

Course No: CH17401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

- Unit-I Sigma Bonded Organometallic Compounds: (16 Contact hours)**
Classification, Stability, Comparison to main Organometallic Compounds, Routes of synthesis, Reactions. Decomposition Pathways: Choice, α and β 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 Pi-bonded Organometallic Compounds: (16 Contact hours)**
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 Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)**
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 Fluxional Organometallic Compounds and Synthetic Reactions involving Organo-metallics (16 Contact hours)**
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 η^1 Cyclopentadienyls and η^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:

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

Course No: CH17402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

Unit-I Basics of Photo-Chemistry (16 Contact hours)

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. Jablonski diagram.

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

Unit-II The Chemistry of Excited State Molecules (16 Contact hours)

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 Redox Reactions by Excited Metal Complexes (16 Contact hours)

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)₃]²⁺ and [Os (bipy)₃]²⁺.

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

Unit-IV Solar Energy-Prospects and Challenges (16 Contact hours)

Solar energy storage, solar energy conversion, Metal complex sensitizers and electron relays in photochemical splitting of water, Nitrogen fixation and CO₂ 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: CH17403CR
Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

Unit-I Iron Storage, Transport and Oxygen carriers: (16 Contact hours)

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 Metallo-enzymes and Electron Carriers (16 Contact hours)

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

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

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 B₁₂: Introduction, Structure and Derivatives of B₁₂ and mechanism of alkylation reaction. Role of vitamin B₁₂.

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

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

Unit-III Metal-ion Induced Toxicity and Chelation Therapy (16 Contact hours)

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- 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 Metal Salts and Metal Complexes in Therapeutics (16 Contact hours)

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: CH17404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

Unit-I Structure and Nomenclature of Heterocyclic compounds (16 Contact hours)

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 ¹HNMR).

Unit-II General Approach to Synthesis of Heterocyclic compounds (16 Contact hours)

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 Monocyclic Heterocycles (16 Contact hours)

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 Bicyclic Heterocycles (16 Contact hours)

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.

Books Recommended:

1. Heterocyclic Chemistry, 5th 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: CH17405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

- Unit-I Terpenoids and Carotenoids (16 Contact hours)**
Introduction, classification, general methods of isolation, separation.
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 α -terpineol, abietic acid and β -carotene.
- Unit-II Alkaloids (16 Contact hours)**
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 Steroids (16 Contact hours)**
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 Oesterone, Androsterone, Testosterone and Progesterone.
Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis of Cortisone, aldosterone and synthesis of cholecalciferol.
- Unit-IV Natural Plant Pigments and Porphyrins (16 Contact hours)**
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, Quercitin & Genestein.
Porphyryns: 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: CH17406CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 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_{2a}. 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, koshlands 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⁺, NADP⁺, 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, carbonylic, thiols sulphides 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, chloroamphenicol and ciprofloxacin. Tetracyclins.

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

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

Cardiovascular Drugs: Introduction, cardiovascular diseases, synthesis of Amylnitrate, sorbitrate, quinidine, verapamil, 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). 3rd Edition.
3. Medicinal Chemistry, Ashutosh Kar. (Wiley Eastern-1993).
4. Biochemistry, Biotechnology and Clinical Chemistry of Enzymes. Trevor Palmer (EWP)
5. Organic Chemistry by I.L.Finar Vol. II (ELBS Longman)
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. Chemistry of Natural Products. S.V. Bhat, B.A. Nagasampagi, M. Siva Kumar. Narosa Publishing House, New Delhi.

Course No: CH17407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

Unit-I Electronic Structure Theory, Hartree-Fock Method (16 Contact hours)

Review: Electronic Hamiltonian, antisymmetrized wave function, Slater determinant. Hartree-Fock self-consistent field method. One and two-electron integrals in the light of minimal basis H₂ system.

Hartree-Fock 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.

Basis Sets: Slater-type orbitals, Gaussian basis sets. Model SCF calculations on H₂/HeH⁺

Unit-II Configuration Interaction and Semiempirical methods (16 Contact hours)

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

Semiempirical methods: The ZDO approximation; the PPP method, brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional Methods and Molecular Properties (16 Contact hours)

Density Functional Theory: Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation of DFT, n- and v- representabilities, E_x&E_c functionals; the local density and local spin density approximations, gradient corrected and hybrid functionals.

