Course No: CH18401CR
Title: Organo-Transition Metal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Continuous Assessment: *20 marks* ***End Term Exam:*** *80 Marks*

Unit-I Sigma Organometallic Compounds: (16 Contact hours)

Classification of σ OTMC, Mechanistic pathways of kinetic instability (water, oxygen and heat), Routes of synthesis and reactions of σ OTMC, Decomposition Pathways: Choice, and mechanisms. Alpha, Beta hydrogen transfer reactions. Intramolecular elimination of alkane, Cyclometallation, Stability from bulky substituents, Agostic alkyls, Umpolung.

Metal Hydride Complexes: Synthesis, Characterization & Chemical reactions, Non classical Hydrides: Bonding and significance of Kuba's type complexes.

Unit-II Pi- Organometallic Compounds: (16 Contact hours)

Classification, Comparison of σ and π OTMC, Structure and comparative bonding in Metal-alkene, alkyne, allyl, 1, 3-butadiene and Cyclobutadiene Pi- systems.

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

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

Unit-III Catalytic Processes involving Transition Metal Organometallic Compounds: (16 Contact hours)

Mechanistic aspects: Oxidative addition, Insertion reactions and water gas shift reaction(WGSR). Designing of a homogenous Transition Metal catalyst. Tolman Catalytic loop, Catalytic efficiency: TOF, TON and e.e.

Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefinmetathesis. Monsanto acetic acid and Reppe reaction.

Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.Asymmeteric,Photo redox catalysis and supported Organometallic Catalysis (brief idea)

Carbon-Carbon coupling reactions (Suzuki and Heck).

Unit-IV Fluxional Organometallic Compounds and Synthetic Reactions involving Organo-metallics (16 Contacthours)

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^1Cyclopentadienyls and η^3–allyls.

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

Synthetic Reactions involving Organometallics:

Reactions of coordinated ligands, carbon monoxide, alkyls, alkenes (Green, Mingo's rules). Role of organo-iron compounds as synthons, Activation of small molecules:prospectus and challenges. Selected reactivities for activation of Carbon monoxide, Carbon dioxide and Alkanes.

Books Recommended:

1. The Organometallic Chemistry of Transition Metals; 2nd and 4thedn; Robert. H . Crabtree; Wiley; 1994, 2004.
2. Fundamental Transition Metal Organometallic Chemistry; Luke hart; Brooks / Cole;1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra& Singh ; New age international2000
4. Principles and Applications of Organo Transition Metal Chemistry; Collman&
5. Finke; University Science Books;1994.
6. Principles of Organometallic Chemistry; 2ndedn.;P.Powel; Chapman & Hall;1998.
7. Metallo-Organic Chemistry; A.J.Pearson;Wiley.
8. Mechanisms of Inorganic and Organo metallic reactions; Twigg; Plenum press1983.
9. Reaction Mechanism of Inorganic and Organometallic systems; 2ndedn.; Robert .b. Jordan1998.
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: CH18402CR

Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*

Continuous Assessment: *20 marks* ***End Term Exam:*** *80 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 & intra-ligand 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: Chemical actinometry.Time Resolved Spectroscopies: Time correlated Single photon counting technique, Time Resolved Transient Absorption Spectroscopies: 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. Quantum Yields of a unimolecular and bimolecular photo-chemical reaction; Quenching and Stern-Volmer plots.

Properties of thexi states; Determination of excited state dipole moments &acidity constants. Photosubstitution and photo-reduction of Co (III) complexes.Photo-substitution chemistry 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 $[Os\ (bipy)_3]^{2+}$ complexes: Structure, excited state properties and photo chemistry as sensitizers

Photochemical supra-molecular 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.Semiconductor-liquid junction solar cells: Dye sensitized and quantum dot sensitized solar cells.Metal oxide semiconductor based photo-splitting of water.

