Seyhan, 3rd Ed. (AITBS)
15. Spectroscopic Methods in Organic Chemistry- Forth Edition, D.H. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990.
16. Organic Spectroscopy- Second Edition, W.Kemp, ELBS Macmillan, 1987.
17. Applications of absorption spectroscopy of Organic Compounds J.R.Dyer, Prentice Hall of India, New Delhi, 1984.
18. Spectrometric identification of Organic Compounds-Fourth Edition, R.M. Silverstein: G.C. Vassiliou and T.C. Merrill, John Wiley, Singapore, 1981.
19. Introduction to spectroscopy-D.L. Pavia, G.M. Lampman, G.S. Kriz, 3rd Ed. (Harcourt college publishers).

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S. V. K. P. & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)
SECOND SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2019-20 Admitted batch)

(19OCHT24) Paper – IV: PHYSICAL CHEMISTRY-II

UNIT-I

Physical methods of molecular structural elucidation: NMR: Principle and theory, Nature of spinning particle and its interaction with magnetic field, Chemical shift and its origin, Spin-Spin interaction, Application of NMR to structural elucidation: Structure of ethanol, dimethylformamide, styrene and acetophenone.

Electron Spin Resonance: Principle and experimental technique- g-factor, presentation of ESR spectra, line shapes and line widths- hyperfine interactions - applications of ESR studies to the structure of free radicals and metal complexes, zero point splitting, Kramers degeneracy.

UNIT-II:

Thermodynamics-II: Brief review on entropy; entropy changes accompanying specific process – expansion, phase transition, heating, measurement of entropy, Nernst heat theorem; Third law of thermodynamics- Determination of the absolute entropy of solids, liquids and gases - Apparent exceptions to Third law of thermodynamics.

Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles, Thermodynamic probability, Most probable distribution Law – Partition Function, (Definition and significance): Molar and molecular partitions - translational, rotational, vibrational and electronic partition functions- Relation between thermodynamic functions (E , H , S , G and C_v) and the partition functions

UNIT-III:

Electrochemistry I: Electrochemical cell- Galvanic and electrolytic cell, Concentration cell with and without transference, Effect of complexation on redox potential – ferricyanide / ferrocyanide couple, Iron (III) phenanthroline / Iron (II) phenanthroline couple, Determination of standard potential, solubility product and activity coefficients from EMF data.

Bjerrum theory of ion association (elementary treatment) - Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient, Debye-Huckel theory of electrolytic solutions, Debye-Huckel limiting law (derivation not required), Calculation of mean ionic activity coefficient, Limitations of Debye-Huckel theory, Effect of dilution on equivalent conductance of electrolytes - Anomalous behavior of strong electrolytes, Debye Huckel-Onsagar equation - verification and limitations, Fuel Cells.

UNIT-IV:

Electrochemistry II: The electrode-electrolyte interface, The electric double layer, The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model.

Electrodes: Charge transfer reactions at the electrode-electrolyte interface, Exchange current density and over-potential, Derivation of Butler-Volmer equation, High field approximation, Tafel equation, Low field equilibrium, Nernst equation, Voltammetry - Concentration polarization, experimental techniques.

Books:

1. Text book of Physical Chemistry by Samuel Glasstone, McMillanPub
2. Physical Chemistry by W.J.Moore, PrenticeHall
3. Physical Chemistry by G.W. Castellan, Narosha PublishingHouse
4. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
5. Modern Electrochemistry, 2A & 2B, JOM Bockris & A.K.N.Reddy, Plenum publishers
6. Introduction to Electrochemistry, S.Glasstone.
7. Fundamentals of Molecular Spectroscopy, Banwell
8. Spectroscopy by Straw & Walker.
9. Statistical thermodynamics, M.C.Gupta
10. Statistical Thermodynamics, M.Dole

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SECOND SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2019-20 Admitted batch)

LABORATORY WORK (6 hrs/ week)

(19OCHP25) Practical-1: INORGANIC CHEMISTRY PRACTICAL –II

Quantitative analysis:

Volumetric:

1. Determination of Ferric iron by photochemical reduction
2. Determination of Nickel by EDTA
3. Determination of Calcium and Magnesium in a mixture by EDTA
4. Determination of Ferrocyanide by Cericsulphate
5. Determination of Copper(II) in presence of iron(III)

Gravimetric:

6. Determination of Zinc as Zincpyrophosphate
7. Determination of Nickel from a mixture of Copper and Nickel.

Reference books:

Vogel's textbook of quantitative chemical analysis, 5th edition by G.H. Jeffery et al.

(19OCHP26) Practical-2: ORGANIC CHEMISTRY PRACTICALS –II

Systematic qualitative analysis of an organic mixture containing two compounds

Identification of method of separation and the functional group(s) present in each of them and preparation of one solid derivative for the confirmation of each of the functional group(s).

