SEMESTER – I ORGANIC CHEMISTRY-1- PCH701S

Objective:

- **T**o appreciate the applications of stereochemistry
- **T**o learn various reactions and rearrangements involving reactive intermediates like carbocations, carbanions,free radicals, carbenes and nitrenes
- **T**o learn the applications of oxidation and reduction reactions in organic synthesis

Unit I: STEREOCHEMISTRY -I (12 hrs)

Review of basic principles of stereochemistry – R, S notation of biphenyls and allenes. Fischer projection. Inter conversion of Sawhorse, Newman and Fischer projections. Molecules with one

And two asymmetric centres. Eg. Erythro and threo compounds. Asymmetric synthesis. Cram's rule. Geometrical isomerism, E, Z - nomenclature of olefins, Geometrical and opical isomerism of disubstituted cyclopropane, cyclobutane and cyclopentanes. Stereo specific and stereo selective reactions.

Unit II PHYSICAL ORGANIC CHEMISTRY (12 hrs)

Introductory physical organic chemistry : Acids and Bases, HSAB, equilibrium constant, thermodynamic effect, kinetic effects – thermodynamic and kinetic control of organic reactions. Hammond postulate, Curtin – Hammett principle – Hammett equation – Application to organic reactions. Methods of determining reaction mechanism – Kinetic and Non-kinetic methods.

UNIT – III REACTIVE INTERMEDIATES (12 hrs)

Structure, reactivity, formation, stability and reactions involving free radicals, benzynes, carbenes and nitrenes. Long and short lived free radials . Addition of free radicals to olefinic double bonds. Aromatic radical substitutions: Decomposition of diazocompounds, phenol – coupling, sandmeyer reaction , Gomberg reaction, Pschorr reaction, Ulmann reaction, Hunsdiecker reaction.

UNIT IV MOLECULAR REARRANGEMENTS (12 hrs)

Structure, reactivity, formation, stability and the following rearrangements involving carbocations and carbanions: Wagner – Meerwein, Pinacol – Pinacolone ,Tiffeneau- Demjanov, Beckmann, Dienone – phenol ,Favorski, Wittig, Neber ,Stevens and Sommelet- Houser rearrangements. Hofmann, Curtius, Lossen, Schmidt and Wolff Rearrangements.

Unit V OXIDATION AND REDUCTION (12 hrs)

Mechanism – study of the following oxidation reactions–oxidation of alcohols with Cr(VI)and Mn reagents – oxidation of methylene to carbonyl, oxidation of aryl methanes – Etard reaction – allylic oxidation of olefins. Formation of C = C bonds-Wittig reaction, Formation of C – C bonds by dehydrogenation, dehydrogenation by quinines, $Hg(OAc)_2$ and $Pb(OAc)_4$. Formation of C – C bond by phenol coupling and acetylene coupling – allylic oxidation-SeO_2, oxidation of alcohol, glycols, halides and amines to aldehydes and ketones , oxidation of Oleffinic double bonds and unsaturated carbonyl compounds – oxidative cleavage of C – C bond. Synthetic importance of clemmensen and wolf Kishner reductions – modification of Wolf-Kishner reduction – Birch reduction, MPV reduction. Catalytic hydrogenation and Sommelet reaction. Reduction with $LiAlH_4$, $NaBH_4$, tritertiarybutoxy aluminium hydride, Sodium cyanoborohydride , trialkyl tin hydride and hydrazines.

Text Books:

1. E. L. Eliel "Stereochemistry of carbon compiounds", John Wiley, 1997.
2. P.S. Kalsi Stereochemistry, Conformation and mechanism, 6th edition ., New Age International (P) Ltd. 2005.
3. Seyhan Ege, Organic Chemistry, AITBS, 2001.
4. F. A. Carey and R. J. Sundberg, Advanced organic chemistry, Plenum publishers Ltd. 2000.

Reference Books:

1. R.O.C. Norman, J.M. Coxon, Principles of organic synthesis, ELBS publications, 1994.
2. C. K. Ingold, Structure and Mechanism in Organic chemistry, Cornell Univ. Press.
3. Michael Smith, Organic synthesis, McGraw Hill, 1996.
4. W. Carruthers, J.Coldham, Modern methods of Organic synthesism IV edition, Academic press, 1989.
5. Clayden, Greeves, Warren, Wothers, Organic chemistry, Oxford University Press.
6. Reinhard Brukner, Advanced Organci chemistry, Academic press, Elseiver, 2002
7. Neil Isaacs, Physical Organic chemistry, ELBS, 1987.

SEMESTER – I INORGANIC CHEMISTRY – I - PCH702S

Unit- I – Isomerism in Coordination Complexes - ORD and CD [12 Hrs]

1.1Isomerism in complexes-ionization isomerism, hydrate isomerism, linkage isomerism, ligand isomerism, Co-ordination isomerism and polymerization isomerism- Geometrical and optical isomerism in 4 and 6 coordinated complexes

1.2 Chirality and nomenclature of chiral complexes; Optical Rotatory Disperision and circular dichroism.

Unit – II – Macrocyclic Ligands and CFT [12 Hrs]

2.1 Macrocyclic Ligands: Thermodynamic and Kinetic template effect – Structure, Stability and applications of porphyrins, corrins, Schiff bases, crown ethers and crypts.

2.2.Crystal field theory- Splitting of d-orbitals in octahedral, tetrahedral and square planar complexes- crystal field stabilization energy-calculation of CFSE in octahedral complexes- Spectrochemical series -low spin and high spin complexes-explanation of magnetic properties and color of complexes using CFT.

Unit-III – Thermodynamic and Kinetic stability of Complexes [12 Hrs]

3.1.Metal-Ligand Equilibria in Solution: Stepwise and overall formation constants and thier interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin.

3.2.Determination of stability constants by Potentiometric, Polarograpy and Spectrophotometric techniques.

Unit-IV - Molecular Polyhedra: Boron hydrides and Metal Clusters **[12 Hrs]**

1.1.Boron Hydrides: Closo, nido and arachno boranes – styx numbers – Hydro Borate ions – Carboranes – Metallocarboranes.

1.2. Metal Clusters: Structure and bonding of Binuclear compounds – $Re_2Cl_8^{2-}$ and $Mo_2Cl_8^{2-}$ - Three atom clusters – $Re_3Cl_{12}^{3-}$ and Fe_3CO_{12} – Four atom tetrahedral clusters – Co_4CO_{12} and Ir_4CO_{12} - Six atom clusters Rh_6CO_{16}.

Unit-V - Polyacids and Inorganic polymers [12 Hrs]

5.1.Polyacids: Isopolyacids and hetereopolyacids of vanadium, chromium, molybdenum and Tungsten.

5.2.Inorganic Polymers: Silicates – structure, properties and applications – polysulphur – nitrogen compounds and poly-organophosphazenes.

Text Books :

1. J.E. Huheey, Inorganic Chemistry, 5th Edn., Harper International.1993.
2. F.A.Cotton, G.Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.1985.
3. M.F.Purcell, J.C.Kotz, Inorganic Chemistry,Saunder, 1977.
4. N.N.Greenwood , A.Earnshaw , Chemistry of the Elements, 2nd Edn.,BH,1997.
5. D.F.Shriver, P.W.Atkins, C.H.Langford, 3rd Edn. Inorganic Chemistry, ELBS.1999.