Brief idea of Molecular mechanics methods, force fields.

Molecular Properties: Potential energy surfaces; molecular geometry and its optimization, Hessian Matrix and normal modes, vibrational frequencies, thermodynamic properties. Dipole moments, atomic Charges.

Unit-IV Use of Quantum Chemistry Software: Gaussian (16 Contact hours)

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

1. A single point energy calculation: HCHO /CH₃.CHO, HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization CH₂O → HCOH
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarizability.
6. Stationary points characterization –C₃H₅F
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 O₃.
 - b) Density Functional Theory: CO₂ structure and atomization energy.
 - c) Butane / Isobutane isomerization energy, rotational barrier in n-butane.
9. Chemical reactions and reactivity:
 - a) Hydration enthalpy of the reaction $\text{H}^+ + \text{H}_2\text{O} \rightarrow \text{H}_3\text{O}^+$
 - b) Potential energy surfaces. Reaction path following (IRC calculation)
 $\text{CH}_2\text{O} \rightarrow \text{HCOH}$
 - c) Heat of formation of CO₂ via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

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

Course No: CH17408CR

Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

Unit-I Instrumental Methods in Electrochemistry (16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.

Overview of electrode Processes: Faradaic and Non-Faradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1st and 2nd law of diffusion,

Electrochemical Techniques:

Electrophoresis: Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Constant-Current coulometric titrations.

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

Unit-II Applied Electrochemistry (16 Contact hours)

Electrochemistry of redox enzymes: Direct and mediated electron transfer, Enzyme modified electrodes-challenges and applications. Mechanism and approach to bioelectrosynthesis, examples of bioelectro synthesis-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, Discharge plot, Ragone plot. Batteries: Measures of battery performance. 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, basic fuel cell operation, kinetics of fuel cell reactions. Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Unit-III Classical Statistical Mechanics and Ensemble concept (16 Contact hours)

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. Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand

partition function, virial coefficients in the classical limit, second and third virial coefficients.

Unit-IV Applied Statistical Mechanics (16 Contact hours)

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, influence of wavelength for the Planck distribution, Bose-Einstein condensation.

Statistical thermodynamics of solutions: Lattice model, regular solution theory, statistical mechanics of polymer solution, Flory-Huggins theory.

Statistical mechanics of solids: Einstein and Debye models (Partition function, Average energy and heat capacity), limitations of the models.

Books Recommended

1. Electrochemical Methods Fundamentals and Applications, 2nd Edition, Allen J. Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
3. Understanding Voltammetry, 2nd Edition, Imperial College Press.
4. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
5. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
6. Modern Electrochemistry 2B, 2nd Edition, J. O'M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
7. Statistical Thermodynamics, M. C. Gupta, (New Age International, 1993).
8. Statistical Thermodynamics-Fundamentals and Applications, N.M. Laurendeau, Cambridge University Press, 2005.
9. Statistical Mechanics, D.A. McQuarrie, (Viva, 2003).
10. Introduction to Statistical Thermodynamics, Chandler, (OUP, 1987).
11. Statistical Thermodynamics and Kinetic Theory, C. E. Hecht, (Dover, 1990).
12. Statistical Mechanics –Principles and Applications, Hill, Dover, 1987.
13. Statistical Thermodynamics for Chemists, A. Ben-Naim, (Plenum, 1992).
14. An introduction to Statistical Thermodynamics, Hill, (Addison-wesley, 1987).

Course No: CH17409CR
Title: Chemistry of Materials (04 Credits)

Max. Marks: 100

Ist Unit Exam: 25 marks

End Term Exam (units III & IV): 50 Marks

Duration: 64 Contact hours

IInd Unit Exam: 25 marks

Unit-I Surfactant mixtures, Stimuli responsive surfactants and block copolymers (16 Contact hours)

Surfactant-Surfactant Interactions: Mixed micelle formation, mixed monolayer formation, synergism, Clint and Rubingh's models of mixed micelle formation. Importance and practical applications of mixed surfactant systems.

