

M.Sc.,ORGANIC CHEMISTRY SYLLABUS

SEMESTER -I PAPER-I: GENERAL CHEMISTRY-I

UNIT-I

[12 Hours]

Rotational spectra of diatomic molecules-rigid rotor-selection rules-calculation of bond length-isotopic effect, second order stark effect and its applications, Infrared spectra of diatomic molecules-harmonic and an harmonic oscillators. Selection rules-overtone-combination bands calculation of force constant, an harmonic constant and zero point energy. Fermi resonance, simultaneous vibration rotation spectra of diatomic molecules.

UNIT-II

[12Hours]

Raman effect-classical and quantum mechanical explanations-Rotational Raman and vibrational Raman spectra, Electronic spectra of diatomic molecules-Vibrational coarse structure-intensity of spectral lines - Franck Condon principle-applications, Rotational fine structure-band head and band shading, Charge transfer spectra.

UNIT-III [12Hours]

Spin Resonance Spectroscopy: Principle and theory of NMR spectroscopy-Nature of spinning particle and its interaction with magneticfield.Chemicalshiftanditsorigin.Spin-Spininteraction-experimental methods. Application of NMR to structural elucidation-Structure of ethanol, dimethyl formamide, styrene and acetophenone. Principle and theory of ESR-g-factor, hyperfine interactions-applications of ESR studies to the structure of free radicals, metal complexes.

UNIT-IV [12Hours]

Basic concepts of Symmetry and Group theory – Symmetry elements, symmetry operations and point groups – Schoenflies symbols – Classificationofmoleculesintopointgroups–AxiomsofGrouptheory–Groupmultiplication tables for C_{2v} and C_{3v} point groups –Similarity Transformationand classes – Representations – reducible and irreducible representations, Mulliken symbols, Orthogonality theorem and its implications, character table and its anatomy.

UNIT-V

[12Hours]

Basic components of Computers, higher and lower level languages, Microsoft Fortran: constants, variables and operators, arithmetic expressions, assignment and replacement statements, Input and Output statements–Format free and Format directed I/O statements – Iw, Fw.d, Ew.d and Gw.dformat specifications, conditional and unconditional statements – Logical IF, Block IF and Go To statements, Dostatement–syntax and rules.

Application of Chemical Problems:

Flowcharts and Programs for

1. Statistical Analysis calculation of arithmetic mean, mean deviation, variance and standard deviation of replicate measurements.
2. Solution of Quadratic equation – calculation of the roots of a quadratic equation.
3. Calculation of the pH and hydrogen ion concentration of an aqueous solution of a strong acid taking into account the auto ionization of water.
4. Calculation of the root of a polynomial using Gauss-Newton method –Application to Vander-Waal's equation.
5. Calculation of the rate constant of a first order reaction or calculation of molar extinction coefficient using Beer-Lambert's Law by Linear least-squares method.

Text Books:

1. Symmetry and Spectres copy of Molecules, KVeeraReddy, New Age International Publishers.
2. Physical Chemistry by Peter Atkins and JuliodePaula, Oxford University Press.
3. Chemical Applications of Group Theory, F.A.Cotton Wiley Eastern Limited NewDelhi.
4. Group Theory and its Applications to Chemistry, K.V.Raman, Tata McGraw–Hill Publishing Company Ltd., NewDelhi.
5. Computer programming in Fortran-IV by V.Rajaraman, Prentice-Hall of India Pvt. Ltd., NewDelhi.
6. Molecular Spectroscopy, -Gordon M.barrow
7. Fundamentals of Molecular Spectroscopy–Ban well.

PAPER-II: INORGANIC CHEMISTRY-I

UNIT-I

[12Hours]

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 $p\pi-d\pi$ bonding, Bent's rule, Non-valence cohesive forces.

Application of MO theory to square planar ($PtCl_4^{2-}$) and octahedral complexes (CoF_6^{3-} , $Co(NH_3)_6^{3+}$). Walsh diagrams for linear (BeH_2) and bent (H_2O) molecules

UNIT-II

[12Hours]

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallo carboranes, Boron–Nitrogen ($H_3B_3N_3H_3$), Phosphorus–Nitrogen ($N_3P_3Cl_6$) and Sulphur–Nitrogen (S_4N_4 , $(SN)_x$) cyclic compounds. Structure and bonding in higher boranes with (special reference to B₁₂ icosahedra). Electron counting rules in boranes – Wades rules (Polyhedral skeletal electron pair theory).

Polyacids: Introduction to polyacids- Types of polyacids- Isopolyacids, Isopoly molybdates, Isopoly tungstates, Isopoly vanadates, Structures of Polyacids $[Mo_7O_{24}]^{6-}$, $[V_{10}O_{28}]^{6-}$ and $[W_4O_{16}]^{8-}$, Heteropoly acids-properties of heteropoly acids and salts, structures of heteropoly acids and theories, Mialali copause and Roscneium theories, Pauling's theory and keggins theory, applications of polyacids.

UNIT-III

[12Hours]

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 theorem (static and dynamic Jahn-Teller theorem) and its consequences, nephelauxetic effect, applications and limitations of CFT; ligand field theory Experimental evidences for covalence in complexes. Molecular Orbital Theory of bonding for Octahedral, tetrahedral and square planar complexes. π -bonding and MOT-Effect of π -donor and π -acceptor ligands on Δ_o . Experimental evidence for π -bonding in complexes.

UNIT-IV

[12Hours]

Electronic spectra of transition metal complexes:

Term symbol-Free Ion terms and Energy Levels: Configurations, Terms, States and Microstates, calculation of Microstates for P^2 and d^2 Configuration, Russell-Saunders Coupling Schemes, J-J Coupling scheme, derivation of terms for various configurations P^2 and d^2 configuration, spectroscopic Ground state, Hole Formalism, Energy ordering of terms (Hund's Rules), Selection rules: Laporte orbital selection rule, spin selection rules. Splitting of energy levels and spectroscopic states Orgel diagrams of d^1 to d^9 metal complexes. Interpretation of electronic spectra of aquo complexes of Ti(III), V(III), Cr(III), Mn(II), Fe(II), Fe(III), Co(II), Ni(II) and Cu(II). Calculation of inter electronic and spectral parameters for d^8 metal complexes.