(19OCHP27) Practical-3: PHYSICAL CHEMISTRY PRACTICALS –II

1. Distribution of iodine between CHCl_3 and water
2. Distribution of I_2 between CHCl_3 and aq. KI solution- calculation of equilibrium constant and concentration of given KI solution.
3. Determination of Coordination number of cuprammoniumcation.
4. Titration of mixture Strong acid and weak acid versus Strong base by conductometry.
5. Titration of Strong acid Vs Strong Base pH -metry.
6. Titration of mixture of $(\text{NaHCO}_3 + \text{Na}_2\text{CO}_3)$ Vs HCl pH-metry.
7. Titration of Fe^{+2} Vs $\text{K}_2\text{Cr}_2\text{O}_7$ potentiometry
8. Verification of Beer-Lambert's law by Iron-thiocyanate system colorimetry.

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THIRD SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2019-20 Admitted batch)

(19OCHT31) Paper-I: ORGANIC REACTION MECHANISMS-I & PERICYCLIC REACTIONS

15 Hrs

UNIT – I

A) Aliphatic Nucleophilic Substitution

Neighboring group participation by Bromine, Phenyl group. Non-Classical carbocations, NGP by Pi bond, Sigma bond and Cyclopropyl group, SN at Allylic carbon (allylic rearrangements), SN at Aliphatic trigonal carbon, SN at Vinylic carbon. Ambident nucleophiles, Hydrolysis of esters ($B_{AC}^{-2}Ac^{+2}, A_{AC}^{-1}, A_{AL}^{-1}, B_{AL}^{-1}$). Mechanism of esterification of carboxylic acid with an alcohol using DCC, Mayers Synthesis of aldehydes, ketones and carboxylic acids Mitsunobu reaction, Von-Braun reaction

B) Aliphatic Electrophilic Substitution

Mechanisms of SE^2 , SE^{-1} , SE^1 . Hydrogen as electrophile: Hydrogen exchange; Migration of double bonds. Halogen electrophiles. Mechanism of Halogenation of aldehydes and ketones; HVZ reaction; Halogenation of Sulfoxides & Sulphones, Nitrogen Electrophiles: Aliphatic diazo coupling, Diazo transfer reaction. Carbon as Leaving groups: Decarboxylation of Aliphatic Acids; Dakin – West reaction; Haller–Bauer reaction.

15 Hrs

UNIT – II

Principles of asymmetric synthesis:

Introduction and terminology: Topicity in molecules Homotopic, stereo heterotopic (enantiotopic and diastereotopic) groups and faces, symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereo selective reactions: Substrate stereo selectivity, product stereo selectivity, enantioselectivity and diastereoselectivity. Conditions for stereo selectivity: Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio. Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR; Chiral derivatizing agents, chiral solvent, chiral shift reagents and Chiral HPLC.

UNIT – III

Pericyclic Reactions-I

Molecular orbital symmetry, frontier orbitals of ethylene, 1, 3 Butadiene, 1, 3, 5- Hexatriene, allyl system, classification of pericyclic reactions FMO approach, Woodward- Hoffman correlation diagram method and perturbation of molecular (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions. Electrocyclic Reactions: Conrotatory and disrotatory motions ($4n$) and ($4n+2$), allyl systems Cycloadditions: Antarafacial and suprafacial additions, notation, of cycloadditions, ($4n$) and ($4n+2$) systems with a greater emphasis on ($2+2$) and ($4+4$) - cycloadditions, ($2+2$) - additions of ketenes and chelotropic reactions.

15 Hrs

UNIT-IV

Pericyclic Reactions-II

FMO approach and perturbation of molecular (PMO) approach for the explanation of sigma tropic rearrangements under thermal and photochemical conditions. Suprafacial and antarafacial shifts of H Sigmatropic shift involving carbon moieties, retention and inversion of configurations, ($3, 3$) and ($5, 5$) sigmatropic rearrangements detailed treatment of Claisen and Cope rearrangements, aza-Cope rearrangement and Barton reaction.

15 Hrs

Text Books and Reference Books:

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
2. Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.
3. Pericyclic reactions by S.N. Mukharji, Memilan.
4. Mechanisms and Theory in Organic Chemistry by T. H. Lowery and K.S. Rich gardson.
5. The modern structural theory in Organic Chemistry by L. N. Ferguson, Pretice Hall
6. Physical Organic Chemistry by jack Hine, Mc. Graw Hill
7. Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourth edition, Kluwer academic publishers, New York
8. Organic Synthesis, Christine Willis and Martin Willis, Oxford Chemistry primers.
9. Principles of Organic Synthesis, ROC Norman and JM Coxon, third edition, CBS, Publisher, Delhi.
10. Organic Synthesis, M. B. Smith, Mc Graw Hill, International Edition.
11. Organic Chemistry, Clayden, Greeves and Stuart Warren.
12. Modern Organic Synthesis-an introduction by George S. Zweifel and Michael H. Nantz, W. H. Freeman & company, New York.
13. Pericyclic Reactions — a problem solving approach, Lehr and Merchand
14. Conservation of Orbital Symmetry by Woodward and Hoffmann.