Stimuli-Responsive Surfactants: Introduction and applications: Biosurfactants, redox, photochromic, thermoreversible, pH-sensitive, cleavable and magnetic surfactants.

Block Copolymers: Introduction: classification, micellization of diblock and triblock copolymers. Introduction to pH-, thermo- and Photo-responsive block copolymers. Applications.

Unit-II Hydrogels and microemulsions (16 Contact hours)

Hydrogels: Introduction, Types of Hydrogels, Preparation, Properties and characterization of Hydrogels, Biomedical applications of Hydrogels.

Microemulsions: Emulsions and microemulsions, Physicochemistry of Microemulsions: Formation, Stability, and Droplet Clustering, Percolation Phenomenon in Microemulsions. Applications of microemulsions in cosmetics and detergency, pharmaceuticals, soil decontamination, enhanced oil recovery and biocatalysis.

Unit-III Langmuir Blodgett Films, Liquid crystals and Fullerenes (16 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.

Fullerenes: Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes).

Unit-IV Optical materials and Ionic conductors (16 Contact hours)

Optical materials: Luminescence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducting lasers and quantum dot lasers. Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials.

Ionic Conductors: Introduction to ionic conduction and mechanism. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy

mechanism. Super-ionic conductors: Diffusion and transition superionic conductors and mechanism of conduction in superionic conductors; examples and applications of ionic conductors.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 4th Edition, 2012.
2. R. D. Vold and M. J. Vold, "Colloid and Interface Chemistry", Addison-wesley, 1982.
3. .D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
4. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998.
5. D. Fennell Evans, H. Wennerstrom, "The Colloidal Domain where physics, chemistry, biology and technology meet" VCH, New York, 1994.
6. Robert J. Hunter, "Foundations of Colloid Science", Oxford University Press, New York, 2007.
7. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
8. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
9. N. Hadjichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
10. Introduction to Solids, Azaroff, Tata McGraw,1993.
11. SolidState Chemistry and its Applications, West, Wiley,1989.
12. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
13. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
14. Principles of Solid State, H. V. Keer, Wiley Eastern.
15. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
16. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
17. M. Sirousazar, M. Foroug, K. Farhad, Y. Shaabani and R. Molaei, Hydrogels: Properties, Preparation, Characterization and Biomedical, Applications in Tissue Engineering, Drug, Delivery and Wound Care, IN Advanced Healthcare Materials, Wiley online Library, 2014.

Course No: CH17410DCE

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

Max. Marks: 100
External Exam: 75 Marks.

Duration: 64 Contact hours
Internal Assessment: 25 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 (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 AgNO_3 over Pt & Calomel assembly using $\text{I}^- \backslash \text{I}_2$ redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard 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 (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.Girolomi; 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: CH17411DCE

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

Max. Marks: 100

External Exam: 75 Marks.

Duration: 64 Contact hours

Internal Assessment: 25 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 β -carotene from tomato and their characterization using UV- spectroscopy.
- (2) Isolation of limonene from its natural source and physicochemical analysis.
- (3) Assay of Belladonna for Hyoscyamine.
- (4) Assay of lemon from 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 of separated components 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 5th 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.

Course No: CH17412DCE

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

Max. Marks: 100

External Exam: 75 Marks.

Duration: 64 Contact hours

Internal Assessment: 25 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.

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl₄ 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 AgNO₃
2. Thermodynamics of a chemical reaction by EMF-method.
3. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of BaCl₂ and K₂SO₄/ (NH₄)₂SO₄
3. Estimation of the concentrations of H₂SO₄, CH₃COOH and CuSO₄ in a mixture.