UNIT-V

[12Hours]

Tanabe-Sugano diagrams for d^1 – d^9 octahedral and tetrahedral transition metal complexes of 3d series. Calculation of Dq , Racah Parameter

(B) and nephelauxetic parameter (β), Charge transfer ($L \rightarrow M$ and $M \rightarrow L$) spectra of metal complexes.

Magnetic properties of metal Complexes: Types of magnetic behavior, Temperature independent paramagnetism. Magnetic properties of transition and inner transition metal complexes– spin and orbital moments–quenching of orbital momentum by crystal fields in complexes. Magnetic susceptibility and its determination by Gouy's method, and Faraday's method. orbital contribution to magnetic moment (O_h and T_d Complexes)

Textbooks:

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).

PAPER:INORGANICCHEMISTRYLABORATORY-I

Synthesis of Inorganic Metal Complexes: Synthesis of 3d transition metal complexes of tetrahedral, square planar and octahedral geometries.

- (i) Preparation of Tetra ammine Copper(II) sulphate monohydrate
- (ii) Potassium tris-oxalate of cerate(III) trihydrate
- (iii) Tris-thiourea copper (I) sulphate

Systematic Semi micro Qualitative Analysis of Inorganic six radical mixtures

In systematic Semi micro qualitative inorganic analysis, inorganic mixture contains three cations and three anions. The analysis involves identification and confirmation of cations and anions containing one less familiar cation (Tungsten, Molybdenum, Zirconium, Thorium, Titanium, Uranium, Cerium, Vanadium, Lithium, Berkelium Etc. and one interfering anion

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, K, Li

Note: A minimum of 4 inorganic mixtures must be analysed in this Semester

REFERENCE BOOKS:

1. Practical Inorganic Chemistry, G.Marr and B.W.Rockett.
2. Practical Inorganic Chemistry by G.Pass H.Sutchiffe, 2nd John Wiley & Sons.
3. Experimental Inorganic/ Physical Chemistry, M.A.Malati, Horwood Publishing, Chichester, UK (1999)

PAPER-III:ORGANICCHEMISTRY-I

UNIT-I

Aliphatic Nucleophilic Substitutions: The SN₂, SN₁, SN_i and SET mechanisms. Substitution reactions of ambident nucleophiles, anchimeric assistance, the neighbouring group mechanism: neighbouring group participation by O, N, S, halogens, aryl groups, alkyl and cyclo alkyl groups in nucleophilic substitution reactions. Sigma, Pi bond participation in acyclic and bicyclic systems (Non-classic carbocations). Nucleophilic Substitution at allylic, trigonal and Vinylic carbons. Effect of substrate, attack in nucleophile, leaving group and reaction medium.

UNIT-II

Aliphatic Electrophilic Substitutions: SE₁ SE₂ and SE_i mechanisms. Reactivity-effects of substrate, leaving group and solvent. Reactions-hydrogen exchange, migration of double bonds, halogenations of aldehydes, ketones, carboxylic acids, acylhalides, sulfoxides and sulphones.

UNIT-III

Stereo chemistry and conformational analysis : Optical Isomerism: optical activity, molecular dissymmetry and chirality-elements of symmetry. Fisher's projection D,L. and R,S. configurations-relative and absolute configurations optical isomerism due to asymmetric carbon atoms – optical isomerism in biphenyls, allenes and spirans- optical isomerism of nitrogenous compounds, racemisation and resolution.

Geometric isomerism: E,Z-configurations, properties of geometric isomers. Conformational analysis: Conformations of acyclic molecules –alkanes and substituted alkanes-compound showing intra molecular hydrogen bonding. Conformations of cyclohexane, mono and disubstituted cyclohexanes and decalins, effect of conformations on reactivity.

UNIT-IV

Chemistry of heterocyclic compounds : Structure, reactivity and synthesis of reduced three membered Heterocycles: (a) Oxirane: Sharpless method, Sharpless epoxidation, Jacobsen epoxidation, etc, (b) Aziridine; four membered Heterocycles: (a) Oxetane (b) Azetidine; five membered Heterocycles: (a) Pyrrole: PaalKnorr, Hantzsch Methods, etc,(b) Thiophene: Paal Knorr, Hinsberg method, etc. (c) Furan: PaalKnorr, Fieser-Benary, Industrial Method, etc.; (d) Pyrazole, Imidazole, Oxazole, Thiazole; Six membered Heterocycles: (a)Pyridine, Pyridazine, pyrimidine and Pyrazine; Aromatic heterocyclics: a) Indole: Fischer indole synthesis, Bischler synthesis, Madelung synthesis, Domino and cascade methods of indole synthesis, (b) Quinoline and Isoquinoline, (c) Coumarins and Chromones.

UNIT-V

Chemistry of Natural Products

- A) **Terpenoids:** - Occurrence, Isolation, isoprene rule, structure elucidation and synthesis of α -Terpineol and α -pinene
- B) **Steroids:-** Nomenclature of steroids, structure elucidation and synthesis and stereo chemistry of cholesterol and progesterone
- C) **Lipids:-** Classification, chemistry, properties and function-free fatty acids, triglycerides, phospholipids, glycolipids & waxes conjugated lipids-lipoproteins

Reference Books

1. Advanced Organic Chemistry: Reactions Mechanism and Structure by Jerry March, McGraw-Hill and Kogakush.
2. Organic Chemistry Vol.I (Sixth Ed.) and Vol.II (Fifth Ed.) by I.L. Finar ELBS.
3. Organic Chemistry (fifth Ed.), by Morrison and Boyd, PHI, India.
4. Organic Chemistry (fifth edition) by Francis A. Carey Tata McGraw Hill publishing Company Limited, New Delhi.
5. Stereochemistry of Organic compounds by Ernest L. Eliel, Samuel H. Wilen
6. Chemistry of natural products by S.V. Bhat, B.A. Nagasampangi and M. Sivakumar, Narosa Publishing House, 6th reprint 2010

