

**Course No: CH14401CR**  
**Title: Organo-Transition Metal Chemistry (04 Credits).**

*Max. Marks: 100*  
*External Exam: 80 Marks.*

*Duration: 64 Contact hours*  
*Internal Assessment: 20 Marks*

**Unit-I** **(16 Contact hours)**

**Sigma Bonded Organometallic Compounds:**

Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways:  $\alpha$  and  $\beta$  hydrogen transfer. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung. Metal Hydride Complexes: Synthesis, Characterization and Chemical reactions, Non-classical Hydrides (Kubas complexes).

**Unit-II** **(16 Contact hours)**

**Pi-bonded Organometallic Compounds:**

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.

Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, Structure and bonding of Ferrocene.

Compounds with Transition Metal to Carbon multiple bonds: Alkylidene (Schrock and Fischer) Synthesis; Structural characteristics; Nature of bonding. Reactions and their synthetic applications.

**Unit-III** **(16 Contact hours)**

**Catalytic Processes involving Transition Metal Organometallic Compounds:**

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.

Asymmetric and supported Organometallic Catalysis (brief idea)

**Unit-IV** **(16 Contact hours)**

**Fluxional Organometallic Compounds and Synthetic Reactions involving Organometallics:**

**Fluxional Organometallic Compounds:**

Characteristics ; Rates of rearrangement and Techniques of study. NMR study of Fluxional behavior, Classification of Fluxional Organometallic Compounds. Mechanism of Fluxionality in compounds of  $\eta^1$  Cyclopentadienyls and  $\eta^3$ -allyls.

Stereochemical non rigidity in case of coordination numbers- 4 & 5 (cis-trans, atomic inversion, Berry Pseudorotation).

### **Synthetic Reactions involving Organo- metallics:**

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules).

Activation of small molecules: Carbon monoxide, Carbon dioxide and Alkanes.

Role of organo-iron as synthons, Carbon-Carbon coupling and its reactions (Suzuki and Heck).

### **Books Recommended:**

- The Organometallic Chemistry of Transition Metals; 2nd edn; Robert. H . Crabtree; Wiley; 1994.
- Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole; 1985.
- Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2000
- Principles and Applications of Organo Transition Metal Chemistry; Collman & Finke; University Science Books; 1994.
- Principles of Organometallic Chemistry; 2nd edn.; P.Powel; Chapman & Hall; 1998.
- Metallo-Organic Chemistry; A.J.Pearson; Wiley.
- Mechanisms of Inorganic and Organo metallic reactions; Twigg; Plenum press 1983.
- Reaction Mechanism of Inorganic and Organometallic systems; 2nd edn.; Robert .b. Jordan 1998.
- Inorganic Chemistry ; 4th edn.; Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;1983
- Modern Inorganic Chemistry; William. A. Jolly; McGraw Hill; 1985.

**Course No: CH14402CR**  
**Title: Photo-Inorganic Chemistry (04 Credits)**

*Max. Marks: 100*  
*External Exam: 80 Marks.*

*Duration: 64 Contact hours*  
*Internal Assessment: 20 Marks*

**Unit-1** **(16 Contact hours)**

**Basics of Photo-Chemistry:**

Absorption; mechanism of absorption of light

Transition moment integral, Einstein's treatment, molar integrated absorption intensity, natural radiative lifetime & the calculation of life times.

Excitation; d-d transition, charge transfer & intraligand transitions and selection rules.

Excited states; term symbols, splitting of terms in ligand field, Orgel diagram; electrostatic description of spin allowed d-d transitions & energy level diagrams depicting excited states.

Frank Condon principle, shapes of absorption & emission bands.

Fate of excited states; energy dissipation by radiative and non-radiative processes. Jablonoski diagram.

Tools and Technique: Light source, measurement of light intensity, chemical actinometry. Flash photolysis.

**Unit-II** **(16 Contact hours)**

**The Chemistry of Excited State Molecules:**

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non-adiabatic. Properties of the excited states; Determination of dipole moments & acidity constants of excited state molecules.

Photosubstitution and photo reduction of Co (III) complexes. Photosubstitution reaction of Cr (III) and Rh (III) complexes.

Organometallic-Photochemistry: Reactions of metal carbonyls, cleavage of metal-metal bond.

**Unit-III** **(16 Contact hours)**

**Redox Reactions by Excited Metal Complexes:**

Energy transfer under conditions of weak and strong interaction. Excited state electron transfer. Marcus-Hush model. Conditions of the excited states to be useful as redox reactants.

Photochemical electron transfer, [Ru (bipy)<sub>3</sub>]<sup>2+</sup> and [Os (bipy)<sub>3</sub>]<sup>2+</sup>.

Photochemical supramolecular devices: devices for photo-induced energy or electron transfer, Devices for information processing, photo-chemically driven molecular machines.

## Unit-IV

(16 Contact hours)

### Solar Energy-Prospects and Challenges:

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO<sub>2</sub> reduction. Inorganic photolithography.

Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

### Books Recommended:

1. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
2. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
3. Inorganic Chemistry; 4\* edn; Huheey; Harper & Row; 1990.
4. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
5. Chemistry of Light; Suppan, Royal Society; 1994.
6. Photochemistry, Carol J. Wayne and Richard P. Wayne; Oxford University Press; 1996.
7. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
8. Inorganic Photochemistry; J.Chem Edu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.

## Course No: CH14403CR

### Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: 100

External Exam: 80 Marks.

Duration: 64 Contact hours

Internal Assessment: 20 Marks

#### A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminechlorocobalt (III) chloride.
- Preparation of trans dichloro bis (ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris (ethylenediamine) nickel (II) chloride dihydrate and its conversion to bis (ethylenediamine) nickel (II) chloride.
- Preparation of bis (acetylacetonato) copper (II) dihydrate.
- Preparation of pentaamminechlorocobalt (III) chloride and study of Linkage isomers by its conversion to pentaamminenitritocobalt (III) chloride and to nitro isomer followed by IR Characterization.