G. Dynamic Electrochemistry

1. To estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry to determine the formal potential and diffusion coefficient of [Fe(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. To 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: CH17413DCE

Title: Supramolecular Chemistry (02 Credits)

Max. Marks: 50

Duration: 32 Contact hours

Ist Unit Exam: 25 marks

IInd Unit (Term end) Exam: 25 marks

- Unit-I Supramolecular Interactions (08 Contact hours)**
Definition and Development of Supramolecular Chemistry. Nature of Supramolecular Interactions.
Hard Soft Acid Base Concept- Concept, Classification, Symbiosis. Utility in drug design and molecular recognition. Soft Ligands for Soft Metal Ions-Mixed Crown Ethers and Mixed Cryptands.
- Unit-II Supramolecular Receptors (08 Contact hours)**
Cation Receptors: Supramolecular Cation Coordination Chemistry, EDTA- The Supramolecular Host. Introductory account of Cation Receptors - Podands, Corands, Cryptands, Spherands and Calixarenes.
Anion Receptors: Scope and Challenges, Anion Hydrophobicity-Hofmeister Series, Introductory Account of Anion Receptors - Cyclophanes, Pyrolles, Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.
Ion-Pair Receptors: Concept and Significance
- Unit-III Crystal engineering and Supramolecular Motiffs (08 Contact hours)**
Crystal Engineering: Introduction, Tectons and Synthons. Hydrogen Bond- Introduction, Criteria Nature and Importance.
Self Assembly: Scope and Objectives. Concepts and Classification. Introductory Account of Coordination Capsules, Catenenes, Rotaxenes and Molecular Knots.
- Unit-IV Network Solids and Molecular Devices (08 Contact hours)**
Network Solids: Concepts and Classification, Network Topology. Zeolites: Structure, utility and limitations. Metal Organic Frameworks-Introduction and application in catalysis and Gas storage.
Molecular Devices: Philosophy of Molecular Devices, Photophysical Fundamentals and Mechanism of Energy and Electron Transfer, Introductory Account of Molecular Wires, Molecular Switches and Molecular Motors.

Books Recommended

1. Supramolecular Chemistry. Jonathan W. Steed and Jerry L. Atwood. **Wiley 2nd Edn.**
2. Supramolecular Chemistry - Fundamentals and Applications. A. Katsuhiko and K. Toyoki. **Springer.**
3. Crystal Engineering. G. R. Desiraju, J. J. Vittal and A. Ramanan. **World Scientific, 1st Edn.**
4. Organic Crystal Engineering: Frontiers in Crystal Engineering. E. R. T. Tiekink, J. Vittal and M. Zaworotko. **Wiley, 2010.**
5. Frontiers in Crystal Engineering. Edward R. T. Tiekink (Editor), Jagadese Vittal (Editor). **Wiley, 2005.**
6. An Introduction to Supramolecular Chemistry. Asim K. Das, Mahua Das, **CBS Publishers and Distributors Pvt Ltd. 2005.**
7. Chemical Reviews. Vol. 115, Issue 15, year **2015**, Pages 6999-8156
8. Introduction: Supramolecular Chemistry. F. Huang and E. V. Anslyn. Chem. Rev. **2015**, 115, 6999–7000.
9. Supramolecular materials. D. B. Amabilino, D. K. Smith and J. W. Steed. Chem. Soc. Rev., **2017**, 46, 2404—2420
10. A Bond by Other Name. G. R. Desiraju. Angew. Chem. Int. Ed. **2011**, 50, 52-59.
11. The Weak Hydrogen Bond: In Structural Chemistry and Biology. G. Desiraju, T. Steiner. **Oxford, IUCr Monograph on Crystallography.**

Course No: CH17414DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: 50
Ist Unit Exam: 25 marks

Duration: 32 Contact hours
IInd Unit (Term end) Exam: 25 marks

Unit-I (A) Oxidative and Reductive Processes in Organic Synthesis (8 Contact hours)

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 LiAlH_4 and NaBH_4 Bouveault-Blanc reduction. Reduction of Epoxides, Nitro, Nitroso, Azo and Oxime groups. Reductions using Tributyl Tin Hydride.

(B) Protection and Interconversion of Functional Groups (8 Contact hours)

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-II Designing Organic Synthesis (16 Contact hours)

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.

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

Two group disconnections: Reterosynthetic analysis of 1, 2- difunctional compounds (1,2 – diols), 1,3- difunctional compounds (1,3-dioxygenated compounds, α , β -unsaturated carbonyl compounds, 3-amino alcohols and 3- amino ketones), 1,4- and 1,5- difunctional compounds.