PhotochemicalNitrogen fixation and CO2 reductionwith metal complexes. 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; WileyEastern, 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.ChemEdu.;Vol .60, No.10,1983.
9. Applications of Inorganic Photochemistry; J. Chem. Edu.; Vol.74, No 69. 1997.
10. Principles and applications of Photochemistry, Brian,Wardle, Wiley 2009

Course No: CH18403CR

Title: Bio-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*

Continuous Assessment: *20 marks* ***End Term Exam:*** *80 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 enzymeaction.

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

Biological chemistry of Molybednum: uptake of Molybednum; 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_{12}: Introduction, Structure and Derivatives of B_{12} and mechanism of alkylation reaction. Role of vitamin B_{12}.

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 ChelationTherapy (16 Contact hours)

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

Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN- Metal ion promoted Carcinogenesis and probable mechanism ofaction.

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 Medicine and Biology

(16 Contact hours)

Treatment of essential trace and ultra-trace element deficiencies: Manganese, Iron, Copper, Cobalt, Zinc, Molybdenum, Silicon, Nitrogen and Phosphorus.

Metal salts as anti-acids, antiseptics and diuretics.

Metal complexes as drugs: Gold, Rhodium and arsenicals.

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

Metal Complexes as anti-virals, anti-bacterials and anti-fungals; Labile and robust metal complexes; probable mechanism of action.

Books Recommended:

1. Bio inorganic Chemistry -An introduction; Ochai, Allyn and Bacon;1977.
2. Inorganic Aspects of Biological and Organic Chemistry; Hanzilik; Academic;1976.
3. The Inorganic Chemistry of Biological processes; 2nd edn.; Hughes ; Wiley;1973.
4. A Text book of Medicinal aspects of Bio inorganic Chemistry; Das; CBS;1990.
5. The Biological Chemistry of Elements; Frausto de Silva; Williams; Clarenden;1991.
6. Principles of Bio inorganic Chemistry; Lippard, Berg; Univ. Science Books; 1994.
7. Inorganic Chemistry in Biology; Wilkins C & Wilkins G; Oxford;1997.
8. Metal -Ions in Biochemistry; P. K. Bhattacharya; Narosa Publishing House;2005.
9. Bio-Inorganic Chemistry; Robert W. Hay; Ellis Horwood Ltd; 1984.
10. Concepts and Models in Bio-Inorganic Chemistry; Heinz-Bernhard Kraatz; Wiley; 2006.

Course No: CH18404CR
Title: Seminar in Inorganic Chemistry (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: CH18405CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Continuous Assessment: *20 marks* ***End Term Exam:*** *80 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 heteroaeromatic heterocycles.

Tautomerism in heterocycles, Meso-ionic systems.

Spectroscopic properties of heterocycles (UV,Visible and ^{1}HNMR).

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,Thiepins.

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 Stutt gart,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: CH18406CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Continuous Assessment: *20 marks* ***End Term Exam:*** *80 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

Terpenoids: Introduction. Isoprene rule, classification. General methods of Isolation, separation and characterisation. Structure determination and synthesis of following representative examples of terpenoids.

Monoterpenoids: Citral, Geraniol, α- Terpineol or Limonene, Camphor or α – Pinene.

*Sesquiterpenoids***:** Farnesol or Juvenile hormone, Zingibrene and α – Santonin.

*Diterpenoids***:** Phytol.

*Triterpenoids***:** Squalene.

Carotenoids: Structure synthesis and importance of β-Carotene.

Biogenesis of Terpenoids.

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. General methods of syntheses of flavanoids,

Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & 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.2,1.L. Finar (Addison Wisley 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: CH18407CR
Title: Bio-Organic and Medicinal Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Continuous Assessment: *20 marks* ***End Term Exam:*** *80 Marks*

Unit-I Bio-Organic 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 PGF2a. 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 Bio-Organic II (16 Contact hours)

Enzymes : Introduction, nomenclature & classification.. Activation & inhibhion 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 catalsed by co-enzymes: coenzyme A, thiamine pyrophosphate. pyridoxal phosphate, NAD+, NADP+, FMN, FAD and Lipoic acid.