#### B:- Total analysis of a Coordination compound for determination of various components present. (1- Experiment)

#### C: - Separation by Column Chromatography and Estimations: (5 Experiments)

- Separation of Permanganate and Bichromate ions on Alumina column and their Estimation from Beer Law plots.
- Determination of Ionisable chloride in a Complex by cation exchange column (separation followed by Mohr's titration of elute for estimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTA titrations.
- Separation of two Cobalt (III) complexes viz  $[\text{Co}(\text{NH}_3)_6] \text{Cl}_3$  and  $[\text{Co}(\text{NH}_3)_5 \text{Cl}] \text{Cl}_2$  on Silica column.
- Ion exchange separation of Hydration / ionization isomers of Chromium (III) Chloride ( $\text{CrCl}_3$ ).

#### D: - Potentiometric Titrations: (6 Experiments)

- Standardization of an Iron (ii) solution with a standard dichromate solution over Pt & Calomel assembly.
- Determination of purity of Ce (IV) Sulphate with a standard Iron (II) solution over Pt & Calomel assembly.
- Estimation of Iodide with Standard  $\text{AgNO}_3$  over Pt & Calomel assembly using  $\text{I}^- \backslash \text{I}_2$  redox couple.

- Simultaneous determinations of Chloride and Iodide ions with Standard  $\text{AgNO}_3$  over Ag-Glass electrode assembly.
- Determination of the purity of  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$  over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii) solution and in order to establish the composition of the complex  $\text{K}_2\text{Zn}_3[\text{Fe}(\text{CN})_6]_2$

**E: - pH-metric Titrations: (2 Experiments)**

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.

**F: - Conductometric Titrations: (2 Experiments)**

- To determine the solubility and solubility product of a sparingly soluble salt ( $\text{BaSO}_4$ ) in water.
- To determine the basicity of sodium potassium tartarate by Conductometric method.

**G:- Spectrophotometry: (5 Experiments)**

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$  in acidic medium.

**H: - Flame Photometry: (2 Experiments)**

- Simultaneous determination of Sodium and Potassium in the given mixture.
- Determination of Cadmium and Magnesium in tap water.

**Books Recommended:**

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education 2002
- Synthesis and Technique in Inorganic chemistry, G. S. Grlomi; R.J. Angleci 3rd edn.; University Science Books.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI Academic Press.
- Experimental Inorganic / Physical Chemistry; Mounir A. Malati Horwood/1999.
- Quantitative Chemical Analysis; 5th edn.; Harris; Freeman; 1999.
- Advanced Practical Inorganic Chemistry; Adams; Raynor, Wiley; 1995.
- Advanced Experimental Inorganic Chemistry; Ayodha Singh; Campus Books 2002.

**Course No: CH14404CR**  
**Title: Heterocyclic Chemistry (04 Credits)**

*Max. Marks: 100*  
*External Exam: 80 Marks.*

*Duration: 64 Contact hours*  
*Internal Assessment: 20 Marks*

**Unit I (16 Contact hours)**

**Structure and Nomenclature of Heterocyclic compounds:**

Introduction and significance of heterocycles in day to day life.

**Nomenclature of Heterocycles:** Monocyclic, bicyclic and polycyclic heterocycles, Hantzsch-Widman and replacement methods of nomenclature.

**Structural features:** Non-aromatic, aromatic and heteroaromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV, Visible and <sup>1</sup>HNMR).

**Unit II (16 Contact hours)**

**General Approach to Synthesis of Heterocyclic compounds:**

Reactions most frequently used in heterocyclic ring synthesis like C-C bonding, C-heteroatom bonding, typical reactant combinations, Electrocyclic processes in heterocyclic ring synthesis, Nitrenes in heterocyclic synthesis, Hantzsch Pyridine, Skraup quinoline, Bischler-Napieralki Isoquinoline, Knorr Pyrrole, Paal-Knorr, Fischer – Indole synthesis.

**Unit III (16 Contact hours)**

**Monocyclic Heterocycles:**

Structure, Synthesis and Reactions of Oxirane, Thirane, Azetidine, Pyrrole, Furan, Thiophene, Diazenes, Pyrimidines, Pyridine. Chemistry of five membered heterocycles with two heteroatoms like 1,3-Azoles, 1,2- Azoles. Chemistry of Six membered rings like Azines and seven membered heterocycles like Azepine, Oxipene, Thiopins.

**Unit IV (16 Contact hours)**

**Bicyclic Heterocycles:**

Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan, Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

**Recommended Books:**

1. Heterocyclic Chemistry, 5<sup>th</sup> Ed. J.A. Joule and K. Mills, (Wiley-2010).
2. Essentials of Organic Chemistry, Paul M Dewick, (Wiley-2006).
3. Heterocyclic Chemistry, J.A. Joule and G.F. Smith, (Chapman and Hall-1996).
4. The Chemistry of Heterocycles Theophil Eicher and Siegfried Hauptmann, (George Thieme Verlag Stuttgart, New York -1995).
5. Heterocyclic Chemistry, Raj K. Bansal, (New Age International Publisher-2006).
6. Heterocyclic Chemistry, R.R. Gupta, M. Kumar, V. Gupta, (Springer-2006).

**Course No: CH14405CR**  
**Title: Chemistry of Natural Products (04 Credits)**

*Max. Marks: 100*  
*External Exam: 80 Marks.*

*Duration: 64 Contact hours*  
*Internal Assessment: 20 Marks*

**Unit-I** **(16 Contact hours)**

**Terpenoids and Carotenoids:**

Introduction, classification, general methods of isolation and separation and biosynthesis.

*Essential oils:* Separation using Gas Liquid Chromatography and High Performance Liquid Chromatography. Physical, chemical and spectral methods of structure elucidation.

Structure determination, stereochemistry and synthesis of  $\alpha$ -terpineol, abietic acid and  $\beta$ -carotene.

**Unit-II** **(16 Contact hours)**

**Alkaloids:**

Introduction, classification, nomenclature, qualitative tests, pharmaceutical applications and general methods of isolation. Physical, Chemical & Spectral methods of structure elucidation.

Stereochemistry, synthesis and biosynthesis of Quinine, Morphine and Reserpine.

**Unit-III** **(16 Contact hours)**

**Steroids:**

Introduction, nomenclature, classification & stereochemistry. Physical, Chemical & Spectral methods of characterization. Qualitative tests.

*Cholesterol:* Isolation, clinical significance, chemical properties, structure elucidation, total synthesis & relationship with bile acids.