Reference Books

1. B.Douglas, D.McDaniel, J.Alexander, Concepts and Models of Inorganic Chemistry, 3rd Edn., John Wiley,2001.
2. J.D.Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.
3. W.L.Jolly, Modern Inorganic Chemistry, 2nd Edn., McGraw-Hill,1991

SEMESTER - I QUANTUM MECHANICS AND MOLECULAR - PCH 703S STRUCTURE

Unit I Quantum Chemistry I **[12 Hrs]**

1.1 Inadequacy of classical theory – Bohr's quantum theory and subsequent developments – the Compton effect – wave particle duality – uncertainty principle.

1.2 Wave equation for electrons – quantum mechanical postulates – the operators – Hermitian property. 1.3 Schrodinger equation – elementary application of Schrodinger's equation – the particle in box (one, two and three dimensional cases)

Unit II Quantum Chemistry II **[12 Hrs]**

2.1 The harmonic Oscillator – the rigid rotor – particle in a ring Schrodinger equation for hydrogen atom (no derivation is required) and the solution.

2.2 The origin of quantum numbers (angular momentum and spin) – their physical significance.

Unit – III Quantum Chemistry **[12 Hrs]**

3.1 Approximation methods – perturbation and variation methods – application to hydrogen, helium atoms – R.S. Coupling and term symbols for atoms in the ground state.

3.2 Born Oppenheimer approximation – valence bond theory for Hydrogen molecule – LCAO – MO theory for diatomic and polyatomic molecules.

3.3 Concept of hybridization – Huckel theory for conjugated molecules (ethylene, butadiene and benzene)

3.4 Semi empirical methods – slater orbital and HF- SCF methods.

Unit IV Empirical MO theory **[12 Hrs]**

4.1 The simple Huckel method – Assumptions – Determinant, Energies and wave functions – Extended Huckel method – overlap – population analysis.

4.2 FMO theory – Interaction and Walsh diagrams – Non crossing rule – s-p mixing – hybridization – conjugation and Hyperconjugation – FMOs of functional groups – isolobal analogy.

Unit V

5.1 Basics of Popular quantum chemical calculations: Hamiltonian and wave functions – Roothan's equations.

5.2 Fock matrix – SCF procedure – Interpretation of LCAO – MO- SCF results – unrestricted open – shell Hatree – Fock – theory- Basis sets – semi empirical methods – Density functional Theory – Hellmann – Feynman theorem.

Text Books

1. R. K. Prasad, Quantum Chemistry, Wiley Eeastern, New Delhi, 2nd edition,1992.

Further reading

P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford 3rd edition, 1983.

SEMESTER – I BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY - EPCH 704T

Unit – I

1.1 Metal Storage Transport and Biomineralization. Ferritin, Transferrin, and siderophores

1.2 Calcium in biology

Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins

Unit – II

2.1 Metalloenzymes – zinc enzymes – carboxypeptidase and carbonic anhydras. Iron enzymes – catalase, peroxidase and cytochrome P – 450. Copper enzymes – superoxide dismutase. Molybdenum oxatransferase enzymes – xanthine oxidase. Coenzyme vitamin B_{12}

Unit – III

3.1 Metal – Nucleic Acid Interactions

Metal ions and metal complex interactions. Metal complexes – nucleic acids

3.2 Metals in Medicine

Metal deficiency and disease, toxic affects of metals, metals used for diagnosis and Chemotherapy with particular reference to anticancer drug.

Unit – IV

Supramolecular Chemistry – I

4.1 Concepts, Nature of Supramolecular interactions, preorganization and design principles.

4.2 Molecular recognition: Recognition, complementarity - Spherical and tetrahedral recognition – Recognition of ammonium ions, neutral molecules.

4.3 Molecular receptors – Crown ethers, Cryptands, Calixarenes - design principles -

4.4 Anion Coordination chemistry and Recognition of Anionic substrate.

4.5 Co-receptor molecules - dinuclear and polynuclear metal ion cryptates - ditopic, heterotopic co-receptors - multiple recognition in Metalloreceptors.

Unit – V

5.1 Supramolecular Chemistry – II

Supramolecular devices: Light Conversion and Energy Transfer Devices, Photoinduced Electron Transfer Devices

5.2 Molecular wires, switchable molecular wires, photo switching devices.

1.3 Supramolecular racks, ladders, grids. Cation and anion binding hosts: Cryptands,

1.4 Supramolecular chemistry in biology.

Text Books:

1. Asim K. Das, Bioinorganic Chemistry, Vikas.
2. J. M. Lehn, Supramolecular Chemistry, Concepts and perspectives, VCH, 1995.
3. J. W. Steed, J.L. Atwood, Supramolecular Chemistry, A concise Introduction, John Wiley, 2000.
4. J.E.Huheey, Inorganic Chemistry, 5th edition, Harper international, 1993.
5. Ivano Bertini, Harry. B.Gray, J. Lippard, Valentine, Bioinorganic chemistry, 1998.

Reference Books:

1. J.L. Atwood, J.E.D. Davies, D.D. Mac Nicol, F. Vogtle, J.M. Lehn, Comprehensive Supramolecular Chemistry, Pergamon, 1996.
2. Albert L. Lehninger, David Lee Nelson, Michael M. Cox, Principles of Biochemistry, 4th Ed, 2005
3. P.S. Kalsi, Bioinorganic and Supramolecular chemistry, 2007.
4. R.W. Hay, Bioinorganic chemistry, Ellis Harwood, 1987.

SEMESTER - II ORGANIC CHEMISTRY – II - PCH 805S

Objectives:

- To learn the aspects of substitution reactions and its applications.
- To appreciate the principles of addition and elimination reactions.

UNIT – I : STEREOCHEMISTRY – II **12 Hrs.**

Conformations of some simple 1,2 – disubstituted ethane derivatives. Conformational analysis of disubstituted cyclohexanes and their stereochemical features. Conformation and reactivity of substituted cyclohexanol(oxidation and acylation), cyclohexanone.(reduction) and cyclohexane carboxylic derivatives (esterification and hydrolysis). Conformation and mechanism of cis and trans decalin and 9 – methyl decalin.

UNIT – II:

ALIPHATIC NUCLEOPHILIC AND ELECTROPHILIC SUBSTITUTION. 12 Hrs.

Substitution at saturated reaction center (carbon). SN1, SN2,SNi mechanisms – Reactivity, structural and solvent effects. Neighbouring group participation – substitution in Norbornyl and bridgehead systems – Substitution at carbon doubly bonded to oxygen. Alkylation and acylation of active methylene carbon compounds, hydrolysis of esters. SE1, SE2, SEi mechanisms – reactivity. Hell-Volhard-Zelinsky reaction, Stork – enamine reaction. Decarboxylation of aliphatic acids.

UNIT – III ADDITION AND ELIMINATION REACTIONS **12 Hrs**

Electrophilic, nucleophilic and free radical mechanisms of addition to carbon – carbon multiple bonds – isolated and conjugated multiple bonds. Hydration, hydroxylation, hydroboration. Stereochemical aspects to be studied wherever applicable.Nucleophilic addition reactions of carbonyl compounds: Aldol, Perkin, Stobbe, Claisen, Dieckmann,Benzoin condensation. Mannich, Reformatsky, Grignard, Robinson Annulation and Shapiro reactions.