PAPER: ORGANIC CHEMISTRY LABORATORY-I

Synthesis of Organic compounds

Synthesis, purification and characterization of about ten organic compounds involving one or two stages. List of some suggested compounds

1. β -Naphthyl methyl ether from β -Naphthol
2. m-dinitrobenzene from Nitrobenzene
3. Azodye from primary amine
4. Aromatic acid from ester
5. Benzanilide from aniline
6. p-nitro aniline from Acetanilide
7. p-Bromoacetanilide from aniline
8. Phthalimide from phthalic acid
9. 1,2,3-Tribromobenzene from aniline
10. Benzanilide from Benzophenone

Text Books:

1. A Textbook of Practical Organic Chemistry by A.I. Vogel, ELBS and Longman group.
2. Practical Organic Chemistry by Mann and Saunders, ELBS and Longman group.

PAPER-IV:PHYSICALCHEMISTRY-I

UNIT-I

[12Hours]

Basic concepts of second law of Thermodynamics-Entropy-Entropy changes accompanying different processes-Entropy changes in an ideal gas, entropy changes in the mixing of ideal gases, entropy as a function of V and T and entropy as a function of P and T- Entropy change in isolated systems-Clausius inequality-Helmholtz and Gibbs energy -Maxwell relations – Criteria for spontaneity-variation of Gibbs energy with temperature and pressure for solids, liquids and gases-Concept of fugacity-determination of fugacity coefficient of gases-Thermodynamics of phase transitions-Concept of chemical potential-Location of phase boundaries-(Clausius-Clapeyron equation for Liquid- Vapour, Solid -Liquid and Solid-Vapour boundaries)-Ehrenfest classification of phases.

UNIT-II

[12Hours]

Thermodynamics of mixtures-partial molar quantities-experimental methods of determination of partial molar quantities -Gibbs-Duhem equation and Duhem-Margules equation-Thermodynamics of mixing of liquids (ΔH_{mix} , ΔG_{mix} and ΔS_{mix})-Thermodynamics of ideal solutions-Raoult's law-Thermodynamics of colligative properties of dilute solutions - concept of activity and activity coefficient-Experimental determination of activity coefficient-Thermodynamic concept of equilibrium, variation of equilibrium with temperature (Van'tHoff equation) and pressure-Nernst heat theorem, Third law of thermodynamics-exceptions to third law of thermodynamics.

UNIT-III

[12Hours]

Surface tension-Capillary action-Adsorption-Adsorption isotherms-Freundlich adsorption isotherm, Langmuir adsorption isotherm-limitations -BET adsorption isotherm-estimation of Surface area. 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.

UNIT-IV

[12Hours]

Chemical Kinetics: Theories of reaction rates-Collision theory-Limitations, Transition state theory. Lindeman's theory of uni molecular reactions -Limitations. Diffusion controlled reactions. Effect of ionic strength on rates of reactions-Primary and secondary salt effects. Effect of dielectric constant on reactions-kinetic isotope effect-Primary and secondary isotopic effects-Effect of substituent-Linear free energy relationships-Hammett equation-limitations-Tafel equation. Kinetics of consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation).

UNIT-V

[12Hours]

Specific and general acid-base catalysis. Skrabal diagrams. Steady state approximation-Enzyme catalysis- Michaelis -Menten mechanism. Derivation of Kinetic equation and Kinetic parameters. Lock and Key hypothesis-pH dependence of enzyme catalyzed reactions. Fast reactions- different methods of studying fast reactions- flow methods, relaxation methods-temperature jump and pressure jump methods.

Text Books:

1. Physical Chemistry by Peter Atkins and JuliodePaula, Oxford University Press.
2. Chemical Kinetics by K.J.Laidler, McGrawHill Pub.
3. Physical chemistry by K.L.Kapoor

Reference Books:

1. Thermodynamics for Chemists, Samuel Glasstone
2. Physical chemistry by Puri, Sharma and Pathania
3. Micelles, Theoretical and applied aspects, V.Moroi, Plenum publisher

PAPER: PHYSICAL CHEMISTRY LABORATORY-I

Conductometry

- Conductometric titration of strong acid(HCl) vs strong base(NaOH)
 - Conductometric titration of weak acid (CH_3COOH) vs strong base NaOH)
 - Conductometric titration of mixture of acids ($\text{HCl} + \text{CH}_3\text{COOH}$) vs strong base (NaOH)
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- Determination of Cell constant of conductivity cell
 - Determination of Dissociation constant of weak acid by conductometric Method
 - Determination of Critical solution temperature of phenol-Water system
 - Determination of effect of electrolyte (NaCl) on the miscibility temperature of Phenol Water system
 - Determination of composition of Cuprammonium cation using partition Coefficient method
 - To verify Langmuir and Freundlich isotherm for absorption of acetic acid onto activated Charcoal

SEMESTER –II

PAPER-I:GENERALCHEMISTRY-II

Unit-I

[12Hours]

Wave equation–interpretation of wave function – properties of wave function – normalization and orthogonalisation, operators– linear and non-linear commutators of operators, Postulates of quantum mechanics, setting up of operators observables– Hermitian operator – Eigen values of Hermitian operator.

Unit-II

[12Hours]

Wave mechanics of simple systems with constant potential energy, particle in one dimensional box–factors influencing colour–transition– dipole integral, symmetry arguments in deriving these selection rules-the concept of tunneling–particle in a three dimensional box, Rigidrotor, wave mechanics of systems with variable potential energy-simple harmonic oscillator-solution of wave equation-selection rules.