*Sex hormones:* Introduction, isolation, clinical & commercial significance, color reactions, structure determination and partial synthesis of Androsterone, Testosterone and Progesterone.

*Glucocorticoids & Mineral Corticoids:* Introduction and partial synthesis. Mechanism of action and synthesis of cholecalciferol.

**Unit-IV** **(16 Contact hours)**

**Natural Plant Pigments and Porphyrins:**

Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)

*Flavonoids:* Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.



Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercetin & Genestein.

*Porphyrins*: Structure determination and total synthesis of haemoglobin. Structural comparison with chlorophyll.

**Books Recommended:**

1. Chemistry of Natural Products; S. V. Bhat, B. A. Nagasampagin. (Narosa 2005).
2. Organic Chemistry, 5th Ed. Vol.2, I.L. Finar (Addison Wesley Longman-2000).
3. New Trends in Natural Product Chemistry, Atta-ur-Rahman (Harward Academic Press).
4. Chemistry of Natural Products, N.R. Krishnaswamy (University Press-1999).
5. Flavanoids; Oyvind M. Andersen and Kenneth R. Markhan. (Taylor & Francis -2006)

## Course No: CH14406CR

**Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)**

**Max. Marks: 100**

**External Exam: 80 Marks.**

**Duration: 64 Contact hours**

**Internal Assessment: 20 Marks**

### 1. Multistep synthesis of drugs/ organic compounds involving name reactions

- (1) Synthesis of local anesthetics
- (2) Synthesis of analgesics
- (3) Synthesis of sulphur drugs
- (4) Synthesis using microwaves: Alkylation of diethyl malonate with benzoyl chloride
- (5) Skraup synthesis : Preparation of quinoline from aniline.
- (6) Beckmann rearrangement.

### 2. Extraction/Estimation of Organic compounds from natural sources

- (1) Isolation of lycopene and  $\beta$ -carotene from tomato. Characterisation of lycopene/ $\beta$ -carotene by UV-absorption process.
- (2) Isolation of limonene from its natural source and physicochemical analysis.
- (3) Assay of Belladonna for Hyoscyamine.
- (4) Assay of lemon for citric acid and vitamin-C
- (5) Isolation of cholesterol from gallstone
- (6) Assay of coke (soft drink)

### 3. Column Chromatography

Separation of two component solid mixture. Identification using physical, chemical and spectral techniques.

### 4. Spectrophotometric estimation (UV/visible)

- (1) Vitamin-C ( Ascorbic acid )
- (2) Caffeine from tea.
- (3) Cholesterol
- (4) Aspirin

### 5. Electrophoresis/ Paper chromatography

Separation and identification of amino acids by electrophoresis / Paper chromatography.

### 6. Spectroscopy

Identification of Organic compounds through interpretation of their spectra ( UV, IR, PMR, CMR and Mass spectra to be provided).

### Books Recommended :

1. Comprehensive Practical Organic Chemistry, V.K. Ahluwalia, Renu Aggarwal (Univ. Press India Limited -2000 ).
2. Vogel's Text Book of Practical Organic Chemistry, B.S.Furniss, A. J. Hannaford (AWL 5<sup>th</sup> Ed.-1998).
3. Organic Laboratory Techniques , Donald .C. Pavia, Gary . M. Lampman ( SCP 3rdEd.-1999)
4. Experiment Organic Chemistry, John.C. Gilbert., Stephen.F.Martin (SCP -1998 )
5. Advanced Practical Organic Chemistry Vol. II, Jag Mohan ( Himalaya Pub. House First Ed.-1992 V

**Course No: CH14407CR**  
**Title: Computational and Quantum Chemistry (04 Credits)**

*Max. Marks: 100*  
*External Exam: 80 Marks.*

*Duration: 64 Contact hours*  
*Internal Assessment: 20 Marks*

**Unit-I: Numerical Methods (16 hrs)**

Basic theory, discussion of algorithms and errors for following numerical methods:

**a. Solution of Equations: ....5 hrs**

Newton-Raphson method for solving polynomial equations. Gaussian elimination, and Gauss-Siedel method. Pivoting strategy. Convergence. Errors and ill-conditioning.

**b. Numerical calculus and interpolation ....6 hrs**

Solutions of simple differential equations by Taylor series and Runge-Kutta methods.

Numerical Integration: Trapezoidal rule, Simpson's method; Lagrange's interpolation & Cubic splines, errors in integration formulae.

**c. Eigenvalues and Matrix Diagonalization: ... 5 hrs**

Eigenvalue problem, diagonalization of a matrix, Jacobi and Householder methods, analysis of errors.

**Unit-II: Electronic Structure Theory, Hartree-Fock Method (16 hrs)**

Hamiltonian and wave function for multi-electron systems: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis  $H_2$  system.

HF Equation, Fock, Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equation. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure. ...8 hrs

Slater-type orbitals, Gaussian basis sets. Model SCF calculations on  $H_2 / HeH^+$  ...2 hrs

**Configuration Interaction:** Electron correlation, configuration interaction (CI), configuration state functions, Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ methods; Size consistency problem. Moller-Plesset and Coupled Cluster methods.

.....6 hrs

### **Unit-III: Density Functional and Semi-Empirical Methods**

**(16 hrs)**

**Density Functional Theory:** Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, the local density approximation,  $E_x$  &  $E_c$  functionals.

...6hrs

**Semiempirical methods:** The ZDO approximation; brief idea of CNDO, INDO and NDDO methods. Introduction to MNDO, AM1 and PM3 methods.

Molecular mechanics methods, force fields. ...6 hrs

**Molecular Properties:** Basic ideas about molecular geometry and its optimization: quasi-Newton & steepest descent methods. Molecular vibrational frequencies, thermodynamic properties. ...4 hrs

### **Unit- IV: Use of Quantum Chemistry Software : Gaussian**

**(16 hrs)**

A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package..