Unit-III Medicinal Chemistry I (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 introdction/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. Lipophillic constant, Hamett constant, steric parameters and Hansch analysis.

Unit-IV Medicinal Chemistry I (16 Contact hours)

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

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

Anti-neoplastic drug: Introduction; cancer chemotherapy, carcenoolytic 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). 3rd 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: CH18408CR
Title: Seminar in Organic Chemistry (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: CH18409CR

Title: Computational and Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*

Continuous Assessment: *20 marks* ***End Term Exam:*** *80 Marks*

Unit-I Numerical Methods-I

(a) Numerical solution of equations (12 Contact hours)

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

Solution of Equations:Bisection, false-position, Newton-Raphsonmethod 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.

Eigenvalues and Matrix Diagonalization: Eigenvalue problem, diagonalization of a matrix, Jacobi and Householder methods.

(b) Numerical differentiation (4 Contact hours)

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

Numerical differntiation:Solutions of simple differential equations by Taylor series and Runga-Kutta methods.

Unit-II Numerical Methods-II

a) Numerical Integration (3 Contact hours)

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

Numerical integration:Newton-Cotes formulae, Romberg integration, errors in integration formulae.

b) Interpolation and Curve Fitting (7 Contact hours)

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

Lagrange's interpolation method, Newton's divided differences, Cubic spline, piecewise interpolation.

Least squares approximation, linear and quadratic.

c) Use of Mathematica/Scilab/Excelin numerical methods (6Contact hours)

The mathematica/Scilab/Excel package will be used for the solution of some of the problems covered under the above three units.

Unit-III *ab initio* Calculations of Electronic Structure

a) **Hatree-Fock Self Consistent field method: (8 Contact hours)**

Hartree-Fock method: Coulomb and exchange operators and integrals, restricted Hartree-Fock formalism, Roothaan equations: the Fock matrix elements, Koopman's theorem, Matrix form of Roothaan equation. Self Consistent Field procedure. Slater-type orbitals (STOs), Gaussian type orbitals (GTOs), Basis Sets: minimal basis set, split-valence basis set, Polarization basis sets. Model SCF calculations on H_2 /HeH^+.

b) Beyond Hatree-Fock method: (8 Contact hours)

Electron correlation: Configuration state functions, configuration interaction (CI)and its calculations. Brief idea of Moller-Plesset (MP) and Coupled Cluster (CC) methods.

Density Functional Theory (DFT): Introduction,electron probability density, Hohenberg-Kohn theorems and Kohn-Sham formulation of DFT, the local density density approximations.

Unit-IV Semi-Empirical Methodsand use of Gaussian quantum mechanical package

Semi-empirical methods: (5 contact hours)

Recap of HMO theory, PPP method, brief idea of CNDO, INDO and NDDO methods.

Use of Gaussian Quantum Chemistry Software: **(11 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 /CH_3CHO,HCHOMOs.
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization $CH_2O \rightarrow HCOH$
4. NMR properties of ethane, ethene and ethyne.
5. Frequency Calculations: Input, Formaldehyde frequencies, Normal modes, zero point energy, thermodynamic properties, polarizability, hyperpolarazability.
6. Stationary points characterization –C_3H_5F
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_3.
   b) Density Functional Theory: CO_2 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 $H^+ + H_2O \rightarrow H_3O^+$
   b) Potential energy surfaces. Reaction path following (IRC calculation)
   $CH_2O \rightarrow HCOH$
   c) Heat of formation of CO_2 via an isodesmic reaction
10. Solvation models: Formaldehyde Frequencies in Acetonitrile