UNIT-III

[12Hours]

Hydrogen atom-solution of $R(r)$, $\theta(\theta)$ and $\Phi(\phi)$ equations-probability density in orbital's-shapes of orbitals. Perturbation theory-time independent perturbation (only first order perturbation is to be dealt with) – application to ground state energy of hydrogen and helium atom

UNIT-IV

[12Hours]

Variation principle-applications to hydrogen and helium atoms-calculation of zero point energy of harmonic oscillator-many electron atom- Comparison between Perturbation and variation theorems. Hartee-Fockself-consistent field method and introductory concepts of Density functional theory (DFT).

UNIT-V

[12Hours]

Valence bond approach-directed valence-hybridization-covalent bond-calculation of ionic and covalent bond contributions in hydrogen molecule. Molecular orbital theory–LCAO approximation–hydrogen moleculeion–hydrogen molecule (fundamental concepts only)–The electronic transitions in the hydrogen molecule.

PAPER-II: INORGANIC CHEMISTRY-II

UNIT-I

[12Hours]

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

Re_2Cl_8^2 , Mo_2Cl_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-Zintlions, Chevrel phases.

UNIT-II

[12Hours]

Organo metallic 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, CH_3 , $\text{Mn}(\text{CO})_5$; S, CH_2 , $\text{Fe}(\text{CO})_4$; P, CH, $\text{Co}(\text{CO})_3$ Synthesis, structure, bonding and reactions of metallocenes with special reference to ferrocene

UNIT-III

[12Hours]

Metal Lig and equilibrium solution:

Step wise and overall formation constants and their interaction. Trends in step wise constants ((statistical effect and statistical ratio), factors affecting the stability of metal complexes; Stability correlations - Irving -William's series, Pearson's theory of hard and soft acids and bases (HSAB), Application of HSAB: Biological functions and toxicology of metals, and medicinal applications; chelate effect and its thermodynamic origin

UNIT-IV

[12Hours]

Determination of stability constants of complexes by spectrophotometric method ((Job's method) and pH-metric method (Bjerrum's).

Reactivity of metal complexes-inert and labile complexes. Explanation of lability on the basis of valence bond and crystal field theories.

UNIT-V

[12Hours]

Reaction Mechanisms of Metal Complexes:

Reactivity of metal complexes, inert and labile complexes, Kinetics and mechanisms of substitution reactions, kinetics of substitution reactions in octahedral complexes, acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reactions, substitution reactions in square planar complexes, Trans effect, Mechanism of trans effect, Electron transfer reactions— concept of complementary and non-complementary reactions with examples, inner sphere and outer sphere mechanisms, Marcus theory.

Textbooks:

1. Advanced Inorganic Chemistry by F.A.Cotton and R.G.Wilkinson, IV Edition, John, JohnWiley and Sons, NewYork, 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 EasternLtd.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press(1999)
5. Theoretical Inorganic Chemistry, IIEdition by M.C.Day and J.Selbin, Affiliated East-West press Pvt. Ltd., NewDelhi.
6. Mechanisms of Inorganic reactions in solution by D.Benson, MCgrawHill, London, 1968.
7. Inorganic chemistry by K.F.Purcell and J.C.Kotz, W.B.Saunders company, NewYork, 1977.

PAPER:INORGANIC CHEMISTRY PRACTICALS-II

Quantitative analysis:

1. Volumetric methods of Analysis:

- i)Determination of Ferriciron by photochemical reduction
- ii).Determination of Nickel by EDTA
- iii)Determination of Calcium and Magnesium in a mixture by EDTA iv)Determination of Ferrocyanide by Cericsulphate
- v)Determination of Copper(II) in presence of iron(III)

2. Gravimetric methods of Analysis:

- i)Determination of Zinc as Zincpyrophosphate
- ii)Determination of Nickel from a mixture of Copper and Nickel.

PAPER-III:ORGANICCHEMISTRY-II

UNIT-I

- A) **Aromaticity:** Concept of Aromaticity, Aromaticity of five membered, six membered and fused systems-non-benzenoidaromatic compounds:-cyclopropenyl cation, cyclobutadienyldication, cyclopentadienylanion–tropyliumcation and cyclo octatetraenyl di anion – metallocenes, ferrocenes, azulenes, fulvenes, annulenes, fullerenes. Homoaromaticity, Antiaromaticity and Pseudoaromaticity.
- B) **Aromatic Nucleophilic Substitutions:** The S_NAr , S_N1 , benzyne and $SRN1$ mechanisms. Reactivity: Effect of substrate, leaving group and attacking nucleophile. The Von-Richter, Sommet-Hauser and Smiles rearrangements.

UNIT-II

- A) **Reactive Intermediates:** Generation, structure, stability and reactivity of Reactive intermediates: carbanion, carbocation, free radicals, carbenes and nitrenes.
- B) **Name Reactions:-** Wittig reaction, Grignard reaction, Storkenamine reaction, Michael addition, Mannich Reaction, Diel's-Alder reaction and Ene-reaction,

UNIT-III

Molecular Rearrangements:

Types of molecular rearrangements, migratory aptitude;

Rearrangements to electron deficient carbon: Pinacol-pinacolone, Wagner-Meerwein and Benzil-Benzilic acid,

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

Rearrangements to electron deficient oxygen: Baeyer-villiger, Dakin rearrangements;

Other rearrangements: Neber rearrangement and Favorskii rearrangements

UNIT-IV

- A) **UV Spectroscopy:** Various electronic transitions, selection rules, effect of solvent on electronic transitions, the absorption laws, chromophores, auxochromes, bathochromic and hypso chromic shifts, hyperchromic and hypochromic effects, Woodward-Fieser rules for conjugated dienes and carbonyl compounds.
- B) **Infrared Spectroscopy:** Basic principles: types of molecular vibrations, finger print region and identification of functional groups.
- C) **Nuclear Magnetic Resonance Spectroscopy (1H -NMR):** nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shifts, factors affecting the chemical shift, and assignment of chemical shifts.
- D) **Mass Spectroscopy:** Basic principles, nitrogen rule and fragmentation pattern of carbonyl compound and alcohols

UNIT-V

- A) **ALKALOIDS:** Occurrence, Isolation, classification based on nitrogen hetero cyclizing and synthesis of quinine and nicotine
- B) **Peptides and Proteins:** α -Aminoacids, their general properties and synthesis, Synthesis of peptides by Merrifield solid phase synthesis. Primary, secondary and tertiary structures of proteins
- C) **Nucleic acids:** Heterocyclic bases; Purines: Adenine and Guanine; Pyrimidines: Cytosine, Uracil and Thymine; nucleosides, nucleotides Basic concepts of the structures of RNA and DNA

REFERENCEBOOKS:

1. Advanced organic chemistry by Jerry March (4th Edition)Wiley Eastern..
2. Stereo chemistry of carbon compounds by E.Eliel, John Wiley & Sons,Inc.
3. Stereo chemistry of Organic compounds by D.Nasipuri.
4. Chemistry of Natural products by R.S.Kalsi Kalyani Publishers. 1983.