1. A single point energy calculation: HCHO /CH<sub>3</sub>.CO.CH<sub>3</sub>, HCHO MOs
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization
4. NMR properties of ethane, ethane and ethyne
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, polarizability, hyperpolarizability.
6. Stationary points characterization –C<sub>3</sub>H<sub>5</sub>F
7. Model Chemistries: Basis set effect on HF bond length
8. Selecting an appropriate theoretical method:
  - a) Electron correlation and post SCF methods, limitations of Hartree-Fock theory: HF bond energy, Optimization of O<sub>3</sub>.
  - b) Density Functional Theory: CO<sub>2</sub> structure and atomization energy.
  - c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.
9. Chemical reactions and reactivity:
  - a) Electron densities of substituted benzenes.
  - b) Hydration enthalpy of the reaction  $H^+ + H_2O \rightarrow H_3O^+$
  - c) Potential energy surfaces. Reaction path following (IRC calculation)  
 $CH_2O \rightarrow HCOH$
  - d) Heat of formation of CO<sub>2</sub> via an isodesmic reaction

### **Books Recommended:**

1. Quantum Chemistry , Ira. N. Levine, (Prentice Hall, 2009).
2. Quantum Chemistry , D. A. McQuarrie, (University Science Books, 2007).
3. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
4. Methods of Molecular Quantum Mechanics, R. McWeeny, (Academic Press, 2001).
5. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
6. Molecular Quantum Chemistry - Introduction to Advanced electronic structure theory  
- A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
7. Ab Initio Molecular Orbital Theory, by Hehre, Radom, Schleyer and Pople, (Wiley)
8. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang,  
Oxford(1989).
9. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
10. GAUSSIAN Manual

## Course No: CH14408CR

### Title: Self Assembling Colloidal systems and Advanced Electrochemistry (04 Credits)

*Max. Marks: 100*

*External Exam: 80 Marks.*

*Duration: 64 Contact hours*

*Internal Assessment: 20 Marks*

#### Unit-I

(16 Contact hours)

##### **Self-assembly of surfactants and its consequences:**

**Surfactants and Micelles:** Classification of Surfactants, Solubility of Surfactants: Kraft temperature and cloud point, Micellization of surfactants: critical micelle concentration (cmc), aggregation number, counterion binding, factors affecting cmc in aqueous media. Thermodynamics of micellization: pseudophase model and mass action models. Structure and shape of micelles: geometrical consideration of chain packing, variation of micellar size and shape with surfactant concentration.

**Micellar Solubilization and catalysis:** Introduction, factors affecting micellar solubilization: nature of surfactant/solubilize, effect of additive and temperature. Effect of solubilization on micellar structure, cloud point and cmc of surfactants. Solubilization of drugs into micelles and its importance in drug delivery systems and controlled release. Theoretical consideration of reactions in micellar media. Examples of micellar catalysis for hydrolysis, oxidation and reduction reactions.

#### Unit- II

(16 Contact hours)

##### **Self assembly of block copolymers and polymer-surfactant mixtures:**

**Block Copolymers:** Introduction: classification, micellization of diblock and triblock copolymers. Introduction to co-assembly of block copolymers by electrostatic interactions: formation of polyion or block ionomer complexes. Introduction to pH-, thermo- and Photo-responsive block copolymers. Linear-dendrimer block copolymers: introduction, structural peculiarities of their aggregates, potential applications.

**Surfactant-Polymer Interactions:** Effect of polymers on aggregation behavior of surfactants and the factors governing their interaction. Phase behavior of polymer-surfactant mixtures, behaviour of polyelectrolyte-surfactant systems. Technical applications of polymer surfactant systems.

#### Unit-III

(16 Contact hours)

##### **Instrumental Methods in Electrochemistry:**

**Fundamentals:** Electrode potential and its measurement, Standard and formal electrode potentials, three electrode measurements, uncompensated resistance. Overview of Electrode Processes-Faradaic and Nonfaradaic processes, factors affecting electrode reaction rate.

Mass transfer: Convection, migration, diffusion, Fick's 1<sup>st</sup> and 2<sup>nd</sup> law of diffusion, Cottrell equation.

#### Electrochemical Techniques:

Potential Step Methods: Chronoamperometry, Chronocoulometry at macroelectrodes; theory and applications.

Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macroelectrodes theory and applications, Diagnostic criteria of Cyclic Voltammetry.

#### **Unit-IV (16 Contact hours)**

##### **Applied Electrochemistry:**

Electrochemistry of redox enzymes- Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications, mechanism and approach to bioelectrosynthesis, examples of bioelectrosynthesis- oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

Energy storage devices: Desirable characteristics of energy storage devices, Batteries, Classical Batteries (Lead Acid, Nickel-Cadmium, Zinc-Manganese dioxide), Modern Batteries (Zinc-Air, Nickel-Metal Hydride, Lithium Ion Batteries), Supercapacitors.

Fuel cells, Types of Fuel Cells (Alkaline, Phosphoric acid, Polymer Electrolyte membrane and Direct MeOH fuel cell), Biofuel cells.

##### **Books Recommended:**

1. D. Fennell Evans, H. Wennerstrom, "The Colloidal Domain where physics, chemistry, biology and technology meet" VCH, New York, 1994.
2. Robert J. Hunter, "Foundations of Colloid Science", Oxford University Press, New York, 2007.
3. P.C. Heimenz, "Principles of Colloid and Surface Chemistry", Marcel Dekker Inc. New York, 1986.
4. M. J. Rosen, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 2004.
5. R. D. Vold and M. J. Vold, "Colloid and Interface Chemistry", Addison-wesley, 1982.
6. D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
7. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998
8. Colloids and Interfaces with Surfactants and Polymers – An Introduction J. W. Goodwin, 2004, John Wiley & Sons Ltd, ISBN: 0-470-84142-7 (HB) ISBN: 0-470-84143-5 (PB).
9. Frederik Wurm, Holger Frey: Linear–dendritic block copolymers: The state of the art and exciting, perspectives, *Progress in Polymer Science* 36 (2011) 1–52
10. M.J.Lawrence & G.D.Rees, *Advanced Drug Delivery Reviews*, Vol,45,p 898,2000.
11. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
12. I. W. Hamley, *The Physics of Block Copolymers* (Oxford University Press, Oxford, 1998.
13. P. Alexandridis and J. F. Holzwarth, *Curr. Opin. Colloid Interface Sci.* 5, 312 (2000).
14. N. Hadjichristidis, S. Pispas and G. A. Floudas *Block Copolymers* (Wiley, New York, 2003).