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S. V. K. P. & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)

M.Sc. ORGANIC CHEMISTRY - III SEMESTER SYLLABUS

(With effective from 2019-20 admitted batch)

Paper - II: ORGANIC SPECTROSCOPY-I

UNIT-I

15 Hrs

UV-Visible spectroscopy:

A) Beer-Lambert's law-Deviations from Beers law-Instrumentation-Energy transitions - Simple chromophores Auxochrome, Absorption shifts (Bathochromic, Hypsochromic, Hyper chromic and Hypo chromicshifts) UV absorption of Alkenes-Polyenes unsaturated cyclic systems.

B) UV absorption of carbonyl compounds: α , β -unsaturated carbonyl systems-UV absorption of aromatic systems-geometrical isomerism-acid and base effects-typical examples-calculation of λ max values using Woodward Fieserrules, applications.

UNIT-II

15 Hrs

Infrared spectroscopy:

A) Mechanics of measurement-Fundamental modes of vibrations-stretching and bending vibrations-Factors effectingVibrational frequency-hydrogen bonding.

B) Finger print region and its importance, typical group frequencies for $-\text{CH}$, $-\text{OH}$, N-H , CC , CO and aromatic systems-Application in structural determination-Examples-simple problems.

UNIT-III

15 Hrs

Nuclear Magnetic Resonance Spectroscopy (^1H NMR):

A) Introduction: Basic principle of- NMR Nuclear spin- nuclear resonance-saturation-Relaxation-Instrumentation.

B) Shielding and deshielding of magnetic nuclei-chemical shift and its measurements, factors influencing chemical shift -spin-spin interactions-, factors influencing -coupling constant J and factors effecting J value.

C) ^{13}C NMR Spectroscopy: Similarities and Differences between PMR and CMR, general considerations, chemical shift(aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbon), typical examples of CMRspectroscopy-simple systems.

UNIT IV

Mass spectrometry

(A) Introduction: Ion production- EI, CI, ES, MALDI and FAB- determination of Molecular weight and formulae- Behavior of organic compounds in mass spectrometer. Isotopic Abundance

(B) Mass spectral fragmentation of organic compounds, Common functional groups, molecular ion peak, Meta stable peak, McLafferty rearrangement, Nitrogen rule. Examples of mass spectral fragmentation of organic compounds with respect of their structure determination.

Suggested Books:

1. Spectroscopic Methods in Organic Chemistry- Forth Edition, D.H. Williams and I. Fleming Tata McGraw Hill, New Delhi, 1990.
2. Organic Spectroscopy- Second Edition, W. Kemp, ELBS Macmillan, 1987.
3. Applications of absorption spectroscopy of Organic Compounds J.R. Dyer, Prentice Hall of India, New Delhi, 1984.
4. Spectrometric identification of Organic Compounds- Fourth Edition, R.M. Silverstein: G.C. Vassiliou and T.C. Merrill, John Wiley, Singapore, 1981.
5. Introduction to spectroscopy- D.L. Pavia, G.M. Lampman, G.S. Kriz, 3rd Ed (Harcourt college publishers).
6. Absorption spectroscopy of organic molecules- V.M. Parkhi.
7. Nuclear Magnetic Resonance- Basic principles- Atta-Ur-Rehman, Springer-Verlag, 1986.

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M. Sc. ORGANIC CHEMISTRY - III SEMESTER SYLLABUS

(With effective from 2019-20 admitted batch)

Paper – III: MODERN ORGANIC SYNTHESIS-I

UNIT-I

15 Hrs

Formation of C-C single bonds

Alkylations via enolate, Thermodynamic and kinetic enolate, Asymmetric Aldol reaction:
a) Chiral enolate and achiral aldehyde b) Achiral enolate and chiral aldehyde – explanation by Zimmerman Traxler model; stork enamine reaction and its synthetic applications.
Organo Sulphur chemistry: Umpolung and its synthetic application (Corey Seebach Reaction), Sulphurylides: dimethyl sulphoniummethylide, dimethyloxosulphoniummethylide preparations and their synthetic applications; Organo Palladium Chemistry: Heck Reaction, Stille coupling, Suzuki coupling, Sonogashira coupling, Negeshicoupling, Wacker Oxidation; Organo copper chemistry: Gilman's reagent and synthetic applications; Synthetic applications of carbenes and carbenoids; BaylisHilman reaction.