PAPER:ORGANICCHEMISTRYPRACTICALS-II

Identification of the unknown organic compounds

Systematic identification for organic compounds—preliminary tests, detection of extra elements, solubility, common functional group tests (determination of functional group/s in a single compound, if present), preparation of two rational derivatives

The given organic compound must be identified by comparing the melting point/ Boiling point of the compound and melting points of its derivatives with the literature

List of suggested compounds

Glucose, fructose, benzaldehyde, p-anisaldehyde, p-chloro benzaldehyde, acetophenone, phenol, cresols, naphthols, esters, p-chlorobenzoic acid, aniline, p-toluene, p-anisidine, p-chloroaniline, diphenylamine, N, N-dimethylaniline, benzamide, naphthalene and anthracene.

TEXTBOOKS

1. A Textbook of Practical Organic Chemistry by A.I.Vogel, ELBS and Longman group.
2. Practical Organic Chemistry by Mann and Saunders, ELBS and Longman group.

PAPER-IV:PHYSICAL CHEMISTRY-II

UNIT-I:

[12Hours]

Crystal structure of solids: Fundamental of lattices, unit cell, Bravais lattices, symmetry elements in crystals, packing efficiency, radius ratios; Miller indices. Structures and types of solids. Structure determination by X-ray diffraction (Bragg's equation). Magnetic properties of solids-classification of magnetic materials, Magnetic susceptibility, Measurement of magnetic susceptibility. Electric properties- Band theory, the band structure of metals, insulators, and semi conductors. The temperature dependence of the conductivity of extrinsic semi conductors. Super conductivity and occurrence. Meissner effect. Types of super conductors. Theories of super conductivity-BCS theory.

UNIT-II:

[12Hours]

Classification of polymers-Free radical, ionic and Zeigler-Natta Polymerization-kinetics of free radical polymerization-Techniques of polymerization - Glass transition temperature - Factors influencing the glass transition temperature - Number average and Weight average, Molecular weights-molecular weights determination-End group analysis-Osmometry-Lights cattering and ultra-centrifugation methods.

UNIT-III:

[12Hours]

Electro chemistry I: Ionic mobilities and conductivities-Debye-Huckel theory of strong electrolytes, Debye-Huckelonsag are quation-limitations- mean activity coefficient-Verification of Debye-Huckel limiting law. Electro chemical cell-Galvanic and electrolytic cell. Nernst equation-Concentration cell with and without transference- effect of complexation on redox potential-ferricyanide/ferrocyanide couple, Iron (III) phenonthroline/Iron(II) phenonthroline couple. Fuel Cells-construction-Various types-Examples.

UNIT-IV:

[12Hours]

Electrochemistry II: The electrode-electrolyte interface. The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Sternmodel .Electrodics: Charge transfer reactions at the electrode-electrolyte interface. Derivation of Butler-Volmer equation. High field approximation, Tafel equation, Low field equilibrium, over voltage. Theories of over voltage-Corrosion-Concentration polarization-Polarography-Halfwave potential and Ilkovic equation

UNIT-V:

[12Hours]

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

Text Books:

1. Physical Chemistry by Peter Atkins and JuliodePaula, Oxford University Press.
2. Physical Chemistry by G.W.Castellon, Narosha Publishing House
3. Physical Chemistry by K.L.Kapoor.
4. Principles of photochemistry, Rohitgee Mukhargee.

PAPER:PHYSICAL CHEMISTRY PRACTICALS-II

1. Potentiometric titration of Iron(II)using potassium dichromate
2. Potentiometric titration of strong acid with a strong base using quinhydrone electrode
3. Determination of kinetics of Ester hydrolysis
4. Determination of Equilibrium constant of Potassium Iodide-Iodine system
5. Determination of kinetics of in version of canesugar by polarimetry method.
6. Determination of partial molar volume of solute–H₂O system by apparent molar volume method.

SEMESTER –III
PAPER I - ORGANIC REACTION MECHANISMS, PERICYCLIC REACTIONS AND PHOTOCHEMISTRY

UNIT-I

Radical substitution reactions: Reactivity for aliphatic substrates, reactivity at Bridgehead, Reactivity in aromatic substrates, neighbouring group assistance in free radical reactions, reactivity in the attacking radical, effect of solvent on reactivity, halogenation at an alkyl carbon and allylic carbon, hydroxylation at aromatic carbon by means of Fenton's reagent, formation of cyclic ethers with $Pb(OAc)_4$, Hunsdiecker reaction, Kolbe reaction, Reed reaction and Sandmeyer reaction.

UNIT-II

Elimination reactions: Mechanisms of E2, E1, and E1CB, factors-effects of substrate, attacking base, leaving group and medium. Stereo chemistry of eliminations in acyclic and cyclic systems. Saytzeff elimination, Hoffman elimination and pyrolytic elimination.

UNIT-III

Addition reactions:

(a) Addition to carbon-carbon multiple bonds- Addition reactions involving electrophiles, nucleophiles and free radicals, cyclic mechanisms. Stereo chemistry and reactivity. Hydrogenation of double and triple bonds, Birch reduction, Hydroboration, Michael reaction, Prins reaction. Addition of oxygen and N_2O_4 .