15. Electrochemical Methods Fundamentals and Applications, 2<sup>nd</sup> Edition, Allen J. Bard, Larry R. Faulkner, John Wiley and Sons, INC.
16. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
17. Understanding Voltammetry, 2<sup>nd</sup> Edition, Imperial College Press.
18. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
19. Electrochemistry, 2<sup>nd</sup> Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
20. Modern Electrochemistry 2B, 2<sup>nd</sup> Edition, J. O`M. Bokriss and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
21. Handbook of Electrochemistry, C. G. Zoski (Ed.) Elsevier.



## Course No: CH14409CR

**Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)**

*Max. Marks: 100*

*External Exam: 80 Marks.*

*Duration: 64 Contact hours*

*Internal Assessment: 20 Marks*

### **A. Tensiometry**

1. Investigation of variation of surface tension of n-butanol and sodium chloride solutions with concentration and hence determination of their surface excess concentrations using Gibb's Adsorption Isotherm.
2. Determination of CMC value of a detergent using tensiometry.

### **B. Cryoscopy**

1. Investigation of variation of freezing point depression with concentration & determination of molecular mass.
2. Determination of the degree of dissociation of a salt/weak acid in solution.
3. Determination of activity co-efficient from freezing point measurements.

### **C. Spectrophotometry**

1. To study the complexation reaction between Fe(III) & salicylic acid.
2. Determination of pK value of an indicator.
3. Isolation and spectrophotometric characterization of nucleic acids from Onion or Peas or Liver.
4. Explore the thermodynamics of DNA Melting through spectrophotometry.

### **D. Spectrofluorometry**

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl<sub>4</sub> in ethanol.
2. Using pyrene as probe determine the cmc of a surfactant and site of solubilization of pyrene in the micelle through spectrofluorometry.

### **E. Potentiometry**

1. Precipitation titration of KCl, KBr, KI and their mixture with AgNO<sub>3</sub>
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of formation constant of Ag-NH<sub>3</sub> complex.
4. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

### **F. Conductometry**

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of BaCl<sub>2</sub> and K<sub>2</sub>SO<sub>4</sub>/ (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>
3. Estimation of the concentrations of H<sub>2</sub>SO<sub>4</sub>, CH<sub>3</sub>COOH and CuSO<sub>4</sub> in a mixture.

### **G. Dynamic Electrochemistry**

1. Estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.

2. Using Cyclic Voltammetry determine the formal potential and diffusion coefficient of  $[\text{Fe}(\text{CN})_6]^{3-}$ .
3. Use cyclic voltammetry to determine the concentration of acetaminophen in a given sample.

#### **H. Kinetics**

1. Kinetic Investigation of BZ-Oscillatory reaction
2. Kinetic study of enzyme catalyzed reaction (effect of pH and Temperature).

#### **I. Viscometry and densitometry**

1. Determination of Mol. Mass of a Polymer (Polyvinyl alcohol) using viscosity method.
2. Explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

#### **Books Recommended**

1. Practical Physical Chemistry ----Findley revised by Kitchner.(Longman, 1971)
2. Experimental Physical Chemistry, A. M. Halpern, G. C. McBane, (Freeman, 2006)
3. Experiments in Physical Chemistry, 5th ed. ---- Schoemaker et al. (MGH, 2003)
4. Experimental Electrochemistry----- R. Holze (Wiley-VCH, 2009).

**Course No. CH14410EA**  
**Title: Bio-Inorganic Chemistry (04 Credits)**

*Max. Marks: 100*  
*External Exam: 80 Marks.*

*Duration: 64 Contact hours*  
*Internal Assessment: 20 Marks*

**Unit-I** **(16 Contact hours)**

**Iron Storage, Transport and Oxygen carriers:**

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.

The transport mechanism: uniport, symport and antiport.

Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.

Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.

Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage. Bohr effect and cooperativity in haemoglobin.

Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding.

Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

**Unit-II** **(16 Contact hours)**

**Metallo-enzymes and Electron Carriers:**

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.

Zinc enzymes:- Carboxypeptidase, Carbonic Anhydrase and Alcohol. Dehydrogenase: Introduction, Structure, Mechanism of action and their model compounds.

Molybdenum enzymes: An overview of the major molybdenum enzymes.

Biological chemistry of Molybdenum: uptake of Molybdenum; oxidation states and redox potentials in enzymes and oxygen atom transfer reactions.

Xanthine oxidase and Aldehyde oxidase: Structure and biological role.

Cobalt in Vitamin B<sub>12</sub>: Introduction, Structure and Derivatives of B<sub>12</sub> and mechanism of alkylation reaction. Role of vitamin B<sub>12</sub>.

Electron Carriers: Rubredoxin & Ferridoxin (Structure and biological role).

Blue Copper proteins: Oxidases and Plastocyanin (Structure and biological role).

**Unit-III** **(16 Contact hours)**

**Metal-Ion Induced Toxicity and Chelation Therapy:**

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN<sup>-</sup>  
Metal ion promoted Carcinogenesis and probable mechanism of action.

Therapeutic Aspects of Chelating Drugs :- Conditional stability constant , Stereochemistry, Lipophilicity. HSAB theory and Plasma mobilizing index(PMI).

Types of Chelation Therapy: Single, Double, Synergistic and Mixed ligand chelation therapy.

Therapeutic index of different chelating drugs in metal ion detoxification.  
Radio protective chelating drugs.

Limitations and Hazards of Chelation therapy

#### **Unit-IV**

**(16 Contact hours)**

#### **Metal Salts and Metal Complexes in Therapeutics:**

Treatment of essential metal deficiencies: Iron, Copper and Cobalt. Metal salts as anti-acids, antiseptic and diuretics.

Gold compounds and Rheumatoid arthritis.

Anti-Cancer Drugs: cis-Platin and its derivatives. Structure-function relationship.

Complexes of Rhodium, Gold and Cobalt.

Anti-bacterial, Anti-viral and Anti-fungal activities of Metal Complexes: Labile and Robust metal complexes; Probable mechanism of action.