Books Recommended

1. Data Reduction & Error Analysis, Bevington& Robinson, (McGraw-Hill, 2003)
2. Numerical Methods for Scientists and Engineers, H. M. Antie, (TMH,).
3. Mathematical Methods for Scientists and Engineers, D.A. McQuarie, Viva Books, 1st Ed., 2009.
4. Mathematica Manual.
5. Quantum Chemistry, Ira. N. Levine, (Prentice Hall, 2009).
6. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
7. Quantum Chemistry and spectroscopy, Engel & Reid, Pearson (2007)
8. Modern Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
9. GAUSSIAN Manual, Gaussian Inc
10. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH18410CR
Title: Advanced Electrochemistry and Statistical Mechanics (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Continuous Assessment: *20 marks* ***End Term Exam:*** *80 Marks*

Unit-I Fundamental Concepts of Experimental Electrochemistry

(16 Contact hours)

Fundamentals: Electrode potential and its measurement, standard and formal electrode potentials, three electrode measurements, uncompensated resistance.
Non-Faradaic processes; ideal polarized electrode, capacitance and charge of an electrode, Double-Layer capacitance and charging current in electrochemical measurements.
Faradaic Processes; factors affecting electrode reaction rate and current. Kinetics of electrode reactions; A review of Butler-Volmer model of electrode kinetics and its implications, Marcus theory of heterogeneous charge transfer reactions, Predictions from Marcus theory.
Mass transfer**:** Convection, migration, diffusion, Fick's 1st and 2^{nd} law of diffusion, semi-empirical treatment of steady state mass transfer and transient response.

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

Potential Step Methods: Chronoamperometry, Chronocoulometry at macro electrodes; theory and applications. Cottrell equation. Controlled-Potential coulometry, Amperometric and Constant- Current coulometric titrations.
Potential Sweep Methods: Linear sweep Voltammetry and Cyclic Voltammetry at macro electrodes theory, applications and limitations. An introduction to concept and applications of pulse voltammetry.
Electrophoresis:Factors affecting ion migration, electro-osmosis, theory and applications of capillary electrophoresis.

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.
Ensembles: 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, 2ndEdition, 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 ,(NewAgeInternational,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: CH18411CR
Title: Soft Matter (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
Continuous Assessment: *20 marks* ***End Term Exam:*** *80 Marks*

Unit-I Introduction to Soft Matter, Amphiphiles and block copolymers

(16 Contact hours)

Introduction to Soft Matter: Constituents of soft matter, Intermolecular forces: van der waals, electrostatic forces, covalent bond, hydrogen bond and hydrophobic interactions.viscoelastic response

Amphiphiles: General overview of self-assembly of amphiphiles- spherical micelles, rod-like micelles, vesicles and bilayers;mixed micelle formation and its applications. Introduction and applications of stimuli-Responsive surfactants: 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 Microemulsions and Langmuir Blodgett Films (16 Contact hours)

Microemulsions: Emulsions and microemulsions, Physicochemistry of Microemulsions: Formation, Stability, and Droplet Clustering, Percolation Phenomenon in Microemulsions. Characterization of microemulsions using DLS, conductivity, viscosity and NMR techniques. Applications of microemulsions in cosmetics and detergency, pharmaceutics, soil decontamination, enhanced oil recovery and biocatalysis.

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.

Unit-III Hydrogels and Liquid crystals (16 Contact hours)

Hydrogels: Introduction, Classification of hydrogels based on type of source, crosslinking and composition. Preparation based on type of crosslinking. Introduction to stimuli responsive hydrogels and their types. Rheological properties of hydrogels (steady-state, oscillatory and thixotropic behavior). Characterization of hydrogels.Applications of Hydrogels in adsorption, 3D printing, shape memory materials, drug release and otherbiomedical applications.

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-IV Biological soft matter (16 Contact hours)

Membranes: Lipid bilayer, hydrophobicity: entropy driven interactions, self-assembly. Physics of membranes: elasticity, Helfrich energy. Plasma membrane: architecture, composition, Fluid mosaic model, membrane channels, active pumps, function.

Nucleic acids: DNA and RNA structures, double helix, structure of nucleotides, sugar phosphate backbone, nuclear bases, genetic code.