(b) Addition to carbon-hetero atom multiple bonds: Mechanism and reactivity. Reductions of carbonyl compounds, carboxylic acids, esters, nitriles. Addition of Grignard reagents, Mannich reaction, Reformatsky reaction, Tollen's reaction, Wittig reaction.

UNIT-IV

Pericyclic reactions: Molecular Orbital Symmetry, MO diagrams of ethylene, 1,3 Butadiene, 1,3,5 Hexatriene and allyl system. Woodward- Hoffman correlation diagram method, Frontier molecular orbital approach (FMO) and Perturbation molecular orbital approach (PMO) for the explanation of pericyclic reactions under thermal and photochemical conditions. Classification of pericyclic reactions: Electrocyclic Reactions: Conrotatory and Dis rotatory motions. $4n$ and $4n+2$ electrons systems. Cycloadditions: Antarafacial and Suprafacial additions. $2+2$, $4+2$ cycloadditions and chelotropic reactions. Sigma tropic rearrangements-Suprafacial and Antarafacial shifts of H, Sigmatropic shift involving carbon moieties (1,3), (1,5), (3,3) and (5,5) sigmatropic rearrangements. Claisen, Cope, Oxy-cope and aza- Cope rearrangements. Enereaction.

UNIT-V

Organic Photochemistry: Photochemistry of carbonyl compounds- $n-\pi^*$ and $\pi-\pi^*$ transitions. Norrish type I and Norrish type II cleavages. Paterno-Buchi reactions, Photoreduction, Photochemistry of α,β -unsaturated ketones, photochemistry of enones and cyclohexadienones. Photochemistry of unsaturated systems (Olefins): cis-trans isomerisation, dimerization, and addition. Acetylenes-dimerisation. Photochemistry of 1,3 butadienes, di- π -methane rearrangement. Photochemistry of aromatic compounds – 1,2, 1,3, and 1,4- additions. Photo-Fries rearrangement, Photo-Fries reactions of anilides.

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, Mcmilan.
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

PAPER II- ORGANIC SPECTROSCOPY

UNIT-I

UV SPECTROSCOPY: a) UV spectra of aromatic and heterocyclic compounds, α -diketones, β -diketones, enediones and quinines. Applications of UV Spectroscopy-study of isomerism, determination of strength of hydrogen bonding and conformations of α -substituted cyclohexanones. Steric effect in biphenyls.

UNIT-II

Infrared Spectroscopy: characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, carbonyl compounds, esters, amides, carboxylic acids, anhydrides, lactones, lactams, nitriles and conjugated carbonyl compounds. Effect of hydrogen bonding and solvent on vibrational frequencies.

UNIT-III

Nuclear Magnetic Resonance Spectroscopy (^1H NMR): Nuclear spin, resonance, saturation, shielding of magnetic nuclei, chemical shifts and its measurements, factors affecting chemical shift, chemical and magnetic equivalence of spins, spin-spin coupling, integration, the coupling constant, types of spin-spin couplings, factors influencing coupling constants, first-order and non first order spectra, spin system notations (ABX, AMX, ABC, A2B2 etc.). Simplification of non first order spectra- use of higher magnetic fields, nuclear magnetic double resonance and contact shift reagents. Deuterium exchange, nuclear overhauser effect difference spectra, Study of dynamic processes by Variable temperature (VT) NMR, restricted rotation DMF, cyclohexane ring inversion.

UNIT-IV

Mass spectroscopy: Basic Principles, instrumentation, isotope abundance, the molecular ion, metastable ions, base peak, fragment ions, even-electron rule and nitrogen rule. McLafferty rearrangement, ortho effect. retro-Diels- Alder reaction, Fragmentation processes- fragmentation associated with various functional groups (alkanes, cycloalkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amides, amines, alkyl chlorides and alkyl bromides).

UNIT-V

Structural elucidation of Organic compounds by a combined application of the UV, IR, NMR and MASS spectral data.

Reference books:

1. Spectroscopic identification of organic compounds by RM Silverstein, G C Bassler and T B
2. Morrill Organic Spectroscopy by William Kemp
3. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
4. Modern NMR techniques for chemistry research by Andrew B Derome
5. NMR in chemistry - A multinuclear introduction by William Kemp
6. Spectroscopic identification of organic compounds by P S Kalsi
7. Introduction to organic spectroscopy by Pavia
8. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
9. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman

PAPER III – ORGANIC SYNTHESIS

UNIT-I

Formation of Carbon-Carbon (C-C) single bonds:

A) Alkylations via enolate anions-1,3-dicarbonyl and related compounds, direct alkylation of simple enolates, imine and hydrozone anions, enamines. The aldol reaction, umplog (dipole inversion).

B) Via Organometallic reagents- organ palladium, organo nickel and organo copper reagents

UNIT-II

Formation of carbon-carbon double bonds:

β - Elimination reactions, Pyrolytic syn eliminations, alkenes form hydrazones, 1,2-diols, sulfones, sulphoxide-sulphonate rearrangement, the Wittig and related reactions

UNIT-III

Organic polymers Introduction to organic polymers, general properties and classification of polymers. Methods of polymerization: (a) Addition polymerization-Definition, synthesis and applications, vulcanization. (b) Condensation polymerization- Definition, synthesis and applications. Radical polymerization. (With atleast two examples in each category)

UNIT-IV

Reactions of unactivated carbon-hydrogen bonds Unactivated carbon-hydrogen bonds: Definition, mechanism and synthetic applications- The Hoffmann-Loeffler-Freytag reaction(HLF reaction)-cyclisation reactions of Nitrenes-the Barton reaction-Photolysis of organic hypohalites-hypochlorites, hypobromites and hypoiodites,

UNIT-V

Asymmetric Synthesis Topocity – Prochirality – Substrate selectivity – Diastereoselectivity and enantioselectivity –Substrate controlled methods – use of chiral substrates – examples Auxiliary controlled methods – Use of chiral auxiliaries – Chiral enolates – alkylation of chiralimines- Reagent controlled methods – Use of chiral reagents – Asymmetric oxidation – Sharpless epoxidation – Asymmetric reduction – borate reagents.