#### **Books Recommended:**

1. As listed for Course No. CHM—101 (Inorganic chemistry-M.Sc. 1st Semester! From serial No. 1 to 5.
2. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon; 1977.
3. Inorganic Bio-chemistry—Vol. 1&2; Eichhorn; Elsevier, 1973.
4. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic; 1976.
5. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley; 1973.
6. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS; 1990.
7. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarendon; 1991.
8. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
9. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford; 1997.
10. Bio inorganic Chemistry ; K. Hussain Reddy; New Age International (P) Ltd; 2005.
11. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House; 2005.

**Course No: CH14411EA**  
**Title: Bio-Organic and Medicinal Chemistry (04 Credits)**

*Max. Marks: 100*

*External Exam: 80 Marks.*

*Duration: 64 Contact hours*

*Internal Assessment: 20 Marks*

**Unit-I**

**(16 Contact hours)**

**Vitamins:** Source, structure and synthesis of vitamins – Vitamin A, Vitamin B-Complex (Thiamine riboflavin, folic acid); Vitamin B-12 (Structure only) Vitamin C, E, K, H and D.

**Prostaglandins :** Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors- Woodward synthesis of PGF<sub>2α</sub>. Cyclo-heptane precursors -Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

**Nucleic Acids:** Structure of nucleotide, nucleosides, RNA and DNA, role of nucleic acids in protein synthesis, genetic code and heredity. DNA finger printing

**Unit-II**

**(16 Contact hours)**

**Enzymes :** Introduction, nomenclature & classification.. Activation & inhibition of enzymes. Mechanism of enzyme action- Fischer lock and key, Koshland's induced fit hypothesis, displacement reactions & coupling of ATP. Enzyme mechanism of chymotrypsin lysozyme & carboxypeptidase.

**Co-Enzymes:** Cofactors derived from vitamins, coenzymes, prosthetic groups. Apoenzyme. Structure, biological function and mechanism of reactions catalysed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD and Lipoic acid.

**Unit-III**

**(16 Contact hours)**

**Drug Design:** Classification and sources of drugs, concept of lead compounds and lead modification. Analogues, prodrugs, factors governing drug design.

**Structure activity relationship (SAR),** Isosterism, bioisosterism, changing the size and shape, changing the number of methylene groups in chain, changing the degree of unsaturation. Effect of introduction of methyl groups, halogens, hydroxyl, carbonyl, thiol, sulphide groups and introduction/removal of ring systems on pharmacological activity.

**Quantitative structure activity relationships (QSAR):** Theories of drug activity, Clark's occupancy theory, the rate theory, two state theory. Lipophilic constant, Hammett constant, steric parameters and Hansch analysis.

**Unit-IV**

**(16 Contact hours)**

**Antibiotics:** Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Penicillins-classification and structures. Synthesis of Penicillins, V, G, chloramphenicol and ciprofloxacin. Tetracyclins.

**Psychoactive Drugs:** Introduction, CNS depressants, CNS stimulants, sedatives and hypnotics, barbiturates. Synthesis of diazepam, phenytoin and glutethimide.

**Anti-neoplastic drug:** Introduction; cancer chemotherapy, carcenolytic antibiotic, plant derived anti-cancer agents (Taxol )role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

**Cardiovascular Drugs:** Introduction, cardiovascular diseases, synthesis of Amylnitrate. sorbitrate, quinidine, verapanil, methyl dopa and atenolol

**Books Recommended:**

1. Introduction to Medicinal Chemistry, Alex Gringauz (Wiley- VCH-1997).
2. Medicinal Chemistry- An Introduction, Gareth Thomas (Wiley-2000). 3<sup>rd</sup> Edition.
3. Medicinal Chemistry, Ashutosh Kar. (Wiley Eastern-1993).
4. Biochemistry, Biotechonolgy and Clinical Chemistry of Enzmyes. Trevor Palmer ( EWP ).
5. Organic Chemistry by I.L.Finar Vol. II ( ELBS Longamnn)
6. Lehninger's Principles of Bio-chemistry, D.L. Nelson. M.Cox Worth publications,2000.
7. Introduction to nucleic acids and related natural products Ulbight (Oldborn Press )
8. Chemsitry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Naroosa Publishing House, New Delhi.

## Course No: CH14412EA

### Title: Non-Equilibrium & Statistical Thermodynamics (04 Credits)

*Max. Marks: 100*

*External Exam: 80 Marks.*

*Duration: 64 Contact hours*

*Internal Assessment: 20 Marks*

#### Unit- I

(16 Contact hours)

##### Non-equilibrium Thermodynamics:

Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity. Gibb's equation, entropy production, entropy production due to matter flow, heat flow, charge flow & chemical reactions.

Concept of forces & fluxes, Onsager's theory of irreversible processes- phenomenological laws, their domain of validity. Chemical reactions near equilibrium. Transformation properties of forces and fluxes. Electrokinetic phenomena.

#### Unit-II

(16 Contact hours)

##### Classical Statistical Mechanics and Ensembles:

Equations of Motion; Newton, Lagrange and Hamiltonian. Classical partition function, phase space and the Liouville equation, Kinetic theory of gases, equi-partition of energy, Maxwell's velocity distribution

Concept of ensembles, ensemble average and postulate of equal a priori probability. Canonical, grand-canonical and Micro-canonical ensembles. Ensemble partition functions and related thermodynamic functions. Ideal gas in canonical and Grand canonical ensemble.

#### Unit-III

(16 Contact hours)

##### Quantum Statistics:

Quantum Statistics : Fermi-Dirac and Boson-Einstein statistics, Nuclear spin statistics, symmetry and nuclear spin, Ortho and Para nuclear spin states, Ortho and Para Hydrogen and Deuterium, CO

Application of grand partition function to Boson-Einstein and Fermi-Dirac statistics. Ideal Fermi-Dirac gas: Electrons in metals, Ideal Photon gas: Black body radiation

#### Unit- IV

(16 Contact hours)

##### Statistical Thermodynamics of Interacting Systems:

**Statistical thermodynamics of solids;** Thermodynamics of point defects, Heat capacity of solids, Einstein and Debye models (Partition function, Average energy and heat capacity). Limitations of the models. ...5 hrs

Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand partition function, virial coefficient in the classical limit, second and third virial coefficients.

Statistical thermodynamics of solutions: Lattice model, regular solution theory, Statistical Mechanics of polymer solution.