Multistep Synthesis: Application of reterosynthetic analysis in designing /achieving syntheses of some complex molecules (for example Brufen, benziodarone, Juvabione, warfarin and brevicomin (Examples other than these may also be included).

Books Recommended

1. Designing Organic Synthesis, S. Warren ;Wiley; 2013.
2. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin; Verlage VCH;1986.
3. Principles of Organic Synthesis 2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
4. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 2007.
5. Organic Chemistry, 10th edn;. T. W. G. Solomons and Craig B. Fryhle ; Wiley-2012.
6. Organic Chemistry; Clayden, Greeves, Warren and Wothers ; Oxford University Press-2012.
7. Organic Chemistry, David Klein; John-Wiley-2012.
8. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6th Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH17415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: 50
Ist Unit Exam: 25 marks

Duration: 32 Contact hours
IInd Unit (Term end) Exam: 25 marks

Unit-I

- (a) Numerical solution of equations (8 Contact hours)**
Basic theory, discussion of algorithms and errors for following numerical methods:
Solution of Equations: Bisection, false-position, Newton-Raphson method for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning.
Linear Simultaneous equations: Gaussian elimination and Gauss-Siedel method. Pivoting strategy. Errors and ill-conditioning.
Eigen values and Matrix Diagonalization: Eigen value problem, diagonalization of a matrix, Jacobi and Householder methods.
- (b) Numerical differentiation and integration (8 Contact hours)**
Basic theory, discussion of algorithms and errors for following numerical methods:
Numerical differentiation: Solutions of simple differential equations by Taylor series and Runge-Kutta methods.
Numerical integration: Newton-Cotes formulae, Romberg integration, errors in integration formulae.

Unit-II

- (a) Interpolation and Curve Fitting (8 Contact hours)**
Basic theory, discussion of algorithms and errors for following numerical methods:
Lagrange's interpolation method, Newton's divided differences, Cubic spline, piece wise interpolation.
Least squares approximation, linear and quadratic.
- (b) Use of Mathematica/Scilab for numerical solution of problems(8 Contact hours)**
The mathematica package will be used for the solution of problems covered under the above three units.

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Computational Chemistry, A. C. Norris, (Wiley.)
3. Computer Software Applications in Chemistry - P. C. Jurs, (John Wiley, 1996.)
4. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
5. Numerical Recipes in Fortran/C, W.H. Press et al., (CUP,1992)
6. Applied Numerical Analysis, Gerald &Wheatly, (Pearson Education, 2002)
7. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
8. Mathematica Manual.

Course No: CH17416DCE
Title: Seminar (02 Credits)

Presentation by a candidate on any topic chosen in consultation with the teacher incharge.

(25 Marks)

Manuscript (on the topic) submission

(25 Marks)

Course No: CH17417GE

Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: 50

Ist Unit Exam: 25 marks

Duration: 32 Contact hours

IInd Unit (Term end) Exam: 25 marks

Unit-I (08 Contact hours)

Introduction, Definition, Classification based on source, Structure, Synthesis and Forces of attraction. Thermosetting and Thermosensitive plastics, Types of Monomers, Homopolymers and Copolymers.

Unit-II (08 Contact hours)

Polymerisation processes, Addition polymerization, Free radical, Cationic, Anionic mechanism of addition polymerization Initiators, Inhibitors and Propagators. Stereochemical control of polymerization- Zeiglar Natta catalysts, Poly condensation; Polymerisation.

Unit-III (08 Contact hours)

Commercially important polymers: Polyesters, Polycarbonates, Polyamides, Polyurethanes, Poly sulphides, Resins: Phenol-formaldehyde and Melamine-formaldehyde resins. Conducting Organic Polymer (elementary idea), Biodegradable polymers

Unit-IV (08 Contact hours)

Natural polymers: Rubber, Vulcanization,

Polysaccharides: Cellulose, Amylopectin and Starch, Proteins; Wool, Silk and Collagen; Regenerated properties.