Elimination reactons: E1, E2 and E1CB mechanism. Hofmann and Saytzeff rules. Dehydration, dehydrohalogenation and dehalogenation. Stereochemistry of E2 elimination in cyclohexane systems. Mechanism of pyrolytic eliminations. Chugaev and Cope eliminations.

UNIT – IV AROMATIC ELECTROPHILIC SUBSTITUTION 12 HRS

The arenium ion mechanism – Orientation and reactivity – typical reactions – nitration, halogenation, alkylation, acylation and diazonium coupling. Reimer-Tiemann, Vilsmeyer- Hack , Gattermann, Kolbe reactions. Synthesis of di- and tri-substituted benzenes. Electrophilic substitution of furan, pyrrole, thiophene and pyridine- N- oxide.

UNIT – V AROMATIC NUCLEOPHILIC SUBSTITUTION 10 HRS

Methods for the generation of benzyne intermediate and reactions of aryne intermediate. Nucleophilic substitution involving diazonium ions. Aromatic nucleophilic substitution of activated halided. Zeigler alkylation. Chichibabin reaction. Problems.

BOOKS RECOMMENDED

1. E.L. Eliel Stereochemistry of carbon compounds, John Wiley, 1997.
2. P.S. Kalsi Stereochemistry , conformation and mechanism, 6th edition, , New Age International (P) Ltd. 2005.
3. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Part A and B, Kluwer Academin/Plenum Publishers,2000.
4. Seyhan Ege, Organic Chemistry, AITBS, 2001.
5. Clayden, Greeves, Warren, Wothers, Organic Chemistry, Oxford Univ Press.
6. Reinhard Brukner, Advanced Organic Chemistry, Academic Press, Elseiver, 2002.
7. Raj.K. Bansal,Organic Reaction Mechanism, 3rd edition, Tata McGraw Hill, 1998.
8. R.O.C. Norman, J.M. Coxon, Principle of Organic Synthesis, ELBS Publications,1994.
9. C.K. Ingold, Structure and Mechanism in Organic Chemistry, Cornell Univ. Press
10. Michael Smith, Organic Synthesis, McGraw Hill, 1996.
11. W. Carruthers, J. Coldham Modern methods of Organic Synthesis, IV Edition, Academic Press, 1989.

SEMESTER – II INORGANIC CHEMISTRY – II - PCH 806T

Unit-I – MO theory of Complexes and Chemistry of Lanthanides and Actinides [12 Hrs]

1.1. Metal-Ligand Bonding: Limitation of crystal field theory, molecular orbital theory-octahedral, tetrahedral and square planar complexes, л-bonding and molecular orbital theory. Jahn-Teller Effect and its consequences.

1.2. The Chemistry of Lanthanides and Actinides: oxidation state, spectral & magnetic characteristics, coordination numbers, stereochemistry, lanthanide contraction-causes, consequences - comparison between 3d and 4f block elements - comparative account of lanthanides and actinides - nuclear and non-nuclear applications.

Unit-II - Electronic Spectra of Transition Metal Complexes [12 Hrs]

2.1. Electronic Spectra of Transition Metal Complexes: Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), Nephlauxetic effect - calculations of Dq, B and β parameters.

2.2. Charge Transfer spectra – Comparison of CT and d-d spectra.

Unit-III - Nanotechnology [12 Hrs]

3.1. Nanotechnology – Introduction – preparatory methods – chemicals methods, thermolysis, pulsed laser method – characterization – particle size determination, SEM, TEM, AFM, XRD, IR and UV - Carbon nanotubes – structure and electrical properties, applications of carbon nanotubes in – computers, fuelcells, chemical sensor and catalysis – Nano structure crystals of metals and their applications – Preparation of Quantum nano structures – Quantum wells, wires and dots – applications of quantum dot laser - biomedical applications of nanotechnology.

Unit-IV - Bioinorganic Chemistry [12 Hrs]

4.1. Bioinorganic Chemistry: Metal Ions in Biological Systems : Essential and trace metals.Na^+/K^+ Pump, Role of metals ions in biological processes, Transport and Storage of Dioxygen : Heme proteins and oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanins and hemerythrin, model systems, synthetic complexes of iron, cobalt and copper.

4.2. Electron Transfer in Biology: Structure and function of metalloproteins in electron transport processes – cytochromes and ion-sulphur proteins, synthetic models.Nitrogenase : Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and structural evidence, nitrogenases model systems.

Unit-V - Nuclear Chemistry [12 Hrs]

5.1. Nuclear Chemistry: Modes of Radioactive Decay : Orbital electron capture: nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters. Nuclear Reaction: Types, reactions, cross section, Q-value, threshold energy, compound nucleus

theory: high energy nuclear reaction, nuclear fission and fusion reactions as energy sources; direct reactions; photonuclear and thermo nuclear reaction.

5.2.Stellar Energy: Synthesis of elements - hydrogen burning, carbon burning, the e, x, r, p and x processes. Nuclear Reactors: fast breeder reactors, particle accelerators, linear accelerators, cyclotron and synchrotron. Radio Analytical Methods: Isotope dilution analysis, Radiometric Titrations, Radio immuno assay, Neutron activation analysis.

Text Books :

1. J.E. Huheey, Inorganic Chemistry, 5th Edn., Harper International.1993.
2. F.A.Cotton, G.Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.1985.
3. M.F.Purcell, J.C.Kotz, Inorganic Chemistry,Saunder, 1977.
4. N.N.Greenwood , A.Earnshaw , Chemistry of the Elements, 2nd Edn.,BH,1997.
5. J.D.Lee, A New Concise Inorganic Chemistry, 3rd Edn., ELBS, 1987.

Reference Books

1. Mich Wilson, Kamali Kanengara, Geoff smith, Michelle Simmons and Burkherd Raguk, Nanotechnology Basic Science and Energy Technologies, Overseas press(I), N.D.2005.
2. R.W.Hay, Bio Inorganic Chemistry, Ellis Horwood, 1987.
3. Lehninger, Principles of Biochemistry, Van Eikeren, 1982.
4. T.M.Loehr, Iron carriers and Iron proteins, VCH, 1989.
5. Arnikar, Essentials of Nuclear Chemistry, 2nd Edn., Sulthan & Chand Publishers, 1991.
6. Gladstone, Source book of Atomic Energy, 3rd Edn., ELBS, 1986.

SEMESTER -II- GROUP THEORY AND ITS - PCH 807T

APPLICATIONS IN SPECTROSCOPY

Unit I Group theory **[12 Hrs]**

1.1Symmetry elements and symmetry operations – group multiplication table – sub groups, similarity transformation and classes – identifications of symmetry operations and determination of point groups.
1.2 Reducible and irreducible representations – direct product representation.

Unit II Applications of Group theory **[12 Hrs]**
2.1 Orthogonality theorem and its consequences – construction of character table for C_2V and C_3V – hybrid orbital in non linear molecules (CH_1, XeF_4, BF_3, SF_6 and NH_3).
2.2 Determination of representations of vibrational modes in non linear molecules (H_2O, CH_4, BF_3 and NH_3).
2.3 Symmetry selection rules of infra red and Raman spectra – application of group theory for the electronic spectra of ethylene and formaldehyde.

Unit III Properties of Molecules **[12 Hrs]**
3.1 Normal modes – Vibrational Analysis and Characterization of Stationary points – Electrical Properties - dipole moments, optical activity, polarizability.
3.2 Magnetic properties NMR chemical shifts, shielding, spin – spin coupling and hyperfine interactions – Thermodynamic properties – IRC and excited state studies.