Proteins: 20 amino acids: structure and function, the peptide bond- primary structure of protein, forces determining protein structure- secondary structure, helix, sheet, turns, super secondary structures and domains, tertiary and quaternary structure of protein.

Macromolecular assemblies: Microtubules and actin filaments.

Books Recommended:

1. M. J. Rosen, J. T. Kunjappu, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 4th Edition, 2012.
2. .D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
3. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998.
4. D. Fennell Evans, H. Wennerstrom, "The Colloidal Domain where physics, chemistry, biology and technology meet" VCH, New York, 1994.
5. Robert J. Hunter, "Foundations of Colloid Science", Oxford University Press, New York, 2007.
6. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
7. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
8. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
9. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
10. Microemulsions: Background, New Concepts, Applications, Perspectives, C. Stubenrauch, Blackwell Publishing Ltd, 2009.
11. 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.
12. Ian W. Hamley, Introduction to Soft Matter: Synthetic and Biological Self-Assembly of Materials, John Wiley & Sons.

Course No: CH18412CR
Title: Seminar in Physical Chemistry (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: CH18413DCE
Title: Advanced Laboratory Course in Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

A: -Inorganic Preparations: (05 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt(III)chloride.
- Preparation of transdicholorobis(ethylenediamine) cobalt (III) chloride and its conversion to cis-isomer.
- Preparation of tris(ethylenediamine) nickel (II) chloride dihydrateand its conversion to bis(ethylenediamine) nickel (II)chloride.
- Preparationofbis(acetylacetonato)copper(II)dihydrate.
- Preparation of pentaamminecholorocobalt(III) chloride and study of Linkage isomers by its conversion topentaamminenitritocobalt(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 andEstimations: (4Experiments)

- Separation of permanganate and dichromateions on Alumina column and their Estimation from Beer Lawplots.
- Determination of lonisable chloride in a Complex by cation exchange column (separation followedbyMohr'stitrationofeluteforestimation).
- Separation of Cobalt (II) and Nickel (II) on anion exchange column followed by estimation through EDTAbacktitrations.
- Ion exchange separationof Hydration / ionization isomers of Chromium (III) Chloride ($CrCl_3$).

D: - PotentiometricTitrations: (7Experiments)

- Fun with Nernst equation: Standardization of an Iron (ii) solution with a standard dichromate solution and calculation of formal and transition potential values.
- Determination of purity of Ce(IV) Sulphate with a standard Iron (II) solution and comparison with Iron (II) dichromate experiment
- Argentometry :Estimation of Iodide with Standard $AgNO_3$ overPt&Calomel assembly using $I^- \setminus I_2$ redox coupleinvolving pseudo indicator action.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$over Ag-Glass electrode assembly and calculations of their corresponding solubility products.
- Purity assessment of $[Co(NH_3)_5Cl]Cl_2$ complex via total chloride content overAg-Glasselectrode assembly.

- Complexometric titration for determination of Ferro cyanide with standard Zinc (ii)

solution andinordertoestablishthecompositionofthecomplex$K_2Zn_3[Fe(CN)_6]_2$

- Complexation effect on redox potential of iron redox couple: Simultaneous potentiometric estimation of iron binary and ternary complex mixtures.

E:- pH-metricTitrations: (3 Experiments)

- Quantitative analysis of Chromate Dichromate mixture by pH Titration.
- Purity of Acetyl Salicylic acid (Asprin) in a commercial tablet by pH Titration.
- Study of pH influence on a pH dependent redox reaction.

F: - ConductometricTitrations: (2Experiments)

- Conductometric investigation of Silver(I) ethylenediaminecomplexation reaction.
- Conductometric analysis of a strong binary acid mixture (HNO_3 and H_2SO_4).