UNIT-II

15 Hrs

Formation of Carbon-Carbon double bonds

Stereochemistry of E_1 and E_2 reactions (Different examples of acyclic and cyclic molecules. Saytzeff rule, Hofmann rules and Bredt's rule); Pyrolytic Syn eliminations (focus should be given on stereochemistry of syn eliminations of amine oxides, xanthates and esters of acyclic and cyclic molecules); Sulphoxide-Sulphenate rearrangement (Mislow-Evans rearrangement); Wittig reaction, Wittig-Horner reaction and stereo chemistry of Wittig reaction; Shapiro reaction, Claisen rearrangement of allyl vinyl ethers, Julia Lythgoe olefination, Mc Murray coupling, Peterson Olefination, Tebbs reagent and its application, Metathesis: Grubbs 1st and 2nd generation catalysts, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, olefination by Nysted reagent.

UNIT-III

15 Hrs

Reactions of Unactivated C-H bonds and organoboranes

The Hoffmann Loeffler- Freytag reaction, Barton reaction and Photolysis of organic hypothalites; Organoboranes: Preparation of Organoboranes viz hydroboration with BH_3 -THF, dicyclohexyl borane, disiamyl borane, tetrakis (t-butyl) borane, 9- BBN, mono isopinocampheyl borane (IPC_2BH_2) and diisopinocampheyl borane (IPC_2BH). Functional group

transformations of Organo boranes-Oxidation, protonolysis and isomerization. Formation of carbon-carbon-bonds viz organo borane carbonylation and cyanidation.

UNIT-IV

Simple applications of Microwave and Ultrasound assisted reactions 15 Hrs

1. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects. Microwave assisted reactions in organic solvents-Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels- Alder reaction, Decarboxylation.
2. Ultrasound assisted reactions: Introduction, Substitution reactions, Addition, Oxidation, Reduction reactions.
3. Click chemistry: criterion for click reaction, Sharpless azides cycloadditions
4. Synthetic applications of PTC and Crown ethers

Textbooks and Books for Reference Books:

- 1) Some Modern Methods of Organic Synthesis W. Carruthers, Third & Fourth Edition, Cambridge University Press, Cambridge, 1988.
- 2) Modern Organic Synthesis-an introduction by George S. Zweifel and Michael H. Nantz, W. H. Freeman & company, New York.
- 3) Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourth edition, Kluwer academic publishers, New York
- 4) Organic Synthesis, Christine Willis and Martin Willis, Oxford Chemistry primers.
- 5) Principles of Organic Synthesis, R.C. Norman and J.M. Coxon, third edition, CBS, Publisher, Delhi.
- 6) Organic Synthesis, M. B. Smith, McGraw Hill, International Edition.
- 7) Organic Chemistry, Clayden, Greeves and Stuart Warren.
- 8) Guide Book to Organic Synthesis (3rd edition), R. Mackie, D. M. Smith and Aitken. 9) Organo Boranes and Silanes, Thomson, Oxford Chemistry primers.
- 10) Strategic applications of named reactions in organic synthesis, Laszlo Kurti and Barbara Czako.
- 11) Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benjamin Inc. Menlo Park, California, 1972.
- 12) Organic Synthesis viz Boranes, Herbert C. Brown, Gray, W. Kramer Alan B. Levy and M. Mark Midland John Wiley & Sons, New York, 1975.
- 13) Organic Synthesis: Special Techniques, V. K. Ahluwalia and Renu Agarwal.
- 14) Organic Synthesis, Jagadamba Singh and Dr. A. Yadav, Pragati Edition.

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S. V. K. P. & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)
THIRD SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS
(With effect from 2019-20 Admitted batch)

(19OCTHE34) Paper - IV: CHEMISTRY OF NATURAL PRODUCTS -I

15 Hrs

UNIT-I:

Alkaloids

Introduction, isolation, general methods of structure elucidation and physiological action, classification based on nitrogen heterocyclic ring, structure, stereochemistry, synthesis of morphine, strychnine, colchicine and reserpine.

15 Hrs

UNIT-II:

Terpenoids:

Occurrence, isolation, general methods of structure determination, isoprene rule, structure determination, stereochemistry, synthesis of Farnesol, Zingiberene, Forskolin, Taxol, Azadirachtin and β -amyrin.

15 Hrs

UNIT-III:

Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and its stereochemistry, Isolation, structure determination and synthesis of cholesterol (total synthesis not expected), androsterone, testosterone and progesterone.