Unit IV Spectroscopy – I
4.1 Interaction of matter with radiation – Einstein theory of transition Probability – Rotational spectroscopy of a rigid rotator – diatomic and polyatomic molecules.
4.2 Vibrational spectroscopy – harmonic oscillator – anharmonicity – vibrational spectra of polyatomic molecules – vibrational frequencies – group frequencies – vibrational coupling overtones – Fermi resonance- Raman Spectra.
4.3 Electronic spectra of polyatomic molecules – group symmetry of molecules and selection rules – types of transition – solvent effects.

Unit – V Spectroscopy – II **[12 Hrs**
5.1 Resonance spectroscopy – Zeeman effect – equation of motion of spin in magnetic fields – chemical shift – spin-spin coupling – NMR of simple AX and AMX type molecules.
5.2 calculation of coupling constants - ^{13}C, ^{19}F, ^{31}P NMR spectra – applications – a brief discussion of Fourier transformation in resonance spectroscopy. Splitting of spin energy level in magnetic field – quantum mechanical treatment.

Text Book

1. C. N. Banwell. 1966, Fundamentals of Molecular Spectroscopy, McGraw Hill.
2. K. V. Raman , Group Theory and its Applications to Chemistry, Tata Mcgraw Hill publishing.Co. 5th edition, 1990.

Further reading

Bhattacharaya. Group Theory and its Applications

SEMESTER - II- REAGENTS AND NAMING - EPCH 808Q

REACTIONS

Objective :

- To inculcate the problem solving nature
- To learn about green chemistry

Unit I STEREOCHEMISTRY AND CONFORMATIONAL ANALYSIS [12 HRS]

Recognition of chiral structures – R & S, E & Z nomenclature,(including allene,biphenyl & spiranes), diastereoisomerism in acyclic systems. Conformational analysis of simple cyclic and acyclic system& their effect on reaction. Inter conversion of Fischer, Newman and Sawhorse projections. Assymetric synthesis newer methods. Enantiotopic and diastereotopic ligands and faces.

Unit II COMMON ORGANIC REACTION MECHANISMS [12 HRS]

Methods of determining reaction mechanism – reactive intermediates – carbocations, carbanions, carbenes, nitrenes, arynes and free radicals. Nucleophilic and electrophilic substitutions and additions to multiple bonds. Elimination reactions. Kinetic isotope effects. Hammett equation – Neighbouring group participation.

Unit III SELECTIVE NAME REACTIONS& REARRANGEMENTS [12 HRS]

Hofmann, Schmidt, Lossen, Curtius, Beckmann, Fries, Claisen, Cope rearrangements. Favorskii, Stork – enamine, Mannich, Michael, Baeyer – Villiger, Shapiro, Hoffmann – Loffler – Freytag reactions. Routine functional group transformations. Hydroboration, Hydroxylation, Oppenaur Oxidation, Meerwein - Ponndorf – Verley, Clemmenson, Wolf Kishner and Birch reductions. Simmons – Smith reaction.

Unit IV reagents in organic synthesis & Photochemistry

Uses of complex metal hydrides, Gilman's reagent, LDA, DCC, 1,3-dithiane, trimethylsilyl iodide, tri-n-butyl tin hydride, osmium tetroxide, SeO2, DDQ, Peterson's synthesis, Wilkinson's catalyst, Baker's yeast, Merrifield resin.

Alpha cleavage given by cyclobutanones - beta cleavage reactions, formation of photoenols and photoenolisation, intermolecular hydrogen transfer &intermolecular photo reduction - Photo rearrangements:photo rearrangements of beta-gamma unsaturated ketones, 1,2 acyl shift - 1,3 acyl shift, aza di-pi methane rearrangement

Unit V GREEN CHEMISTRY **[12 HRS]**

Green Chemistry – Genesis and concept of Green Chemistry, Principles, Strategies Alternative Techniques in Organic Synthesis

Use of microwave, ultrasound, ionic liquids, super-critical solvents in organic synthesis; Multi-component reactions

Text Books :

1. P. S. Kalsi. Organic Reaction stereochemistry & Mechanism. 4th edition . New Age International publishers. 2006.
2. Clayden, Greeves, Warren, Wothers. Organic chemistry. Oxford University Press. 2001.
3. Jerry March. Advanced organic chemistry. 4th edition. Wiley Interscience publications. 1999.
4. Paula Yurkanis Bruice. Organic chemistry . 3rd edition Pearson Education Inc. 2001.
5. Peter sykes. A guide book to mechanism in organic chemistry. Orient Long mann. 2002

Reference Books :

1. Seyhan Ege. Organic Chemistry. 3rd edition. D. C. Health & company.
2. Raj. K. Bansal. Organic Reaction Mechanism. 3rd edition Tata Mc. Graw Hill.
3. V. K. Ahluwalia, R. K. Parashar. Organic Reaction Mechanism. 3rd edition. Narosa publishing House.
4. Coxon, Halton; organic photochemistry, Cambridge university press, 1987

Claiden, Grreeves, warren, wothers; organic chemistry, Oxford university press,2001

SEMESTER –II ORGANIC CHEMISTRY PRACTICAL – I - PCH P201

(Total Marks : 100 External Marks: 60 & Internal Marks: 40)

I. Identification of Compounds in a two component mixture and Preparation of their derivatives and Determination of Boiling Points and Melting Points for Compounds and Melting Point for their derivatives.

II. Organic Preparations (Any Six from the followings)

1.Anthraquinone from Anthracene
2.Benzhydrol from Benzophone
3.Methyl Orange from Sulphanilic Acid
4.p-Nitrobenzoic acid from p-Nitrotoluene
5.m-Nitroaniline from m-Dinitrobenzene
6.Diphenylmethane from Benzylchloride
7.p-Chlorotoluene from p-Toluidine
8.1,2,3,4-Trtrahydrocarbazole from Cyclohexanone
9.Preparation of o-Benzyl Benzoic Acid

Quantum of marks in respect of Practical Examinations :

Qualitative Organic Analysis	:	30 Marks
Preparation	:	15 Marks
Record	:	5 Marks
Practical Viva	:	10 Marks
Total	:	60 Marks

Books Recommended:

1. Vogel, A text book of Practical Organic Analysis, ELBS.
2. Raj K. Bansal, Laboratory manual of Organic Chemistry, Wiley Eastern Ltd.
3. Mann and Saunders, Laboratory manual of Organic Chemistry.

SEMESTER – II INORGANIC CHEMISTRY - PCH P202

PRACTICAL – I

1. Semimicro qualitative analysis of mixture containing two common and two rare cations. The following are the cations to be included- W, Se, Te, Mo, Ce, Th, Ti , Zr, V,U, Li
2. Complexometric titrations (EDTA) – Estimation of Ca, Mg and Zn
3. Preparation of the following
    a) Potassium tris (oxalato) aluminate(III)trihydrate
    b) Tris(thiourea)copper(II) chloride
    c) Sodium bis(thiosulphato)cuprate(II)
    d) Tris(thiourea)copper(II) sulphate
    e) Bis(isothiocyanato)dipyridinemanganese(II)

PRACTICAL EXAMINATION

Continuous internal assessment (CIA) (40 marks)

Based on the periodical evaluation of record and experiments assessed by the staff in charge

External Examination (60 marks)

6 Hrs. Exam Total Marks: 60

1. a) Qualitative analysis (semimicro)(:Mix of 4 radicals anions) 20 Marks
   (2 rare +2 common cations)
2. (a) Preparation 10 Marks
   (b) EDTA (complexometric tiration) 20 Marks
3. (a) Practical Record Note Book 5Marks
   (b) Pratical Viva-Voce 5Marks

SEMESTER – II PHYSICAL CHEMISTRYPRACTICALS -1- PCH P203

Experiments in Thermodynamics, colligative properties, phase rule,Surface Phenomenon, chemical equilibrium and chemical kinetics. Typical examples are given and a list of experiments is also provided from which suitable experiments can be selected as convenient.