Books Recommended

1. Organic chemists : Francis . A. Carey, Robert M. Giuliano. 8th ed. Tata Mc Graw Hill. 2010
2. Polymer chemistry- An introduction. Mallolin. P. Steven, 2nd ed. Oxford University. 1998
3. Organic chemistry: L. G. Wade, Tr. Maya Shankar Singh. 6th ed., 2005, Pearson.
4. Introduction to polymers: 2nd ed. R.J. Young and P.A. Lovell. Chapman and Hill
5. Organic chemistry: David Klein; Willey 2012 .

Course No: CH17418GE
Title: Novel Materials (02 Credits)

Max. Marks: 50
Ist Unit Exam: 25 marks

Duration: 32 Contact hours
IInd Unit (Term end) Exam: 25 marks

Unit-I Block Co-Polymers, Langmuir Blodgett Films and Organic Solids
(16 Contact hours)

Block Copolymers: Introduction: classification, micellization of diblock and triblock copolymers. Introduction to pH-, thermo- and Photo-responsive block copolymers. Linear- dendrimer block copolymers: introduction, structural peculiarities of their aggregates, potential applications.

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.

Organic solids and fullerenes: Organics conductors, organic superconductors. Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors. Carbon nanotubes: Types, Properties and Applications.

Unit-II Optical and Nano-materials:
(16 Contact hours)

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

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

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.

Nanomaterials: Introduction with examples and applications of nanoparticles, nanofibers (nanowires, nanotubes and nanorods) and nanoplates.

Composites: Polymer-nano-object blends, Metal-Matrix composites, self-repairing composites and Nanofluids for Thermal transport.

Books Recommended

1. Solid State Chemistry and its Applications, West, Wiley, 2014.
2. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
3. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
4. Principles of Solid State, H. V. Keer, Wiley Eastern; 2008.
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
7. New directions in solid state chemistry, C.N.R. Rao and J. Gopalakrishnan, Cambridge University Press, 2nd ed.
8. Nanotechnology, An Introduction, J. J. Ramsden, Elsevier, 1st Edition, 2011.
9. Essentials of Nanotechnology, J. J. Ramsden, Jeremy Ramsden and Ventus Publishing ApS, 2009.

Course No: CH17419OE
Title: Food Chemistry (02 Credits)

Max. Marks: 50
Ist Unit Exam: 25 marks

Duration: 32 Contact hours
IInd Unit (Term end) Exam: 25 marks

Unit-I

(16 Contact hours)

(a) Food Components

Chemistry of different components of food: Composition and functions of Sugars, Polysaccharides, Lipids, Proteins, Vitamins and Minerals.

(b) The Chemistry of Food Colours and flavours

Introduction. Pigments in animal and plant tissues: Chlorophyll, Carotenoids, Anthocyanins and other Phenols. Natural and artificial food colorants.

Definition of flavor. Classification of food flavors. Chemical components responsible for the following: Sweetness, Saltiness, Sourness, Bitterness, Astringency, Pungency, Meateness and Fruitiness. Synthetic flavouring.

Unit-II

(16 Contact hours)

(a) The Chemistry of Food Preservatives:

Introduction. Basis of Food Preservation. Food additives: Sodium Chloride, Nitrites, Smoke, SO₂, Benzoates and other Organic acids.

(b) The Undesirables in Food Stuff

Autooxidation and antioxidants. Modified atmosphere and vacuum packaging. Toxins of plant foods. Toxins of animal foods. Toxic agriculture residue Toxic metal residue. Toxins generated during heating and packaging of food. Environmental pollutants of food stuff.

Books Recommended

1. Food Chemistry; Owen R. Fennema; 3rd Ed.; Marcel Dekker, Inc. NY; 2005.
2. Food: The Chemistry of its components; T.P. Coultate; 3rd Ed.; RSC Paperbacks; 1996.
3. Food Flavours; Biology and Chemistry; Carolyn Fisher and Thomas R Scott; RSC Paperbacks; 1997.
4. Food Preservatives; H.J. Russell and G. W. Gould; 2nd ed.; Springer International Edition; 2005.