## **SEMESTER – I ORGANIC CHEMISTRY-1- PCH701S**

#### **Objective:**

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

#### Unit I: STEREOCHEMISTRY -I

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**

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**

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

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.

#### (12 hrs)

#### (12 hrs)

(12 hrs)

# (12 hrs)

#### 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<sub>2</sub>, 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<sub>4</sub>, NaBH<sub>4</sub>, 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, 6<sup>th</sup> 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.

[12 Hrs]

## SEMESTER – I INORGANIC CHEMISTRY – I - PCH702S

#### Unit- I - Isomerism in Coordination Complexes - ORD and CD

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

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

- 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

- 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  $\text{Re}_2\text{Cl}_8^{2-}$  and  $\text{Mo}_2\text{Cl}_8^{2-}$  -Three atom clusters –  $\text{Re}_3\text{Cl}_{12}^{3-}$  and  $\text{Fe}_3\text{CO}_{12}$  – Four atom tetrahedral clusters –  $\text{Co}_4\text{CO}_{12}$  and Ir<sub>4</sub>CO<sub>12</sub> - Six atom clusters Rh<sub>6</sub>CO<sub>16</sub>.

#### - Polyacids and Inorganic polymers Unit-V

- 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.

[12 Hrs]

# [12 Hrs]

[12 Hrs]

#### **Text Books :**

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

#### **Reference Books**

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

## SEMESTER - I QUANTUM MECHANICS AND MOLECULAR - PCH 703T STRUCTURE

## Unit I Quantum Chemistry I

- 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

- 1.1 The harmonic Oscillator the rigid rotor particle in a ring Schrodinger equation for hydrogen atom (no derivation is required) and the solution.
- **1.2** The origin of quantum numbers (angular momentum and spin) their physical significance.

## **Unit – III Quantum Chemistry**

- 1.1 Approximation methods perturbation and variation methods application to hydrogen, helium atoms R.S. Coupling and term symbols for atoms in the ground state.
- 1.2 Born Oppenheimer approximation valence bond theory for Hydrogen molecule LCAO MO theory for diatomic and polyatomic molecules.
- 1.3 Concept of hybridization Huckel theory for conjugated molecules (ethylene, butadiene and benzene)

## Unit IV Empirical MO theory

- 1.1 The simple Huckel method Assumptions Determinant, Energies and wave functions Extended Huckel method overlap population analysis.
- 1.2 FMO theory Interaction and Walsh diagrams- examples benzene,naphthalene, butadiene and cyclo butadiene.

## Unit V

- 5.1 Basics of Popular quantum chemical calculations: Hamiltonian and wave functions Roothan's equations.
- 5.2 Semi empirical methods slater orbital and HF- SCF methods.

## **Text Books**

R. K. Prasad, Quantum Chemistry, Wiley Eeastern, New Delhi, 2<sup>nd</sup> edition, 1992.

**Further reading** P.W. Atkins, Molecular Quantum Mechanics, Oxford University Press, Oxford 3<sup>rd</sup> edition, 1983

# [12 Hrs]

## [12 Hrs]

[12 Hrs]

## SEMESTER – I BIOINORGANIC AND - EPCH 704T SUPRAMOLECULAR CHEMISTRY

#### Unit – I

Metal Storage Transport and Biomineralization. Ferritin, Transferrin, and siderophores
 Calcium in biology

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

#### Unit – II

 $\begin{array}{l} 2.1 \ Metalloenzymes-zinc\ enzymes-carboxypeptidase\ and\ carbonic\ anhydras.\ Iron\ enzymes-catalase,\ peroxidase\ and\ cytochrome\ P-450.\ Copper\ enzymes-superoxide\ dismutase.\\ Molybdenum\ oxatransferase\ enzymes-xanthine\ oxidase.\ Coenzyme\ vitamin\ B_{12} \end{array}$ 

#### 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, 5<sup>th</sup> 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.
- Albert L. Lehninger, David Lee Nelson, Michael M. Cox, Principles of Biochemistry, 4<sup>th</sup> 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

#### **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.

**12 HRS** 

## UNIT – IV AROMATIC ELECTROPHILIC SUBSTITUTION

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, 6<sup>th</sup> 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, 3<sup>rd</sup> 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.

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, Evidences of metal- ligand covalency, TASO-MO concepts of Oh and Td complexes, MO energy level diagrams of sigma- and pi-bonding in Oh complexes, nature of metal- ligand pi-bonds, evidences for pi-back bonding, spectochemical series, and pi-acceptor series. 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<sup>1</sup>-d<sup>9</sup> 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**

- **3.1** Nanotechnology Introduction preparatory methods chemicals methods, thermolysis, pulsed laser method Microwave Synthesis -Basic concepts of Nano science and technology Quantum wire Quantum well Quantum dot Properties and technological advantages of Nano materials Carbon Nanotubes and applications Principles of SEM, TEM and AFM.
- **3.2** Biomedical applications of nanotechnology.