1. Verification of Arrhenius equation
2. Determination of activity and activity coefficient fromfreezing point depression method.
3. Construction of vapour pressure curves for different types of solutions.
4. Molecular modeling
5. Simulations to find out symmetry of the molecule
6. Simulations to find vibrational modes and verification by using group theory.
7. Effect of ionic strength of solvents and solutions.
8. Phase diagram construction involving two component systems.
9. Adsorption isotherm
10. Reaction rate and evaluation of other kinetic parameters using polarimetry, analytical techniques and conductometry.

DETAILS OF LIST OF EXPEIMENTS FOR PHYSICAL CHEMISTRY PRACTICAL – I

1. Determine the temperature coefficient and energy of activation of hydrolysis of ethyl acetate.
2. Study the inversion of cane sugar in the presence of acid using polarimeter.
3. Study the effect of ionic strength on the rate of saponification of an ester.
4. Study the salt effect, solvent effect on the rate law of alkaline hydrolysis of crystal violet.
5. Determine the molecular weight of benzoic acid in benzene and find the degree of association.
6. Determine the activity coefficient of an electrolyte by freezing point depression method.
7. Study the phase diagram from toluidine and glycerine system.
8. Construct the boiling point composition diagram for a mixture having maximum boiling point and minimum boiling point.
9. Determine the partial molal volume of glycine/methanol/formic acid/sulphuric acid by graphical method and by determining the densities of the solutions of different compositions.
10. Determine the strength of hydrogen bond in solutions.

SEMESTER – III ORGANIC CHEMISTRY – III PCH 909S

Unit – I PERICYCLIC REACTIONS (12 hrs)

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3 – butadiene, 1,3,5 – hexatriene and allyl system. Classification. Electrocyclic reactions – cycloadditions and cheleotropic reactions. Sigmatropic rearrangements – Woodward – Hoffmann rules and correlation diagrams.Claisen and Cope rearrangements. Fluxional tautomerism , Ene reaction, Applications of concerted reactions in organic synthesis.

Unit – II ORGANIC PHOTOCHEMISTRY (12 hrs)

Introduction to organic photochemistry ,Photochemical excitations, Fate of the excited molecules, Jablonski diagram, Study of photochemical reactions of alkenes, dienes, aromatic, carbonyl and conjugated systems, Norrish Type-I and IIreactions, Paterno- Buchi reaction, di-pi-methane rearrangement, Applications of photochemical reactions in Organic synthesis.

Unit – III REAGENTS IN ORGANIC SYNTHESIS (12 hrs)

Applications of the following reagents in organic synthesis:AIBN, 9-BBN, DCC, CAN,PCC, Crown ethers, LDA, Lindlar's catalyst, Gilman's reagent, 1,3-Dithiane-Umpolung, Trimethylsilyl iodide, Phase transfer catalysts, Wilkinson's catalyst, Baker yeast, Organo transition metal reagents. Applications of reagents containing silicon, Phosphorus, Sulphur, selenium, palladium, rhodium, and titanium reagents in organic synthesis.

Unit - IV SELECTIVE NAME REACTIONS AND THEIR APPLICATIONS IN ORGANIC SYNTHESIS (12 hrs)

Michael addition , Mannich reaction , sharpless asymmetric epoxidation, Hofmann – Loffler – Freytag reaction , Knoevenagel reaction, Peterson Olefination reaction, Skraup reaction, Barton reaction, Reformatsky reaction,Von Richter reaction, Prevost reaction and Woodward modification of the Prevost reaction.

Unit V AROMATICITY (12 hrs)

Aromaticity of benzenoid, heterocyclic and non benzenoid compounds, Huckel's rule – Aromatic systems with pi electron numbers other than six – non aromatic (cyclo octatetraene etc,) and anti aromatic system (cyclobutadiene etc.) – system with more than 10 pi electrons – Annulenes up to C18 (synthesis of all these compounds is not expected)

Text Books:

1. S. M. Mukherji, "Pericyclic reactions", Mac Millan, India
2. charles H. Deputy abnd Orville, L. Chapmann, "Molecular reaction and photochemistry" Prentice Hall of India Pvt., Ltd., New Delhi.
3. J. D. Coyle, Organic Photochemistry, Wiley, 1985

Reference Books:

1. R.O.C. Norman, J.M. Coxon, Principles of organic synthesis, ELBS publications, 1994.
2. C. K. Ingold, Structure and Mechanism in Organic chemistry, Cornell Univ. Press.
3. F. A. Carey and R. J. Sundberg, Advanced organic chemistry, Plenum publishers Ltd. 2000.
4. Michael Smith, Organic synthesis, McGraw Hill, 1996.

W. Carruthers, J.Coldham, Modern methods of Organic synthesism IV edition, Academic press, 1989.

SEMESTER – III INORGANIC CHEMISTRY – III - PCH 910S

Unit-I - Organometallic Chemistry - I [12 Hrs]

1.1. Organometallic Chemistry: Carbon σ donors: Alkyls and aryls - metalation reactions - Bonding in carbonyls and nitrosyls – Metal carbene and carbyne complexes - Carbon π donors: chain π donor ligands - olefins, acetylene and π-allyl systems - cyclic π donors - synthesis structure and bonding in Metallocenes.

1.2. Organometallic Reactions : Association, substitution, addition and elimination, ligand protonation, electrophilic and nucleophilic attack on ligands. Carbonylation and Decorbonylation, oxidative addition, reductive elimination and fluxionality.

Unit-II - Organometallic Chemistry – II [12 Hrs]

2.1. Organometallic Chemistry - Catalysis: Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or Rhodium catalysts (oxo process), oxidation of olefins to aldehydes and ketones (Wacker process)

2.2. Polymerization of Olefins: Polymerization (Zeigler – Natta Catalyst); cyclo oligomerisation of acetylene using nickel catalyst (Repee's Catlyst); polymer- bound catalysts- Olefin metathesis-ROM & RCM.

Unit-III - Inorganic Spectroscopy - I [12 Hrs]

3.1. Inorganic Spectroscopy: Applications to inorganic systems of the following : ultraviolet, visible, infra-red and Raman spectra of metal complexes, organometallic and simple inorganic compounds with special reference to coordination sites, isomerism.

3.2. Magnetic Susceptibility and measurements – Guoy method, Faraday method, VSM and their applications.

Unit-IV- Inorganic Spectroscopy - II [12 Hrs]

4.1. Inorganic Spectroscopy: ESR introduction – Zeeman Equation, g-value, nuclear hyperfine splitting, interpretations of the spectrum, simple carbon centered free radicals. Anisotropy-g-value and hyperfine splitting constant. McConnel's equation, Krammer's theorem. ESR of transition metal complexes of copper, manganese and Vanadyl ions.