G:-Spectrophotometry: (6 Experiments)

- Estimation of ferrous ions in a water sample with 1,10-Phenanthroline , spectrophotometerically
- Analysis of Ferrous Iron in a Vitamin Pill
- Estimation of inorganic Phosphorus in human serum, byMolybdenumbluemethod.
- DeterminationofIronbyThiocyanateusingJob'sContinuousvariationmethod.
- DeterminationofcompositionofIron(II)—2,2-bipyridylcomplexbyMoleratiomethod.
- Determinationofrateofaquationofcomplex$[Co(NH_3)_5Cl]Cl_2$inacidic medium.

H:Nano chemistry:(2Experiments)

- Synthesizing of silver nanoparticles (Ag NP) via chemical reduction: Understanding the Impact of Size on Silver's Optical Properties.
- Synthesis of CdSeSnano-crystals exhibiting controllable photo-luminescence.

For Demonstration

- Thermal degradation studies of potassium trisoxalatoferratetrihydrate complex.
- Cyclic Voltammetric behavior of trisphenanthrolineiron(II) complex.
- Hands on training of Chem draw, Mercury and Gaussian softwares

Books Recommended:

- Vogel's quantitative analysis 6 Edn. Mendham, Denny; Pearson Education2002
- Synthesis and Technique in Inorganic chemistry , G. S.Girlomi; R.J. Angleci 3rdedn.; University ScienceBooks.
- Synthesis and characterization of Inorganic compounds W.AJolly
- Inorganic syntheses Vols II, VI AcademicPress.
- Experimental Inorganic / Physical Chemistry ;Mounir A. MalatiHorwood/1999.
- Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
- Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ;1995
- Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books2002
- Journal of Chemical Education vol. 88(2), year 2011,pp.220-222.
- Russian Journal of general Chemistry, vol 85, year 2015, pp.959-973.
- Journal of Chemical Education vol. 93(2), year 2016,pp.355-361.
- Journal of Chemical Education vol. 68(8), year 1991,pp.677-678.
- Experiments in Physical Chemistry, 5th ed. --- Schoemaker et al. (MGH,2003)
- Experimental Electrochemistry---R. Holze (Wiley-VCH,2009).

Course No: CH18414DCE
Title: Advanced Laboratory Course in Organic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***Internal Assessment****: 25 Marks*

1. **Multistep synthesis of drugs/ organic coinpouiuls involving name reactions**
   (1) Synthesis oflocal anesthetics
   (2) Synthesis of analgesics .
   (3) Synthesis of sulpha 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 Belladona 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. **Spcctrophotomctric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin
5. **Elcctrophoresis/ Paper chromatography**
   Separation and identification of aminoacids by elcctrophoresis / Paper chromatography.
6. **Spcctroscopy**
   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: CH18415DCE
Title: Advanced Laboratory Course in Physical Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *75 Marks.* ***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 CCl_4 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 $AgNO_3$
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 $BaCl_2$ and K_2SO_4/ $(NH_4)_2SO_4$
3. Estimation of the concentrations of H_2SO_4, CH_3COOH and $CuSO_4$ 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 densitometery

1. Determination of Mol. Mass of a Polymer (Polyv inyl 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.: CH18416DCE

Title: Supramolecular Chemistry (02 Credits))

Max. Marks: *50* ***Duration:*** *32 Contact hours*

Continuous Assessment: *10 marks* ***End Term Exam:*** *40 Marks*

Unit-I Acids and Bases (08 Contact hours)

Revision of Acid-Base Theories.

Hard Soft Acid Base (HSAB) Concept– Introduction, Classification, Symbiosis, Pearson-Pauling Paradox.

Utility of HSAB Concept in Drug Design, Quantitative Analyses of Metal Cations and Prediction of Direction of Inorganic Reactions.

Applications of HASB Concept to Organic Chemistry.

Unit-II Supramolecular Interactions (08 Contact hours)

Definition and Development of Supramolecular Chemistry.

Nature of Supramolecular/Non-Covalent Interactions. Hydrogen Bonding, π-π Interactions, Halogen Bonding, *van derWaal* Interactions. Quantification of non-covalent interactions: d_e-d_i and fingerprint plots.