**Books Recommended:**

1. Thermodynamics of Irreversible Processes, De Groot, Mazur, (Dover, 1986).
2. Introduction to Thermodynamics of Irreversible Processes, I. Prigogine, (Wil-Interscience, 1967.)
3. Thermodynamics for students of Chemistry, Kuriacose, Rajaram, (S. Chand and Co., 1996).
4. Exploring Complexity, I. Prigogine, G. Nicolis, (Freeman, 1998).
5. Molecular Thermodynamics, D. A. McQuarrie, J. D. Simon, USB, 1998.
6. Statistical Thermodynamics, M.C.Gupta, (New Age International, 1993).
7. Statistical Thermodynamics-Fundamentals and Applications, N. M. Laurendeau, Cambridge University Press, 2005.
8. Statistical Mechanics, D. A. McQuarrie, ( Viva, 2003).
9. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
10. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover, 1990).
11. Statistical Mechanics - Principles and Applications, Hill, Dover, 1987.
12. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
13. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley, 1987).



## Course No: CH14413EA

### Title: Organic Synthesis (02 Credits)

Max. Marks: 50

External Exam: 40 Marks.

Duration: 32 Contact hours

Internal Assessment: 10 Marks

#### Unit-I

(8 Contact hours)

##### Oxidative and Reductive Processes in Organic Synthesis:

**Oxidation:** Introduction, Aromatisation of cycloalkanes and alkenes using metal catalysts and DDQ. Oxidation of Alcohols using chromic acid, DCC and Swern reagent. Oppenaur oxidation. Oxidation of ketones. Oxidation at activated carbon-hydrogen bond. Oxidation with Selenium dioxide. Prevost hydroxylation and its modification by Woodward.

**Reduction:** Introduction. Reduction of Alkenes, Alkynes and Aromatic rings.

Reduction of carbonyl compounds: Clemmensen and Wolf-Kishner reductions. Reductions using  $\text{LiAlH}_4$  and  $\text{NaBH}_4$  Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

#### Unit-II

(8 Contact hours)

##### Protection and Interconversion of Functional Groups:

###### Protection of functional groups

Principle of protection of functional groups and its significance. Protection of carbon-hydrogen bonds (in terminal alkynes and Carbon-hydrogen bond of aldehydes), carbon-carbon double bonds, alcoholic and Phenolic hydroxyl groups, amino groups, carbonyl and carboxyl groups.

###### Functional Group Interconversion (FGI) / Transformations.

Significance of Functional Group Interconversion (FGI) / Transformations in Organic synthesis. Methods of transformation of different functional groups into one another. Chemoselectivity.

#### Unit-III

(8 Contact hours)

##### Designing Organic Synthesis-I:

**The disconnection approach:** Introduction to synthons, their types and equivalent reagents. Reversal of Polarity(umpolung). One group, two group and Reteroelectrocyclic disconnections. Reterosynthetic Analysis involving connections and rearrangements. Guidelines for good disconnections.

Reterosynthetic analysis of alcohols, amines (aliphatic and aromatic), alkenes, carbonyl compounds, carboxylic acids and their derivatives using one group disconnecitons and FGIs. Use of acetylenes in the syntheses of above mentioned compounds.

## Unit-IV

(8 Contact hours)

### Designing Organic Synthesis-II:

**Two group disconnections:** Retrosynthetic analysis of 1, 2- difunctional compounds (1, 2 –diols), 1, 3 difunctional compounds (1,3-dioxygenated compounds,  $\alpha$ ,  $\beta$  - unsaturated carbonyl compounds, 3-amino alcohols and 3- amino ketones), 1, 4 and 1, 5-difunctional compounds.

**Multistep Synthesis:** Application of retrosynthetic analysis in designing /achieving syntheses of some complex molecules (for example Brufen, benzydaron, Juvabione, warfarin and brevicomin).

### Books Recommended:

1. Designing Organic Synthesis, S. Warren (Wiley-2002)
2. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin (Verlage VCH-1986).
3. Principles of Organic Synthesis 2nd Ed., R.O.C.Norman (Chapman and Hall-1978).
4. Advanced Organic Chemistry Part B, 5th Ed., F. A. Carey and R.J Sundberg (Springer--2007).
5. Organic Chemistry, 10th Ed., T. W. G. Solomons and Craig B. Fryhle (Wiley-2012).
6. Organic Chemistry, Clayden, Greeves, Warren and Wothers (Oxford University Press-2009).
7. Organic Chemistry, David Klein, (John-Wiley-2012).
8. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6th Ed., J. March, (Wiley-2012).

**Course No: CH14414EA**  
**Title: Inorganic Polymers (02 Credits)**

*Max. Marks: 50*  
*External Exam: 40 Marks.*

*Duration: 32 Contact hours*  
*Internal Assessment: 10 Marks*

**Unit-I** **(8 Contact hours)**

**Introduction to Inorganic Polymers:**

Definition, Classification and Comparison with organic polymers.

Inorganic Polymeric Reactions: Condensation, addition and coordination.

Applications and characterization of Inorganic polymers.

**Unit-II** **(8 Contact hours)**

**Boron-Nitrogen and Sulphur-Nitrogen Compounds:**

Bonding in higher boranes: Types of bonds, empirical rules for bonding in boron clusters, a detailed account of carboranes and metallocarboranes.

Boron-Nitrogen and Sulphur-Nitrogen: Properties, structure, bonding and uses of Borazines, Boron nitride, Polythiazyls and Sulphur Nitrides.

**Unit-III** **(8 Contact hours)**

**Phosphorus Nitrogen Polymers and Polyphosphates:**

Polyphosphazenes, Cyclophosphazenes, Phosphonitrilic halides and Polyphosphates: Preparation, properties, structure, bonding and uses.

**Unit-IV** **(8 Contact hours)**

**Silicon-Oxygen Polymers:**

Silicates: Classification, structure and bonding.

Zeolites: Potential applications as ion exchangers, adsorption agents, catalysts and gas separators.

Silicones and Polysiloxanes: Preparation, properties, bonding and uses.