4.2. Photoelectron spectroscopy (UV and X-ray) – photoelectron spectra – Koopman's theorem, chemical shift and correlation with electronic charges.

Unit-V- Inorganic Spectroscopy -III [12 Hrs]

5.1. Inorganic Spectroscopy: ^{31}P , ^{19}F NMR spectrum of HPF_2, P_4S_3, TiF_4, BrF_5, SF_4, SIF_6^{2-}, $B_3H_8^-$, NF_3, ClO_4^-, $P_4N_4Cl_4F_2$, ClF_3 Phosphorous and Hypophosphorous acid systems - shift reagents.

5.2. NQR - Principles and applications of NQR - Mossbauer spectra – Principle, chemicals shift, Doppler shift - Mossbauer spectra of Fe and Sn systems.

Text Books :

1. J.E. Huheey, Inorganic Chemistry, 5th Edn., Harper International.1993.
2. F.A.Cotton, G.Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.1985.
3. M.F.Purcell, J.C.Kotz, Inorganic Chemistry,Saunder, 1977.
4. R.S.Drago , Physical methods in Inorganic Chemistry , 2nd Edn, ELBS, 1985.

Reference Books :

1. P.Powell, Principles of Organometallic Chemistry, 2nd Edn., ELBS,1991.
2. C.Elshenbroich , A.Slazer , 2nd Edn., VCH, 1992.
3. R.S.Drago , Physical methods in Spectroscopic Techniques, 2nd Edn, ELBS, 1985.

SEMESTER – III STATISTICAL THERMODYNAMICS - PCH 911S AND ITS APPLICATIONS

Unit I Statistical thermodynamics I [12 Hrs]

1.1 Objectives of statistical thermodynamics – concept of thermodynamics and mathematical probabilities – distribution of distinguishable and non distinguishable particles.

1.2 Maxwell Boltzmann , Fermi – Dirac and Bose Einstein statistics – comparison and applications – modes of contribution to energy – Ortho and Para hydrogen – radiation law – electron in metals.

Unit II Statistical thermodynamics II [12 Hrs]

1.1 The partition function –Boltzmann distribution –the interpretation of the partition function – examples of partition function.

1.2 Partition function evaluation of translational, vibrational and rotational partition functions for mono, diatomic and polyatomic ideal gases.

1.3 Thermodynamic functions in terms of partition functions, isotope exchange and dissociation of diatomic molecules – application of partition functions to heat capacities of ideal gases – nuclear partition function – Einstein and Debye models.

Unit III Statistical thermodynamics III [12 Hrs]

Statistical mechanics of ensemble – thermodynamic functions of ensemble- canonical ensemble- properties of canonical ensemble- grand canonical ensemble- micro canonical ensemble.

Unit IV Thermodynamics I [12 Hrs]

4.1 Partial molar properties – Partial molar free energy (Chemical Potential) – Partial molar volume and Partial molar heat content – Their significance and determination of these quantities - Variation of chemical potential with temperature and pressure.

4.2 Thermodynamics of real gases – gas mixture – definition of fugacity – determination of fugacity – variation of fugacity with temperature and pressure.

Unit V Thermodynamics II [12 Hrs]

5.1 Thermodynamics of ideal and non ideal binary solutions – dilute solutions.

5.2 Excess function for non ideal solutions and their determination – the concept of activity and activity coefficients – determination of standard free energies – choice of standard states – determination of activity and activity coefficients for electrolytes by EMF vapour pressure measurements.

5.3 Gibbs Duhem equation and solubility product method – Thermodynamic equilibrium – Three component system.

Text Books:

1. M.C. Gupta. Statistical thermodynamics. 2nd edition.
2. Rajaram and J.C. Kuriacose, Thermodynamics For Students Of Chemistry, New Delhi: Lal Nagin Chand , 3rd editon1986.

Further reading;

P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford 3rd edition, 1983.

SEMESTER – III PHYSICAL METHODS IN - EPCH 912S
ORGANIC CHEMISTRY

UNIT – I UV – VISIBLE SPECTROSCOPY (12 hrs)

Ultraviolet – Visible spectroscopy – Various electronic transitions – Beer-Lambert law,effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Woodward-Fieser rulesfor conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Octant rule, Applications of ORD and CD to stereochemical
assignments.

UNIT – II INFRA RED SPECTROSCOPY (12 hrs)

Infra red spectroscopy – Instrumentation and sample handling. Vibrational frequencies of different functional groups. Effect of hydrogen bonding and solvent on vibrational frequencies, overtones,combination bands and Fermi resonance. FT – IR. IR of gases,solids and polymeric materials.

UNIT – III MASS SPECTROMETRY (12 hrs)

Introduction, ion production – EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, of common functional groups, molecular ion peak, base peak, isotope peaks, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

UNIT – IV ^{1}H -NMR SPECTROSCOPY (12 hrs)

Basic principles. Macroscopic magnetization. General introduction to NMR techniques – CW and FT NMR techniques, magnetic anisotropy,^{1}H NMR spectral parameters – chemical shift, coupling constant, factors affecting chemical shift,coupling constant. Karplus eqution. Proton NMR spectra of simple organic molecules. Simplification of complex spectra. Nuclear Overhauser effect (NOE). Identification of Homotopic, diastereotopic and enentiotopic protons.

UNIT – V ^{13}C NMR SPECTROSCOPY (12 hrs)

^{13}C NMR – proton decoupled and off-resonance spectra. Factors affecting ^{13}C chemical shift – electronegativity. ^{13}C NMR spectra of simple organic molecules. DEPT and SEFT spectra. 2D NMR techniques ^{1}H -^{1}H COSY, ^{1}H - ^{13}C COSY spectra.

Text Books :

1. R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectrometric Identification of Organic compounds, John Wiley.,1997
2. D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw – Hill, 1998.
3. W. Kemp, Spectroscopy, Macmillan Ltd.,1994.

References:

1. J. R. Dyer, Application of spectroscopy of Organic Compounds, Prentice Hall.
2. JagMohan, Spectroscopy of Organic compounds, Narosa Publications.
3. Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rd edition, Brooks/Cole Pubs. Co.

SEMESTER – III HUMAN RIGHTS - ECHR901S

Unit I

Definition of human rights-nature content-characterizes of human rights-classification of human rights-historical development of human rights-reasons for human rights studies today

Unit II

International human rights norms-humanitarian law-declaration covenants-international covenant on economic, social and cultural rights,international convenants on civil and political rights-optional protocol to the international covenant on civil and political rights-human rights treaties,enforcement of human rights law ,universal jurisdiction.

Unit III

International bodies-the united nation organization ,human rights council,other treaty bodies-amesty international –helsinki declaration –regional human rights-africa,America,asia,Europe&oceania.

Unit IV

Contemporary issues on human rights-human right violations-children's rights-women's rights-scheduled caste-minority rights –bonded lalour and wages, torture and death.

Unit v

Human rights and the Indian constitution, fundamental rights in Indian constitution – directive principles of state policy-fundamental duties.

Various commission; National Human Rights Commission- National commission for Women-Women's Rights in India-Consumers protection Act-Rights to information Act- Public Litigation Act and Rights to Education Act.