Reference books:

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
2. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benjamin Inc. Menlo Park, California, 1972.
3. Principles of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
4. Advanced organic chemistry part A & B; Fourth edition; Francis A Cary and Richard J. Sundberg; Kluwer Academic/Plenum Publisher New York, 2000.
5. Organic chemistry Jonathan Clayden, Nick Greeves, Stuart Warren, 2nd Edition, 2012, Oxford University Press.
6. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri.
7. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen.
8. Stereochemistry: Conformation & Mechanism by P S Kalsi.
9. The third dimension in organic chemistry, by Alan Bassendale.
10. Stereo selectivity in organic synthesis by R S Ward.
11. Asymmetric synthesis by Nogradi.
12. Asymmetric organic reactions by J D Morrison and H S Mosher.
13. Principles in Asymmetric synthesis by Robert E. Gawley & JEFFREY AUBE.

Paper IV – Chemistry of Natural Products

UNIT-I

Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Penicillin G, Cephalosporin-C, streptomycin, chloramphenicol and tetracyclins

UNIT-II

Isolation, structure elucidation, stereochemistry, synthesis and biological properties of Terpenes: Forskolin, taxol and β -amyryn

UNIT-III

Isolation, structure elucidation, stereochemistry, synthesis, and biological properties of Alkaloids: Morphine, reserpine and vincristine

UNIT-IV

Natural Flavonoids : Apigenin, flavanones-Hesperetin, Isoflavones-Genistein, Flavonolquercetin, xanthone-Euxanthone.

UNIT-V

Natural Pigments: Introduction structure elucidation and synthesis of quinones-Polyporic acid. Chlorophyll and haemin.

Reference Material:

1. Organic Chemistry, Volume 2, Stereochemistry and chemistry of natural products, I.L.Finar, 5th Edition. ELBS.
2. Chemical Aspects of Biosynthesis, John Mann, Oxford University Press, Oxford, 1996
3. Chemistry of Natural Products. A Unified Approach, N.R. Krishnaswamy, Universe Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.
4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010.

SEMESTER –IV

Paper – I: Modern Synthetic Methodology in Organic Chemistry

UNIT – I

Modern Synthetic Methods: Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction and Ugi reaction. Brook rearrangement; Tebbe olefination. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reaction.

UNIT-II

Multi component Reactions: Passerini reaction, Biginelli reaction, Hantzsch reaction and Mannich reaction.

Metathesis: Grubb's 1st generation and 2nd generation catalyst, Olefin Cross coupling Metathesis (OCM), Ring Closing Metathesis(RCM), Ring Opening Metathesis (ROM) and applications.

UNIT-III

Oxidation: Metal based and non-metal based oxidations of (a) alcohols to carbonyls (Chromium, Manganese, aluminium, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents). (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation.(d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, (e) alkenes to carbonyls with bond cleavage (Manganese, Osmium, Ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation) (g) ketones to ester/lactones (Baeyer-Villiger)

UNIT-IV

Reduction:(a) Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium/Nickel etc; Homogeneous: Wilkinson). Noyori asymmetric hydrogenation. (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations) (c) Hydride transfer reagents-NaBH₄ triacetoxyborohydride, L-select ride, K-select ride, Luche reduction; LiAlH₄, DIBAL-H, and Red-Al.

UNIT-V

NEWER METHODS IN ORGANIC SYNTHESIS:

Green Chemistry: Introduction, principles, atom economy and scope (illustrate with two examples) Microwave induced reactions: Principle conditions, advantages over conventional heating methods-applications

Ionic liquids: Introduction and applications in organic synthesis (illustrate with two examples).

Nanomaterials: Introduction, methods of preparation, applications in organic synthesis Phase-transfer catalysis: solid-solid, solid-liquid systems-mechanism of catalytic action, type of catalysts, application in few important reactions

Reference books:

1. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
2. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.
3. M. B. Smith, Organic Synthesis, 2nd Edition, 2005
4. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.
5. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley-VCH, New York, 2000.

M.SC., CHEMISTRY (FINAL)-IV-SEMESTER SYLLABUS
Paper II- Organic Spectroscopy and Structure determination of natural products

UNIT-I

¹³C NMR spectroscopy

Introduction, ¹³C-chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and aromatic compounds. Types of ¹³C NMR spectra: Proton-coupled, proton- decoupled and OFF-resonance decoupled (ORD) spectra, DEPT. ¹³C-NMR solvents:

UNIT-II

Heteronuclear NMR spectroscopy & Electron Spin Resonance Spectroscopy (ESR):

Heteronuclear couplings: ¹³C-¹H, ¹³C-D, ¹³C-¹⁹F, ¹³C-³¹P, ¹H-D, ¹H-¹⁹F, ¹H-³¹P, ¹H-¹⁵N

ESR Spectroscopy: Principles, hyperfine splitting

UNIT-III

NMR Instrumentation, 2D-NMR techniques

NMR Instrumentation: Types of NMR Spectrometers-Continuous Wave (CW)-NMR, Fourier Transform (FT)-NMR, NMR solvents, sample preparation

2D-NMR techniques: Principles of 2D NMR, Correlation spectroscopy (COSY) HOMO COSY (¹H-¹H COSY), Hetero COSY (¹H, ¹³C COSY, HMQC), long range ¹H,¹³C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.

UNIT-IV

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, and circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Application of the rules to the study of absolute configuration and conformations of organic molecules.