15 Hrs

UNIT-IV:

Flavonoids and Isoflavonoids: Occurrence, nomenclature and general methods of structure determination, Isolation, structure elucidation and synthesis of Kaempferol, Quercetin, Cyanidin, Genestein, Butein and Daidzein. Synthesis of flavonoids and Isoflavonoids.

Books Suggested:

1. Natural Products: Chemistry and Biological Significance, J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe and J. B. Harbome, Longman, Essex.
2. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
3. Chemistry of Organic Natural Products, O. P. Agrawal, Vols. 1 & 2, Goel Pubs.
4. Natural Products Chemistry K. B. G. Torressell, John Wiley, 1983
5. New Trends in Natural Products Chemistry, Atta-ur-Rahman and M. I. Choudhary, Harwood Academic Publisher.
6. Chemistry of Natural products P. S. Kalsi, Kalyani Publishers
7. Biosynthesis of steroids, terpenes and acetogenins, J. H. Richards & J. R. Hendrieson.
8. The biosynthesis of secondary metabolites, R. D. Herbert, Chapman & Hall
9. The Biosynthesis of Secondary Metabolite, R. D. Herbert, Second edn, Chapman and Hall 1984.
10. Chemical aspects of Biosynthesis, John Mann, Oxford University Press, Oxford, 1996.

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S. V. K. P. & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)

M. Sc. (FINAL) ORGANIC CHEMISTRY
III SEMESTER PRACTICAL SYLLABUS

(With effective from 2019-20 admitted batch)

Laboratory Course-1

Multistep Synthesis of Organic Compounds:

100 M

The experiments should illustrate the use of organic reagents:

1. Beckmann rearrangement: Benzanilide from Benzophenone

Benzophenone $\rightarrow$ Benzophenone oxime $\rightarrow$ Benzanilide

2. Benzilic acid rearrangement: Benzilic acid from benzoin

Benzoin $\rightarrow$ Benzil $\rightarrow$ Benzilic acid

3. P-Bromo Aniline from Aniline :

Aniline $\rightarrow$ Acetanilide $\rightarrow$ P-Bromo Acetanilide $\rightarrow$ P-Bromo Aniline

4. Symmetrical Tribromo Benzene from aniline:

Aniline $\rightarrow$ Tribromoaniline $\rightarrow$ Tribromobenzene

5. 2,4,6-trimethylquinoline from p-toluidine

p-toluidine $\rightarrow$ 4-(p-tolylamino) pent-3-ene-2-one $\rightarrow$ 2,4,6-trimethylquinoline

6. 2-phenylindole from phenylhydrazine

phenylhydrazine $\rightarrow$ acetophenonephenylhydrazone $\rightarrow$ 2-phenylindole

Laboratory Course-2

Estimations and Chromatography

100 M

1. Estimation of (a) Glucose (b) Phenol (c) Aniline (d) Acetone (e) Aspirin (f) Ibuprofen

2. Separation by column chromatography: Separation of a mixture of *ortho* and *para* nitroanilines using silicagel as adsorbent and benzene as the eluent. The column chromatography should be monitored by TLC.

Books Suggested

1. Modern Organic Synthesis in the Laboratory *A Collection of Standard Experimental Procedures*, Jie Jack Li, Chris Limberakis, Derek A. Pflum

2. Practical organic chemistry by Mann & Saunders

3. Text book of practical organic chemistry by Vogel

4. Text book of practical organic chemistry including qualitative organic analysis by A.I. Vogel (Longman)

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FOURTH SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2019-20 Admitted batch)

(19OCHT41) Paper- I: ORGANIC REACTION MECHANISMS-II & ORGANIC PHOTO CHEMISTRY

15 Hrs

UNIT – I:

A) Free Radical Reactions:

Neighboring group assistance in free radical reactions; Reactivity for aliphatic substrates; Reactivity in aromatic substrates; Reactivity at bridge head; Allylic halogenations using NBS (Wohl – Ziegler bromination); Hydroxylation at aromatic carbon by Fentons reagent; Oxidation of aldehydes to carboxylic acids; Formation of cyclic ethers using Lead tetra acetate; Formation of hydroperoxides (autooxidation); Coupling of alkynes (Eglinton reaction and Glaser reaction); Arylation of Aromatic compounds by diazonium salts (Gomberg – Bachman reaction); Mechanisms of Sandmeyer reaction, Hunsdiecker reaction, Reed reaction.

B) Rearrangements: Wagner – Meerwein Rearrangement, Demjanov Rearrangement, Wittig Rearrangement and Stevens Rearrangement

15 Hrs

UNIT– II:

Methodologies in asymmetric synthesis

Strategies in Asymmetric Synthesis: 1. Chiral substrate controlled, 2. Chiral reagent controlled and 3. Chiral catalyst controlled.

1. Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2-asymmetric induction, Cram's rule and Felkin-Anh model.

2. Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC_2BH and IPCBH_2 .

3. Chiral catalyst controlled asymmetric synthesis: Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts. Enzymemediated enantioselective synthesis.

15 Hrs

UNIT – III

Photo Chemistry-I

Photochemical energy, Frank Condon Principle, Types of Electronic Excitation and Molecular orbital view of excitation, Jablonski Diagram, singlet and triplet states, photosensitization, quenching, quantum efficiency and quantum yield. Photo Chemistry of Carbonyl Compounds: Norrish Type I reaction (alpha cleavage reaction), Norrish Type – II reaction, Paterno-Buchi reaction, Photo reduction & photo enolisation; photochemical Oxidations [Backstrom mechanism], Photooxidation of alkenes with singlet oxygen.

15 Hrs

UNIT – IV

Photochemistry-II

Di – Pi methane Rearrangement, Oxa di – Pi methane rearrangement; Aza di – Pi methane rearrangement; Photochemistry of Benzene and substituted benzene, 1, 2, 1,3 & 1, 4-additions; Photo Fries rearrangement of Phenolic acetates and Anilides; Photochemistry of unsaturated systems, Cis- Trans Isomerisation of alkenes (Direct and sensitized) (Photoisomerisation of Stilbene), Photochemistry of Butadiene; Dimerisations of alkenes, Intramolecular dimerisation. Photochemical rearrangement of Cyclohexadienones; Photochemistry of alpha, beta Unsaturated ketones (dimerisations and addition across the double bond); Photochemical rearrangement reactions of Cyclohexenone, Photorearrangements of Beta, gamma unsaturated systems (Mechanism of 1, 2 & 1, 3 – acyl shifts); Photochemistry of Nitrite esters (Barton reaction).

Text Books and Reference Books:

1. Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc. Graw Hill and Kogakush.
2. Molecular Reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.
3. Mechanisms and Theory in Organic Chemistry by I. H. Lowery and K.S. Richardson.
4. The modern structural theory in Organic Chemistry by I. N. Ferguson, Prentice Hall.
5. Physical Organic Chemistry by Jack Hine, Mc. Graw Hill.
6. Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourth edition, Kluwer Academic Publishers, New York.
7. Organic Synthesis, Christine Willis and Martin Willis, Oxford Chemistry primers.
8. Principles of Organic Synthesis, R.C. Norman and J.M. Coxon, third edition, CBS, Publisher, Delhi.
9. Organic Synthesis, M. B. Smith, Mc Graw Hill, International Edition.
10. Organic Chemistry, Clayden, Greeves and Stuart Warren.
11. Modern Organic Synthesis-an introduction by George S. Zweifel and Michael H. Nantz, W. H. Freeman & company, New York.
12. Organic Photochemistry by D Coyle.
13. Molecular Photochemistry by Gilbert & Baggo.
14. Organic Photochemistry by Turro.
15. Photochemistry by C. W. J. Wells.

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S. V. K. P. & Dr. K. S. RAJU ARTS & SCIENCE COLLEGE (A)

M. Sc. ORGANIC CHEMISTRY - IV SEMESTER SYLLABUS

(With effective from 2019-20 admitted batch)

Paper – II: ORGANIC SPECTROSCOPY-II

15 Hrs

UNIT-I:

Optical Rotatory Dispersion (ORD) and CD spectroscopy:

- (A) Optical Rotation, Circular birefringence, Circular Dichroism and Cotton effect.
- (B) Optical Rotatory Dispersion: Types of Optical Rotatory Dispersion and CD curves
Similarities and difference between ORD and CD curves. Applications of ORD curves
- (C) The α -halo keto rule - The octant rule-application in structural studies of absolute configuration and confirmations of organic molecules.

UNIT-II

- (A) Improving the PMR spectrum: Chemical and Magnetic Equivalence. Chemical exchange, First and Non-First Order Spectra and analysis of AB, AMX and ABX systems.
- (B) Simplification of complex spectra:- Nuclear Magnetic double resonance, Lanthanide shift reagents, solvent effects, Fourier transforms technique, Nuclear Overhauser Effect (NOE), Deuterium Exchange, spectra at higher fields. Resonance of other nuclei- ^{19}F & ^{31}P
- (C) 2D NMR spectroscopy: Definitions and importance of COSY, DEPT, HOMO-COR, HETCOR, INADEQUATE, INDOOR INEPT, NOESY.

15 Hrs

UNIT-III:

Solution of structural problems by joint application of UV, IR, NMR (^1H & ^{13}C) and mass spectrometry.