Reference Books;

1. Human rights in developing society-Sankar Sen
2. Teaching of human rights-Sergio Baradat Swaronjali Ghosh

SEMESTER – III ORGANIC CHEMISTRY - PCH P304S

PRACTICALS –II

(External Marks : 60 & Internal Marks : 40)

1.a)Preparation of organic compounds involving two stages.
b) Isolationof natural products
i) Isolation of Lycopene from Tomato
ii) Isolation of Citric acid from Lemon
iii) Isolation of Caffeine from Tea .

2. Quantitative Organic analysis
i) Estimation of Phenol
ii) Estimation of Aniline
iii) Estimation of Glucose

Quantum of marks in respect of the Practical Examinations:

1. Preparation and Isolation	20 marks
2.Estimation	25 marks
3. Viva-voce	5 marks
4. Record	10 marks
Total	60 marks.

BOOKS RECOMMENDED:

1. Mann and Saunders, Laboratory manual of Organic Chemistry.
2. Vogel's Quantitative Organic Analysis.
3. R.M. Silverstein, G.C. Bassler and T.C. Morrill, Spectrometric Identification of Organic compounds, John Wiley.,1997
4. D.H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw – Hill, 1998.

SEMESTER – III INORGANIC CHEMISTRY - PCH P305

PRACTICALS –II

- Preparation of coordination complexes , characterization of the products by UV Spectroscopy

a) Sodium hexanitrocobaltate(III)
b) Chloropentamminecobalt(III) chloride
c) Hexamminecobalt(III) chloride
d) Hexamminenickel(II) chloride
e) Potassium tetrachlorocuprate(II)

- Spectral interpretation of some inorganic compounds

3. Colorimetric estimation of metal ions (Fe,Cu,Ni)

4. Estimation of metal ions by Gravimetric and Volumetric analysis(Cu,Ni,Zn,Fe)

EVALUATION PATTERN

Continuous internal assessment (CIA) (40 marks)

Based on the periodical evaluation of record and experiments assessed by the staff in charge

External Examination (60 marks)

6 Hrs. Exam — Total Marks: 60

1. Estimation of metal ions by Gravimetric analysis - 30 marks
2. Volumetric analysis –20 marks
3. Viva Voce – 5 marks
4. Record – 5 marks

SEMESTER – III PHYSICAL CHEMISTRY - PCH P306

PRACTICALS –II

I. **Pulse Polorography.**
1. Determination of Half wave potential of Cd ion in KCl.
2. Determination of Half wave potential of Zn & Mn.
3. Determination of Pb and Cu in Steel.
4. Determination of Ni, Zn and Fe.
5. Analysis of Cu based Alloys.
6. Stability constants for complexes (Pb Oxalate complexes).

II. **UV- Visible Spectrophotometer**
1. Determination of concentration of Potassium Nitrate.
2. Determination of molar extinction coefficient of Potassium dichromate and Potassium permanganate.
3. Determination of concentration of para acetamol in antipyretic drug.

III. **Nephelometer**
1. Nephelometric determination of Sulphate.
2. Nephelometric determination of Phosphate.

IV. Conductometric Titrations.
1. Determination of strength of weak acid (CH_3COOH Vs NaOH)
2. Determination of strength of strong acid (HCl Vs NaOH).
3. Determination of strength of mixture of acids (HCl+CH_3COOH Vs NaOH)
4. Determination of End point in the Precipitation titration (KCl Vs $AgNo_3$)
5. Verification of Ostwald's dilution law.
6. Verification of Onsager's equation.

V. Potentiometric Titrations.
1. Determination of pH of buffer using Quinhydrone elelctrode.
2. Determination of pKa of weak acid using Std. NaoH solution.
3. Determination of strength of FAS using Redox titration (FAS Vs $KMnO_4$).
4. Determination of Single Electrode potential.
5. Determination of strength of strong acid (HCl Vs NaOH).
6. Determination of strength of weak acid (CH_3COOH Vs NaOH)
7. Determination of End point in the Precipitation titration (KCl + KI Vs $AgNo_3$)

VI. **Computational Chemistry.**

1. Computing atomic charges for H_2O molecule by AIM method.
2. Computing molecular orbital coefficients of 1,3-cyclo butadiene by HF method.
3. Geometry optimization of H_2O by HFSCF method.

Scheme of evaluation: (total = 60 marks)

Aim & short procedure	– 10
Record	– 10
Experiment & manipulation	- 30
Viva voce	– 10
Total	- 60

SEMESTER – IV ORGANIC CHEMISTRY – IV PCH 1013S

UNIT – I: ALKALOIDS AND BIO ORGANIC CHEMISTRY

Total synthesis of quinine, morphine , reserpine, cocaine, hygrine and reticulene
Nucleic acids: Types of nucleic acids – DNA & RNA polynucleotide chain. Components –Structure and role of (genetic code) DNA and RNA (Nucleotides only)
.

UNIT – II: PROTEINS

Peptides and their synthesis – synthesis of tripeptide. Merrifield synthesis, End group analysis of peptides, Primary,Secondary and tertiary structure of proteins, Determination of tertiary structure of proteins.

UNIT – III: MODERN SYNTHETIC METHODS, REACTIONS AND REAGENTS

Principles and synthetic processes involving phase transfer catalysis, (Nitriles from Alkyl halides, Alcohol from Alkyl halides) Polymer supported reagents(Synthesis of oligo saccharides), (Microwave assisted Organic synthesis – Esterification, deacetification and hydrolysis)Synthesis of simple organic molecules using standard reaction like acetylation,alkylation of enamines and active methylene compounds, Grignard reactions, Phosphorus and sulphur ylides,Protection and deprotection of functional groups(R-OH, R-CHO, RCO-R , R-NH_2 and R-COOH).

UNIT-IV:

PLANNING ORGANIC SYNTHESIS AND RETROSYNTHETIC ANALYSIS

An introduction to retrosynthesis – Synthon, Synthetic equivalent, Target molecule, Functional group interconversion – Disconnection approach – One group disconnection – Disconnection of simple alcohols, olefins and ketones – Logical and illogical disconnections, Two group disconnection –1,2 – 1,3 – 1,4 – 1,5 and 1,6 – dioxygenated skeletons and dicarbonyls. Retro Diels – Alder reactions.(Synthesis of the following target molecules: cyclohex-3-ene carbaldehyde, 1-phenylpentan-3-one,1-bromo-3-methylbut-2-ene,(E)-3-(4-nitrophenyl)acrylaldehyde,Pentane-2,4-dione,ethyl-2-oxocyclopentane carboxylate,nonane-3,7-dione, 2-amino-3-methyl butanoic acid,2,3-dimethylbutane-2,3-diol)

UNIT- V: HETEROCYCLES, VITAMINS AND STEROIDS

Imidazole, Oxazole, Thiazole, Flavones, isoflavones, anthocyanins, pyrimidines (cytocine and L racil only) and purines(adenine, Guanine only). Synthesis of parent and simple alkyl or aryl substituted derivatives are expected. Synthesis of vitamin A1 (Reformatsky and Wittig reaction methods only). Conversion of cholesterol to progesterone, estrone and testosterone.