UNIT-V

Structure determination of natural products by spectral methods structure elucidation-Spectroscopic techniques IR, UV, ¹H-NMR, ¹³C-NMR, COSY, HETEROCOSY, and MS- natural products- Examples, flavones-Apigenin, flavanones- Hesperetin, isoflavones-Genistein, coumarins-7-hydroxycoumarin, alkaloids-morphine, quinine, terpenoids(-) -Menthol, Steroids-stigmasterol, Glycosides-salicin (Alcoholic β- glucoside)

Text books:

1. Spectroscopy, fourth edition, D. L Pavia, G. M Lampman CENGAGE Learning, 2012
2. Spectroscopic Methods in Organic Chemistry. Forth Edition D. M. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990. For all spectral methods except ORD and CD and ESR.
3. Organic Spectroscopy, Second Edition, W. Kemp, ELBS Macmillan, 1987 for ORD and CD and ESR.
4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010

SEMESTER- IV

Paper – III: DESIGNING ORGANIC SYNTHESIS AND SYNTHETIC APPLICATIONS OF ORGANO- BORANES AND -SILANES

UNIT-I

Disconnection approach –Principles

Introduction, Terminology: Retrosynthesis, Target Molecule (TM), synthon, synthetic equivalent, functional group interconversion (FGI). Linear and convergent synthesis. Criteria for selection of target. Order of events in retrosynthesis with reference to Salbutamol, Proparacaine and Dopamine. Chemoselectivity, Regioselectivity, reversal of polarity and cyclizations. Protecting groups- Principles of protection of alcohols, amine, carbonyl and carboxyl groups

UNIT-II

Synthetic Strategies-One group disconnections

A) Introduction to one group disconnections: C-C disconnection-alcohols and carbonyl compounds; C-X disconnections- alcohols and carbonyl compounds and sulphides two group C-C and C-X Disconnections.

UNIT-III

Synthetic Strategies-Two group disconnections

B) Introduction to Two group C-C disconnections; Diels-Alder reaction, 1,5- difunctionalised compounds, Michael addition and Robinson annulation. Two group C-X disconnections; 1, 1 difunctionalised, 1, 2-difunctionalised and 1, 3-difunctionalised compounds. Control in carbonyl condensations, explanation with examples oxanamide and mevalonic acid.

UNIT –IV

Organoboranes

Hydroboration- Preparation of Organoboranes. Reagents –dicyclohexyl borane, disiamyl borane, tetryl borane, 9-BBN and mono-, di-isopinocampheyl borane. Functional group transformations of Organo boranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organo boranes- carbonylation, cyanoboration.

UNIT –V

Organo Silanes

Preparation and synthetic applications of trimethylsilyl chloride, dimethyl-tbutylsilyl chloride, trimethylsilyl cyanide, trimethylsilyl iodide and trimethylsilyl triflate. Protection of functional groups- Trimethylsilyl ethers, Silyl enol ethers. Synthetic applications of α -silyl carbanions, β -silyl carbonium ions. Peterson's olefination.

Books for Reference:

1. Organic syntheses via boranes / Herbert C. Brown; with techniques by Gary W. Kramer, Alan B. Levy, M. Mark Midland. New York : Wiley, 1975
2. Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
3. Organic Synthesis: The disconnection approach, S. Warrant John Wiley & sons, New York, 1984.
4. Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benzamine, Inc. Menlo Park, California, 1972.
5. Principle of Organic Synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
6. Organic Synthesis: Special techniques. V.K.Ahulwalia and Renu Aggarwal.
7. Organic Synthesis by C Willis and M Willis
8. Problems on organic synthesis by Stuart Warren

SEMESTER-IV
PAPER IV-DRUG DESIGN AND DRUG CHEMISTRY

UNIT I

Basic consideration of drugs

General Classification, nomenclature, drug metabolism. **Development of drugs:** Procedure followed in drug design, concepts of lead compound lead modification, concept of prodrugs, Structure Activity Relationship (SAR)-factors affecting bio-activity-resonance, inductive effect, isosterism, bio-isosterism, spatial considerations, Quantitative Structure Activity Relationships (QSAR)-Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials.

UNIT II

Antineoplastic Agents: Introduction, classification-**alkylating agents**- mechanism and mode of action, nitrogen mustards-synthesis, properties, uses and dosage - Chlorambucil, cyclophosphamide and melphalan. **Antimetabolites**- synthesis, properties, uses and dosage-pyrimidine analogues-5-fluorouracil, purine analogues-6-mercaptopurine, folic acid analogues-Methotrexate. **Antibiotics**-structure, properties and dosage-Doxorubicin, Mitomycin.

UNIT III

Cardiovascular Drugs: Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyphenolol.

UNIT IV

Oral Hypoglycemic Drugs: Introduction, Classification, **Sulphonylureas**- synthesis, mode of action, properties, uses and dosage- tolbutamide, glipizide. **Biguanides**- synthesis, mode of action, properties, uses and dosage-Metformin. **α -glucosidase inhibitors**- synthesis, mode of action, properties, uses and dosage- Miglitol. **Dipeptidyl Peptidase-4 (DPP-4) inhibitors**- synthesis, mode of action, properties, uses and dosage-saxagliptin and sitagliptin

UNIT V

Local Antiinfective Drugs & Antiviral drugs

Local Antiinfective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, ciprofloxacin, norfloxacin, dapson, amino salicylic acid, isoniazid, fluconazole, econazole and chloroquin.

Antiviral Drugs: Introduction, classification based on mechanism of action, Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NRTIs)-Synthesis, metabolism, properties and uses and dosage-Acyclovir, Zidovudine (Anti-HIV agent). Non-Nucleoside or Nucleotide Reverse Transcriptase Inhibitors (NNRTIs)-Synthesis, metabolism, properties and uses and dosage-Nevirapine, Efavirenz. Protease Inhibitors (PIs)- Synthesis, metabolism, properties and uses and dosage-Indinavir. CCR5-Inhibitors- Synthesis, metabolism, properties and uses and dosage-Maraviroc.

SUGGESTED BOOKS FOR READING

1. Text book of medicinal chemistry, Volume 1 & II, Third edition by V Alagarsamy, CBS-publishers
2. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH.
3. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge.
4. An Introduction to Drug Design, S. S. Pandeya and J. R. Dimmock, New Age International.
5. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter.-9 and Ch-14), Ed. M. E. Wolff, John Wiley.
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
7. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
8. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.