Hydrogen bonding: Definition, Nature and Importance. Classification of Hydrogen Interactions. Identification of Weak, Moderate and Strong Hydrogen Bonds.

Organic Complexes: Co-crystals and Molecular Salts.

Unit-III Supramolecular Sensors (08 Contact hours)

Theory of Cation Sensing.SupramolecularCation Coordination Chemistry: EDTA as the Supramolecular Host. Introductory Account of Podands, Corands, Cryptands,Spherands and Calixarenes.

Theory of Anion Sensing. Scope and Challenges in Anion Sensing, Anion Hydrophobicity - Hofmeister Series, Introductory Account of Cyclophanes, Pyrolles,Azacrowns and Metal Based receptors. Hydride Sponge and Anticrowns.

Ion-Pair Receptors*:* Concept and Significance.

Unit-IV Network Solids and Molecular Devices (08 Contact hours)

Zeolites: A Brief Account.

Metal Organic Frameworks - Introduction and application in catalysis and Gas storage..

Charge Transfer Complexes -Photophysical Fundamentals and Mechanism of Energy and Electron Transfer. Organic Conductors and Semiconductors. Organic Light Emitting Diodes (OLEDs) and Transistors.

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,IstEdn**.
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),JagadeseVittal (Editor). **Wiley, 2005.**
6. An Introduction to Supramolecular Chemistry. Asim K. Das, Mahua Das, CBS Publishers and Distributors Pvt Ltd. **2005.**
7. Introduction: Supramolecular Chemistry. Huang,F.;Anslyn. E. V.*Chem. Rev.***2015**, *115*, 6999-77000.
8. Supramolecular materials. Amabilino, D. B.; Smith, D. K.; Steed. J. W. *Chem. Soc.Rev.*, **2017**, *46*, 2404-2420.
9. A Bond by Other Name.Desiraju. G. R.*Angew.Chem.Int.Ed.***2011**, *50*, 52-59.
10. The Weak Hydrogen Bond: In Structural Chemistry and Biology.Desiraju, G.; Steiner. T.**Oxford**,*IUCr Monograph on Crystallography*.
11. Application of the Principle of Hard and Soft Acids and Bases to Organic Chemistry. Pearson, R. G.; Songstad, J. *J. Am. Chem. Soc.* **1967**, *89*,1827-1836.
12. Hydrogen storage in metal–organic frameworks. Murray, L. J.;Dincă. M.; Long, J. R.*Chem. Soc. Rev.*, **2009**,*38*, 1294-1314.
13. Metal–organic frameworks: versatile heterogeneous catalysts for efficient catalytic organic transformations. Chughtai, A. H.; Ahmad, N.;Younus, H. A.;Laypkov, A.;Verpoort, F.*Chem. Soc. Rev.*, **2015**,*44*, 6804-6849.

Course No: CH18417DCE
Title: Designing Organic Synthesis (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Continuous Assessment: *10 marks* ***End Term Exam:*** *40 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**:** lntroduction. 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

14. Designing Organic Synthesis, S. Warren ;Wiley; 2013.
15. Organic Synthesis- concept, methods and Starting Materials, J. Furhop and G. Penzlin; Verlage VCH;1986.
16. Principles of Organic Synthesis2nd edn;. R. O. C. Norman; Chapman and Hall; 1978.
17. Advanced Organic Chemistry Part B, 5th edn.; F. A. Carey and R.J Sundberg ; Springer; 2007.
18. Organic Chemistry, 10th edn;. T. W. G. Solomons and Craig B. Fryhle ; Wiley-2012.
19. Organic Chemistry; Clayden, Greeves, Warren and Wothers ; Oxford University Press-2012.
20. Organic Chemistry, David Klein; John-Wiley-2012.
21. Advanced Organic Chemistry: Reactions, Mechanism and Structure, 6lh Ed., J. March,; Wiley; 2012.
22. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH18418DCE
Title: Applied Electrochemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Continuous Assessment: *10 marks* ***End Term Exam:*** *40 Marks*

Unit-I Electrochemistry for Energy conversion and Energy storage

(16 Contact hours)

Energy conversion devices:

Fuel Cell: Basic principles, advantages and limitations, fuel cell performance.