RECOMMENDED BOOKS

1. Guidebook to organic synthesis by Ramond K. Mackie and David M. Smith, ELBS Publication.
2. Chemistry of alkaloids by Pelletier .
3. Introduction to alkaloids by G.A Swan
4. Organic chemistry V Edition, 1986, Vol – II by I.L. Finar, ELBS Publication
5. Biochemistry by Lubert Stryer,WH.Freeman and Co., New York
6. Organic Synthesis by R.E. Ireland, Prentice Hall of India, Geol Publishing House
7. Principles of organic synthesis by R.O.C . Norman,Champan and Hall,NY, 1980
8. Advanced Organic Chemistry by Francis .A.Carey, Richard J.Sandberg, 3rd Edition, Plenum, Press, New York,1990
9. Advanced Organic Chemistry by Jerry March, IV edition, Wiley Eastern Ltd., New Delhi

Workbook for organic synthesis , The disconnection approach by Stuart Warren, John Wiley & Sons (Asia) Pvt. Ltd.,

SEMESTER – IV INORGANIC CHEMISTRY – IV PCH 1014

Unit-I Reaction mechanism of Transition metal complexes-I [12 Hrs]

1.1 Energy profile of a reaction, inert and labile complexes , substitution reactions of octahedral complexes - , acid hydrolysis , base hydrolysis , conjugate base mechanism , anation reactions.

1.2 Synthesis of Platinum & Cobalt complexes by substitution reactions.

Unit-II - Reaction mechanism of Transition metal complexes-II [12 Hrs]

2.1 Substitution reactions in square planar complexes, mechanism of Substitution reactions- trans effect – theories of trans effect. Reactivity of Platinum complexes, influences of entering , leaving and other groups and central metal ion.

2.2 Inorganic Photochemistry: photo-substitution, photoredox & isomerisation process, application of metal complexes in solar energy conversion.

Unit-III - Electron transfer reactions [12 Hrs]

3.1 Electron transfer reactions: Outer and Inner sphere processes, atom transfer reaction. Formation and rearrangement of precursor complexes, the nature of binding ligand , successor complexes, Marcus theory.

3.2 Complementary, Non-complementary and two electron transfer reactions.

Unit-IV – Solid State Chemistry - I [12 Hrs]

4.1 Solid state reactions : General principles , experimental procedures , coprecipitation as a precursor to solid state reactions , kinetics of solid state reactions.

4.2 Crystal defects and non stoichiometry: perfect and imperfect crystals , intrinstic and extrinsic defects – point defects , line and plane defects , – schottky defects and Frenkel defects. Thermodynamics of schottky defects and Frenkel defect formation , colour centres , non stoichiometry defect.

Unit- V Solid State Chemistry – II [12 Hrs]

5.1 Electronic Properties and Band Theory, band structure of metals , insulators and semiconductors. , intrinstic and extrinsic semiconductors, doping semiconductors, super conductors.

5.2 Optical properties- Optical reflectance , photoconduction- photoelectric effects Magnetic properties- Classification of materials : para, dia, ferro , ferri , antiferro magnetism - magnetic domains , hysteresis.

Text Books :

1. J.E. Huheey, Inorganic Chemistry, 5th Edn., Harper International.1993.
2. M.F.Purcell, J.C.Kotz, Inorganic Chemistry,Saunder, 1977.
3. W.R.West, Solid State Chemistry and its Applications, John Wiley and Sons, New York, 1984.

Reference Books :

1. G.J.Ferraudi, Inorganic Photochemistry,1973.
2. A.W.Adamson, E.D.Fleishcer, Concepts in Inorganic Photochemistry, 1963.
3. L. E. Smart, E. A. Moore, Solid State Chemistry – An introduction 3rd ed, Taylor and Francis group 2005 .
4. F.A.Cotton, G.Wilkinson, Advanced Inorganic Chemistry, 5th Edn., John Wiley.1985.
5. H.V.Keer, Principles of Solid State, Wiley Eastern Limited, 1993.

SEMESTER – IV Reaction kinetics, Electrode kinetics and Photo chemistry PCH 1015T

Unit I Chemical Kinetics I

1.1 Effect of temperature on reaction rates – collision theory of reaction rate – molecular beams – collision cross sections – effectiveness of collisions – probability factor.

1.2 Potential energy surfaces – partition function and activated complex – erying equation – estimation of free energy, enthalpy and entropy of activation and their significance.

1.3 Reactions in solutions – effect of pressure, dielectric constant and ionic strength on reactions in solutions – kinetic isotope effects.

1.4 Acid base catalysis – mechanism of acid base catalysed reactions – Bronsted catalysis law.

Unit II Chemical Kinetics II

2.1 Kinetics of complex reactions, reversible reactions, consecutive reactions, parallel reactions, chain reactions – general treatment of chain reactions – chain length – rice Herzfeld mechanism – explosion limits.

2.2 Catalysis by enzymes – rate of enzyme reactions – effect of substrate concentration, pH and temperature on enzyme catalysed reactions – Inhibition of enzyme catalysed reactions.

2.3 Study of surfaces – Langmuir and BET adsorption isotherms – study of kinetics of surface reactions – catalytic by metals, semiconductor oxides – mechanism of heterogeneous catalytic reactions – the absorption coefficient and its significance.

2.4 Study of fast reactions – relaxation methods – temperature and pressure jump methods – stopped flow and flash photolysis methods.

Unit – III Electrode Kinetics

3.1 Mean ionic activity and mean ionic activity coefficient – concept of ionic strength, Debye- Huckel theory of strong electrolytes – activity coefficient of strong electrolytes – determination of activity coefficient by electrical method – Debye – Huckel limiting law qualitative and quantitative verification – limitation of Debye Huckel limiting law at appreciable concentrations of electrolytes – Huckel equation – Debye – Huckel – Bronsted equation.

3.2 Electrode – electrolyte interface – adsorption at electrified interface – electrified double layer – electro capillary phenomenon – Lipmann equation – structure of double layers – Helmholtz – Perrin, Guoy – Chapman and Stern model of electrical double layers.

3.3 Irreversible thermodynamics – forces and fluxes – linear force – flux relation – phenomenological equations – Onsagers theorem diffusion – electro kinetic phenomena – membrane potential.

Unit IV Photochemistry – I

4.1 Absorption and emission of radiation – Franck – Condon Principle – decay of electronically excited states – Jablonski diagram – radiative and non radiative processes – fluorescence and phosphorescence – spin forbidden radiative transition – internal conversion and intersystem crossing – energy transfer process.

4.2 Kinetics of unimolecular and bimolecular photo physical processes – excimers and exciplexes – static and dynamic quenching – Stern Volmer analysis.

Unit V Photochemistry II **[12 Hrs]**

a. Experimental methods – quantum yield and life time measurements – steady state principle – quantum yield and chemical actinometry.

b. Kinetics of photochemical reactions: hydrogen and halogen reactions, photoredox, photo substitution, photoisomerisation and photosensitized reactions – photovoltaic and photo galvanic cells, photo assisted electrolysis of water, aspects of solar energy conversion.

c. Radiation chemistry – Interaction of high energy radiation with matter – primary and secondary processes – G value – radiolysis of water – hydrated electron.

Text books

1. K.J. Laidler, Chemical Kinetics. New York: Harpet and Row, 2nd Indian edition.., 1987.
2. K.K. Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern Ltd, 1978.

Further reading;

J.Rajaram and J.C.Kuriacose, kinetics and mechanism of chemical transformation. India: Macmillan India Ltd. 1993.

JPCH1016 PROJECT

JPCH1017 SEMINAR & PAPER PRESENTATION