15 Hrs

UNIT-IV

- (A) Separation Techniques: Solvent extraction chromatography-paper-thin layer-column Chromatography, Electrophoresis.
- (B) Instrumentation – Gas Chromatography, High performance Liquid Chromatography, X-Ray diffraction (XRD)

Suggested Books:

1. Spectroscopic Methods in Organic Chemistry- Forth Edition, D.H. Williams and I. Fleming Tata – McGraw Hill, New Delhi, 1990.
2. Organic Spectroscopy- Second Edition, W.Kemp, ELBS Macmillan, 1987.
3. Spectrometric identification of Organic Compounds-Fourth Edition, R.M. Silverstein: G.C.Vassillir and T.C. Merrill, John Wiley, Singapore, 1981.
4. Introduction to spectroscopy-D.L.Pavia, G.M.Lampman, G.S.Kriz, 3rdEd (Harcourt college publishers).
5. "Applications of Optical rotation and Circular Dichroism", G.C. Barret, in "Elucidation of Organic structures by Physical and Chemical Methods" Part I (Eds) K.W. Bentley and G.W.Rirty John Wiley, 1972, Chapter VIII (only those aspects mentioned in the syllabus).
6. Instrumental methods of chemical analysis by H.Kaur, PragatiPrakasan,meerut.
7. Separation Techniques by M.N.Sastri, Himalaya publishing House (HPH), Mumbai.

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M. Sc. ORGANIC CHEMISTRY - IV SEMESTER SYLLABUS

(With effective from 2019-20 admitted batch)

Paper - III: MODERN ORGANIC SYNTHESIS-II

UNIT-I

Organo Silanes

15 Hrs

Synthetic applications of trimethylsilyl chloride dimethyl-t-butyl silyl chloride, trimethylsilyl cyanide, trimethylsilyl iodide and trimethylsilyl triflate, synthetic applications of α -silyl carbanion and β -silyl carbonium ions. Synthetic applications of silyl enol ethers, Preparation and synthetic applications of alkynyl silanes, aryl silanes, allyl silanes and vinyl silanes, Nazarov cyclization, Synthetic conversion of α , β -epoxy silanes, Peterson Olefination, Brook rearrangement and Ruzicka oxidation.

UNIT-II

Oxidation

15 Hrs

Synthetic applications of the following reagents in the oxidation of functional groups like alkenes, alkynes, alcohols, aldehydes and ketones: 1) $\text{Pb}(\text{OAc})_4$ 2) HIO_4 3) SeO_2 4) Collins reagent, Jones reagent, PCC (Corey's reagent), PDC, Baeyer-Villiger oxidation 4) MnO_2 5) KMnO_4 6) OsO_4 7) Swern oxidation, 8) Oxidations by using IBX, TEMPO 9) Bayer-Villiger oxidation 10) Oxidation of alkenes using Woodward and Prevost reagents 11) Oxidation by using DDQ 12) Sharpless asymmetric epoxidation and Sharpless asymmetric dihydroxylation 13) Thallium nitrate

Reduction 15 Hrs

- (1) Catalytic reductions: Homogeneous (Wilkinson's Catalytic reduction) and heterogeneous catalytic reductions and their synthetic applications.
- (2) Reductions by using electrophilic nucleophilic metal hydrides: LiAlH_4 (Various examples of reductions and Cram's rule), related reagents of LAH, NaBH_4 , NaBH_3CN , Trialkyl Borohydrides (Super Hydride and Selectride).
- (3) Reductions by using electrophilic metal hydrides: BH_3 , DIBAL
- (4) Reductions by dissolving metals: Clemmensen reduction, Aldol condensation, Bouveault-Blanc reduction, Birch reduction (Various examples should be discussed).
- (5) Reductions by using Diimide and Wolf-Kishner Reduction
- (6) Reductions by using tri n-butyl tin hydride.

UNIT-IV

Retro Synthetic Analysis

15 Hrs

1. Basic definitions of the following: a) Retro synthetic analysis b) Disconnection c) Target molecule d) Synthons e) Synthetic equivalent f) Functional Group Inter Conversion (FGI) g) Functional Group Addition (FGA)
2. Guidelines for the order of events: One Group C-X disconnections (Carbonyl derivatives, ethers, sulphides and alcohols); Two group C-X disconnections (1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds), One group C-C disconnections (Alcohols and carbonyl compounds, 1,1- C-C, 1,2-C-C and 1,3-C-C). Linear and convergent Synthesis

Textbooks and Books for Reference:

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
2. Modern Organic Synthesis-an introduction by George S. Zweifel and Michael H. Nantz, W.H. Freeman & company, New York.
3. Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourth edition, Kluwer academic publishers, New York.
4. Organic Synthesis, Christine Willis and Martin Willis, Oxford Chemistry primers.
5. Principles of Organic Synthesis, R.C. Norman and J.M. Coxon, third edition, CBS, Publisher, Delhi.
6. Organic Synthesis, M. B. Smith, McGraw Hill, International Edition.
7. Organic Chemistry, Clayden, Greeves and Stuart Warren.
8. Guide Book to Organic Synthesis (3rd edition), R. Mackie, D. M. Smith and Aitken.
9. Organo Boranes and Silanes, Thomson, Oxford Chemistry primers.
10. Strategic applications of named reactions in organic synthesis, Laszlo Kurti and Barbara Czako.
11. Organic Synthesis: The disconnection approach, S. Warren John Wiley & sons, New York, 1984.
12. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benjamin Inc. Menlo Park, California, 1972.

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FOURTH SEMESTER M.Sc. ORGANIC CHEMISTRY SYLLABUS

(With effect from 2019-20 Admitted batch)

(19OCHT44) Paper – IV: BIO-ORGANIC CHEMISTRY

UNIT-I

15 Hours

Biopolymers and Enzymes

Peptides: α -Amino acids, their general properties and synthesis. Synthesis of peptides by Merrifield solid phase synthesis. Chemistry of oxytocin and dolastatin-10.

Enzymes-Oxidoreductases, hydrolases, transferases, synthesis of ATP, Baker's Yeast. Enzyme models.

UNIT-II

15 Hours

Antimalarials & Antibiotics

i. **Antimalarials:** Chemotherapy, synthesis and activity of antimalarial drugs- quinoline group - quinine, acridine group quinaquine and guanidine group - paludrine.

ii. **Antibiotics:** General characteristics, structure- activity relationships, synthesis and activity of antibiotics: Penicillin G, Cephalosporin-C and streptomycin.

UNIT-III

15 Hours

Vitamins

Definition, occurrence, structural formulae, physiological functions and synthesis of Vitamins.

Vitamins: Structure determination and synthesis of Retinol (A), Thiamine (B1), Riboflavin (B2), Pyridoxine (B6) and Biotin(H), Nicotinic acid.

UNIT-IV

15 Hours

Nucleic Acids:

Nucleic acids: Basic concepts of the structures of RNA and DNA and their hydrolysis products, nucleotides, nucleosides and heterocyclic bases, Genetic Code, Finger Print test.

Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples.

Reference Books and Material:

1. Chemical Aspects of Biosynthesis, John Man, Oxford University Press, Oxford, 1996.
2. Chemistry of Natural Products: A Unified Approach, N. R. Krishnaswamy, University Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.
3. Introduction to Organic Chemistry, A. Streitwieser, C.H. Heathcock and E. M. Kosover IV Edition, Mc. Millan, 1992. (For Merrifield synthesis of peptides and also for other aspects of Unit IV)
4. Bio-organic Chemistry, H. Dugas and C. Penney, Springer, New York, 1981.
5. Details of Primary literature: Nomenclature: Structure: Dolastatin-10: JACS, 1987, 109, 6883 (structure), ibid, 1989, 111, 5463, JCS, Parkin I, 1996, 859 (synthesis).

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M. Sc. (FINAL) ORGANIC CHEMISTRY

IV SEMESTER PRACTICAL SYLLABUS

(With effective from 2019-20 admitted batch)

IV SEMESTER

Laboratory Course-1

Chromatographic Separation and Isolation & identification of Natural Products: 100 M

1. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R_f values of known standards.
2. Isolation and identification of Natural Products
 - (a) Isolation of caffeine from tea leaves
 - (b) Isolation of eugenol from cloves
 - (c) Isolation of casein and lactose from milk
 - (d) Isolation of limonene from lemon peel
 - (e) Isolation of piperines from black pepper
 - (f) Isolation of lycopene from tomatoes
 - (g) Isolation of β -carotene from carrots

Laboratory Course-2

100 M

Spectral Identification of Organic Compounds (UV, IR, ¹H- NMR, ¹³C- NMR & MASS).

A minimum of 40 representative examples should be studied

Books Suggested:

1. Ikan, R. *Natural Products, A Laboratory Guide*, 2nd ed.; Academic Press: New York, 1991.
2. Adapted from *Introduction to Organic Laboratory Techniques: A Microscale Approach*. Pavia, Lampman, Kriz and Engel. (1999) Saunders College Publishing.
3. Pharmaceutical drug analysis by Ashutoshkar
4. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
5. Practical pharmaceutical chemistry part-1 and part-2 by A H Beckett and J B Stenlake
6. Practical organic chemistry by Mann & Saunders.
7. Spectrometric Identification of organic compounds, R.M. Silverstein, F.X. Webster and D.J. Kiemle, 7th Ed.,(Wiley).

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