## **Unit-IV - Bioinorganic Chemistry**

#### [12 Hrs]

- 4.1 Bioinorganic Chemistry: Metal Ions in Biological Systems : Essential and trace metals.Na<sup>+</sup>/K<sup>+</sup> 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,
- 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, 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, 5<sup>th</sup> Edn., Harper International.1993.
- F.A.Cotton, G.Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edn., John Wiley.1985.
- 3. M.F.Purcell, J.C.Kotz, Inorganic Chemistry, Saunder, 1977.
- 4. Mick Wilson, Kamali Kannangara, Michells Simmons and Burkhard Raguse, "Nano Technology – Basic Science and Emerging Technologies", 1st edition, Overseas Press,New Delhi,2005.
- Arnikar, Essentials of Nuclear Chemistry, 2<sup>nd</sup> Edn., Sulthan & Chand Publishers, 1991.
- 6. R.W.Hay, Bioinorganic chemistry, Ellis Harwood, 1987.
- 7. A.K.Das, Inorganic Chemistry

## **Reference Books**

- 1. Mich Wilson, Kamali Kanengara, Geoff smith, Michelle Simmons and Burkherd Raguk, Nanotechnology Basic Science and Energy Technologies, Overseas press (1), 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. Gladstone, Source book of Atomic Energy, 3<sup>rd</sup> Edn., ELBS, 1986.
- 6. N.N.Greenwood , A.Earnshaw , Chemistry of the Elements, 2<sup>nd</sup> Edn.,BH,1997.

## SEMESTER – II Group theory and its applications in Spectroscopy PCH 807T

## **Unit I Group theory**

## [12 Hrs]

[12 Hrs]

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

## **Unit II Applications of Group theory**

- 2.1 Orthogonality theorem and its consequences construction of character table for C<sub>2</sub>V and C<sub>3</sub>V – hybrid orbital in non linear molecules (CH<sub>1</sub>, XeF<sub>4</sub>, BF<sub>3</sub>, SF<sub>6</sub> and NH<sub>3</sub>).
- 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**

- 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.

## 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

- 5.1 Resonance spectroscopy Zeeman effect equation of motion of spin in magnetic fields – chemical shift – spin-spin coupling.
- 5.2 calculation of coupling constants <sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>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. 5<sup>th</sup> edition, 1990.

## **Further reading**

Bhattacharaya. Group Theory and its Applications

## [12 Hrs]

#### SEMESTER – II REAGENTS AND NAMING REACTIONS EPCH808Q

**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

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**

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

## [12 HRS]

# [12 HRS]

#### **Text Books :**

- 1. P. S. Kalsi. Organic Reaction stereochemistry & Mechanism. 4<sup>th</sup> edition . New Age International publishers. 2006.
- 2. Clayden, Greeves, Warren, Wothers. Organic chemistry. Oxford University Press. 2001.
- 3. Jerry March. Advanced organic chemistry. 4<sup>th</sup> edition. Wiley Interscience publications. 1999.
- 4. Paula Yurkanis Bruice. Organic chemistry . 3<sup>rd</sup> 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. 3<sup>rd</sup> edition. D. C. Health & company.
- 2. Raj. K. Bansal. Organic Reaction Mechanism. 3<sup>rd</sup> edition Tata Mc. Graw Hill.
- **3.** V. K. Ahluwalia, R. K. Parashar. Organic Reaction Mechanism. 3<sup>rd</sup> edition. Narosa publishing House.

**4.** Coxon, Halton; organic photochemistry, Cambridge university press, 1987 Claiden, Grreeves, warren, wothers; organic chemistry, Oxford university press,2001

## **ORGANIC CHEMISTRY PRACTICAL – I PCH P201**

**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 Analys	is	:	30 Marks
Preparation		:	15 Marks
Record		:	5 Marks
Practical Viva		C	10 Marks
]	Fotal	÷	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.

#### **INORGANIC CHEMISTRY PRACTICAL – I PCH P202S**

#### **Objectives**

- 1. To improve the skill in quant itat ive est imat ion of metal ions by complexometr ic titration.
- 2. To ident ify the methodology to quantitat ively separate and est imate mixture of metal ions.
- 3. To improve the skill in synthesis of inorganic compounds.
- 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 method) Estimation of Ca, Mg and Zn.
- 3. Preparation of the following
  - a) Potassium tris(oxalato)aluminate(III)hydrate
  - b) Sodium bis(thiosulphato)cuprate(II)
  - c) Tris(thiourea)copper(I) sulphate
  - d) Diisothiocyanatodipyridine manganese(II)
  - e) Tetramminecopper(II) sulphate

## PHYSICAL CHEMISTRYPRACTICALS -I 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.