**Books Recommended:**

- Inorganic Polymers F.G-A-Stone & W-A.Graham; Academic Press.
- Inorganic Polymers James. E.Mark, HarryAllock & Roberta West; Prentice Hall.
- Inorganic Polymers NJLRay; Academic Press; 1978.
- Development of Inorganic Polymer Chemistry; Lappert& Leigh; Elsevier; 1962.
- Fluoropolymers; Wall; Wiley; 1972.

**Course No: CH14415EA**  
**Title: Chemistry of Materials (02 Credits)**

*Max. Marks: 50*

*External Exam: 40 Marks.*

*Duration: 32 Contact hours*

*Internal Assessment: 10 Marks*

**Unit-I: Langmuir Blodgett Films and Liquid crystals (8 Contact hours)**

*Langmuir- Blodgett Films:* Introduction and general preparative techniques. LB Films of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications – nonlinear optical effects, conduction, photoconductivity and sensors.

*Liquid Crystals:* Mesomorphism, types of liquid crystals, molecular structural requirement of mesomorphism, properties of liquid crystals, Applications – Liquid crystal displays, thermography, optical imaging and ferroelectric liquid crystals.

**Unit- II: Organic Solids and Molecular Devices (8 Contact hours)**

*Organic solids and fullerenes:* Organics conductors, magnetism in organic materials. Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes)

*Molecular devices:* Molecular rectifiers and transistors, artificial photosynthetic devices, switches and sensors.

**Unit-III: Optical materials (8 Contact hours)**

Luminescence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducting lasers, quantum cascade and quantum dot lasers.

Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

**Unit- IV: Superconductors (8 Contact hours)**

Super conductors: Characteristic properties- Zero resistance, Meissner effect, Heat capacity, Thermal conductivity, absorption of em radiations and Josephson effect. BCS theory of superconductivity, High T<sub>c</sub> superconductivity in cuprates: Structure, preparation and characterization of 1-2-3 materials, mechanism of high T<sub>c</sub> superconductivity.

Unconventional superconductors: Heavy-fermion superconductors, metal-oxide superconductors, organic superconductors, Applications of high T<sub>c</sub> materials.

**Books Recommended:**

1. Introduction to Solids, Azaroff, Tata McGraw,1993.
2. Solid State Chemistry and its Applications, West, Wiley,1989.
3. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
4. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
5. Principles of Solid State, H. V. Keer, Wiley Eastern.
6. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
7. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.

**Course No: CH14416EA**  
**Title: Seminar (02 Credits)**

The Course shall comprise of following two components of 25 marks each and each component would be evaluated in the same manner as project works are evaluated. .

**Part A :** **Marks: 25**

Each student shall submit a seminar report (review) on the topic assigned to him/her by the supervisor concerned. The report would be evaluated on 25 point scale by another teacher of the same branch.

**Part B: Lecture followed by viva-voce** **Marks: 25**

The student shall deliver a lecture on the same topic before all M.Sc. students/Scholars and teachers of the departments followed by an open viva-voce session. This would be conducted by a team of three teachers, one from each branch, who would award marks out of 25 based on the presentation and performance in question answer session.

**Course No: CH14417EO**  
**Title: Chemistry of the Environment (04 Credits)**

*Max. Marks: 100*

*External Exam: 80 Marks.*

*Duration: 62 Contact hours*

*Internal Assessment: 20 Marks*

**Unit –I: Environment and Soils. (16 Contact hours)**

Introduction, Segments of Environment; factors affecting Environment. Biogeochemical cycles of C, N, P, S and O.

Nature and Composition of Soil: Air, Water, Inorganic Components, Organic matter and Humus. Macro and Micronutrients in Soil. Acid--Base and Ion exchange reactions in Soil.

Pollution: Fertilizers, Pesticides, Plastics and Metals.

**Unit-II: Hydrosphere: (16 Contact hours)**

Chemical composition of water bodies: - Lakes & rivers ; Factors determining composition (thermal stratification, acid-base, pE concept).

Aquatic pollution: Inorganic, Organic, Pesticide, Agricultural, Industrial and Sewage. Water quality parameters: Dissolved oxygen, Metals, Content of Chloride, Phosphate, Nitrate, and Microorganisms. Water quality standards.

Analytical Methods for determining BOD, DO, COD, and metals (As, Cd, Hg, Pb & Se) Choice of methods for determination.

Purification and treatment of water (Chlorination, Ozonation, UV radiation)

**Unit-III: Atmosphere. (16 Contact hours)**

Chemical Composition of Atmosphere: particles, ions, radicals and their formation. Vertical profile of atmosphere, Heat budget of earth s atmospheric system. Chemical and Photochemical Reactions in Atmosphere, Photochemical Smog formation; Oxides of N, C, S and their effects, Sun screens ; Ozone chemistry. Pollution by Chemicals (chlorofluorocarbons, hydrocarbons, O<sub>3</sub>)

Green House Effect; Acid Rain; their chemistry and control, Atmospheric Window.

Analytical Methods for measuring Air Pollutants.

Continuous monitoring instruments.

**Unit-IV: Environmental Toxicology and Industrial Pollution. (16 Contact hours)**

Principles of Toxicology; Dose Response Relationship; Risk assessment and management.

Organochlorine Compounds: Accumulation and fate in biological systems. Toxicology of PCBs, Dioxins and Furans; Health effects in humans.

Environmental Estrogens.

Industrial Pollution: - Cement, Sugar, Drug, Paper and pulp. Thermal power plants, Nuclear power plants and Polymers

Radio nuclide analysis: Disposal of wastes and their management..

**Books Recommended:**

1. Environmental Chemistry; Nigel.J.Bunce; Wurez Publishers; 1991.
2. Environmental Chemistry; 2<sup>nd</sup> edn; Colin Baird; Freeman &Co; 1991.
3. A Textbook of Environmental Chemistry; O.D.Tyagi & M.Mehra; Anmol Publishers; 1990.
4. Environmental Chemistry; A.K.De; Wiley Eastern;1995.
5. Environmental pollution Analysis; S.M.Khopkar; Wiley Eastern.
6. Environmental pollution; B.K.Sharma& H.Kaur; Goel Publishers;1996.
7. Environmental Toxicology; Ed.Rose; Gordon & Breach Science Publishers.
8. Environmental Chemistry; S.E.Manahan; Lewis Publishers;2000