Fuel Cell Thermodynamics: Open circuit voltage, efficiency and efficiency limits, efficiency and fuel cell voltage. Operational fuel cell voltage; fuel cell irreversiblities, causes of voltage drop.

Types of fuel Cells: Alkaline, Phosphoric acid, Polymer Electrolyte membrane and direct MeOH fuel cell, biofuel cells.

Energy storage devices:Desirable characteristics of energy storage devices, Discharge plot, Ragone plot.

Batteries: How batteries work, Battery characteristics, Battery specification, Battery components. Primary and secondary batteries, Measures of battery performance. Classical batteries (Lead Acid, Nickel-Cadmium, Zinc-Mangenese dioxide). Modern batteries (Zinc-Air, Nickel- Metal Hydride, Lithium Ion Batteries).

Super-Capacitors: Energy stored in a Capacitor, advantages of electrochemical Super-Capacitor, Hybrid Super-Capacitors.

Unit-II Industrial and Environmental Electrochemistry (16 Contact hours)

Industrial Electrochemistry:

The Chloro-alkali industry: General concepts of brine electrolysis, chlorine cell-technologies, production of potassium hydroxide.

Metal extraction and refining: Electrowinning and electrorefining.

Metal Finishing: Electroplating, anodizing, electrophoretic painting.

Metal Processing: Electroforming, Electrochemical machining, electrochemical etching.**Environmental Electrochemistry**:Positive Features of Electrochemical Remediation. Direct Electrolysis of Pollutants. Indirect Electrolysis of Pollutants. Electroremediation of Soils.

Water Disinfection:Background and Principles. Electrochemical Disinfection of Water, electrodialysis, Photoelectrochemical Disinfection of Air and Water.

Books Recommended

1. Electrochemical Methods Fundamentals and Applications, 2ndEdition, Allen J. Bard, Larry R. Faulkner, John Wiley and Sons, INC.
2. Physical Electrochemistry: Fundamentals, Techniques, and Applications, 2nd Edition, Eliezer Gileadi and Noam Eliaz, 2018, Wiley-VCH.
3. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich,Wiley-VCH.
4. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bockris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
5. Fuel Cell Fundamentals, 3rd Edition, Ryan O'Hayre, Suk-Won Cha, Whitney Colella, Fritz B. Prinz, John Wiley & Sons.
6. Understanding Batteries, Ronald Dell, David Anthony James Rand,Royal Society of Chemistry, 2001.
7. Industrial Electrochemistry, 2nd Edition, D. Pletcher, F. C. Walsh, London, GB. Chapman & Hall.
8. Environmental Electrochemistry, 1st Edition, Krishnan Rajeshwar, Jorge Ibanez, Academic Press, 1997.

Course No: CH18004GE
Title: Synthetic Polymers and their Applications (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Continuous Assessment: *10 marks* ***End Term Exam:*** *40 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: CH18005GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Continuous Assessment: *10 marks* ***End Term Exam:*** *40 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. LBFilms of various compounds (hydrocarbon, liquid crystals compounds and polymers), Applications–nonlinear optical effects, conduction, photoconductivity and sensors.

Organicsolidsandfullerenes: Organics conductors, organic super conductors. Fullerenes-History, bonding , properties, doped fullerenes, fullerenes as super conductors. Carbon nano tubes: Types, Properties and Applications.

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

Luminesenceand phosphors. Lasers - general principle of lasing action, Rubylaser, semiconducing lasers and quantum cascade lasers.

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

LiquidCrystals: 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-Matrixcomposites, 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: CH18004OE
Title: Food Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
Continuous Assessment: *10 marks* ***End Term Exam:*** *40 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, Meatiness 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, SO_2, 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.