Course No: CH15401CR

Title: Organo-Transition Metal Chemistry (04 Credits).

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

External Exam: *80 Marks* ***Internal Assessment****: 20 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.

Asymmeteric 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; 6th edn; Robert. H . Crabtree; Wiley; 2014.
2. Fundamental Transition Metal Organometallic Chemistry; Charles M. Lukehart; Brooks / Cole; 1985.
3. Organometallic Chemistry; 2nd edn ; Mehrotra & Singh ; New age international 2007
4. Principles and Applications of Organotransition Metal Chemistry; Collman & Finke; University

Science Books; 1994.
5. Principles of Organometallic Chemistry; 2nd edn.; P.Powel; Chapman & Hall; 1998.
6. Metallo-Organic Chemistry; A.J.Pearson; Wiley.
7. Mechanisms of Inorganic and Organo metallic reactions; Twigg; Plenum press 1983.
8. Reaction Mechanism of Inorganic and Organometallic systems; 3rd edn.; Robert .B. Jordan, Oxford University Press 2007.
9. Inorganic Chemistry ; 4th edn.; J. Huheey ; E. Keiter & R. Keiter; Addison-Wesley ;2009
10. Modern Inorganic Chemistry; William. A. Jolly; 2nd edn. McGraw Hill; 1991.
11. Principles of Inorganic Chemistry; 1st edn.; Brain W. Pfennig; Wiley; 2015.

Course No: CH15402CR
Title: Photo-Inorganic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

Unit-1 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. Jablonoski 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 & nonadiabatic.
Properties of thexi 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 CO_2 reduction. Inorganic photolithography.
Supramolecular photochemistry in natural systems: photosynthesis, bacterial photosynthesis and artificial photosynthesis.

Books Recommended:

1. Principles and Applications of Photochemistry, B. Wardle, John Wiley, 2009
2. Ligand Field Theory and Its Applications; B. A. Figgis and M. A. Hitchman; Wiley India, 2000
3. Reaction Mechanisms of Inorganic and Organometallic Systems; 2nd edn.; Jordon; Oxford; 1998.
4. Inorganic Chemistry; G. Wulfsberg; Viva Books, 2000.
5. Mechanism of Inorganic Reactions; Katakis, Gordon; Wiley; 1987.
6. Inorganic Chemistry, Principles of structure and reactivity; 4th edn; J. E. Huheey, E. A. Keiter and R. L. Keiter. Pearson Education Inc.2003
7. Mechanism of Inorganic Reactions, 2nd edn, Basalo, Pearson; Wiley Eastern, 1997.
8. Chemistry of Light; Suppan, Royal Society; 1994.
9. Photochemistry, C. J. Wayne and R. P. Wayne; Oxford University Press; 1996.
10. Fundamentals of Photochemistry; C Rohatgi, Mukhergi; Wiley Eastern.; 1992
11. Inorganic Photochemistry; J.Chem. Edu.;Vol .60, No.10,1983.

Course No: CH15403CR
Title: Advanced Laboratory Course in Inorganic Chemistry
(04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

A: - Inorganic Preparations: (5 Experiments)

- Preparation of tetraamminecarbonatocobalt (III) nitrate and its conversion to pentaamminecholorocobalt (III) chloride.
- Preparation of trans dicholoro 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 pentaamminecholorocobalt (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 lonisable 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 $[Co(NH_3)_6]\ Cl_3$ and $[Co\ (NH_3)_5\ Cl]\ Cl_2$ 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 I^- \ I2 redox couple.
- Simultaneous determinations of Chloride and Iodide ions with Standard $AgNO_3$ over Ag-Glass electrode assembly.
- Determination of the purity of $[Co\ (NH_3)_5Cl]\ Cl_2$ over Ag-Glass electrode assembly.
- Complexometric titration for determination of Ferro cyanide with standard Zinc (II) solution and inorder to establish the composition of the complex $K_2Zn_3[Fe(CN)_6]_2$

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: (6 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.
- Spectrophotometric determination of inorganic phosphorus in human serum.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ 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:

1. Chromatography: Basic Principles, Sample Preparations and Related Methods; 1st edn; E. Lundanes; L. Reubsaet; T. Greibrokk; Wiley-VCH; 2013
2. Vogel's quantitative analysis; 6th edn.J. Mendham, R.C.Denny;J. D. Barnes; M.J. Kthomas; Pearson Education; 2002
3. Analytical chemistry; 6th edn.; G. D. Christian; John Wiley; 2003
4. Modern Analytical Chemistry; D. Harvey; McGraw-Hill Higher Education; 2000
5. Principles and Practice of Analytical Chemistry; 5th edn.; F. W. Fifield; D. Kealey; Balckwell Sciences; 2000.
6. Chromatographic methods; 5th edn.; A. Braithwaite; F.J. Smith; Kluwer Academic Publishers; 1999
7. Essence of Chromatography; 1st edn.; C. F. Poole; Elsevier; 2003
8. Synthesis and Technique in Inorganic chemistry; 3rd edn; G. S. Girlomi; R. J. Angleci; University Science Books; 1999
9. Synthesis and characterization of Inorganic compounds; W. A Jolly; Prentice-Hall; 1970
10. Inorganic syntheses; Vols II, VI; Academic Press.
11. Experimental Inorganic / Physical Chemistry ; M. A. Malati; Horwood;1999.
12. Quantitative Chemical Analysis ; 5th edn.; Harris ; Freeman ; 1999.
13. Advanced Practical Inorganic Chemistry ; Adams ; Raynor, Wiley ; 1995.
14. Advanced Experimental Inorganic Chemistry ; Ayodha Singh ; Campus Books 2002

Course No: CH15404CR
Title: Heterocyclic Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks* ***Internal Assessment****: 20 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 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: CH15405CR
Title: Chemistry of Natural Products (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks* ***Internal Assessment****: 20 Marks*

Unit-I Terpenoids and Carotenoids (16 Contact hours)

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

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

Structure determination, stereochemistry and synthesis of α-terpeneol, 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 Androsterone, Testosterone and Progesterone.

Glucocorticoids & Mineral Corticoids: Introduction and partial synthesis. Mechanism of action 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 flavanoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.

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: CH15406CR

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

Max. Marks: *100* ***Duration:*** *128 Contact hours*
External Exam: *80 Marks.* ***Internal Assessment****: 20 Marks*

1. **Multistep synthesis of drugs/ organic compounds involving name reactions**
   (1) Synthesis of local anesthetics
   (2) Synthesis of analgesics .
   (3) Synthesis of 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 b-carotene from tomato. Characterisation of lycopene/P-carotene by uv -absorption process.
   (2) Isolation of limonene from its natural source and physicochemical analysis.
   (3) Assay of Belladona for Hyoscyamine.
   (4) Assay of lemon for citric acid and vitamin-C
   (5) Isolation of cholesterol from gallstone
   (6) Assay of coke (soft drink)
3. **Column Chromatography**
   Separation of two component solid mixture. Identification using physical, chemical and spectral techniques. Paper Chromatography
4. **Spcctrophotometric estimation** (UV/visible)
   (1) Vitamin-C (Ascorbic acid)
   (2) Caffeine from tea.
   (3) Cholesterol
   (4) Aspirin

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 V

Course No: CH15407CR
Title: Advanced Quantum Chemistry (04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks* ***Internal Assessment****: 20 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 H_2 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: Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2 /$HeH^{+.}$

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; brief idea of CNDO, INDO and NDDO methods. The MINDO, MNDO, AM1 and PM3 methods.

Unit-III Density Functional and Semi-Empirical Methods (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 functional.

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 /CH_3.CO.CH_3, HCHO MOs
2. Geometry Optimization: Input and Output for ethene, fluoroethene, propene conformers
3. Transition state optimization
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) Electron densities of substituted benzenes.
   (b) Hydration enthalpy of the reaction $H^+ + H_2O \rightarrow H_3O^+$
   (c) Potential energy surfaces. Reaction path following (IRC calculation) $CH_2O \rightarrow HCOH$
   (d) Heat of formation of CO_2 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. Molecular Quantum Chemistry - Introduction to Advanced electronic structure theory - A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).
6. Modern Electronic Structure Theory, D. R. Yarkouy (ed). (World Scientific, 1995)
7. Ab Initio Molecular Orbital Theory**,** by Hehre, Radom, Schleyer and Pople, (Wiley)
8. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989).
9. Molecular Modeling, Principles and Applications, A. R. Leach, Prentice-Hall, 2001
10. GAUSSIAN Manual, Gaussian Inc
11. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc

Course No: CH15408CR
Title: Statistical Mechanics and Advanced Electrochemistry
(04 Credits)

Max. Marks: *100* ***Duration:*** *64 Contact hours*
External Exam: *80 Marks* ***Internal Assessment****: 20 Marks*

Unit-I 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 coefficient in the classical limit, second and third virial coefficients.

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

Unit- II Quantum Statistics (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.

Heat capacity of solids, Einstein and Debye models (Partition function, Average energy and heat capacity). Limitations of the models.

Unit-III 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 1^{st} and 2^{nd} law of diffusion, Cottrell equation.

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

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

Unit-IV 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 bioelectrosysnthesis- oxidation of alcohols, synthesis of dihydroxy acetone phosphate, site specific oxidation of sugars, reduction of carbonyl compounds, hydrogenation.

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

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

Books Recommended

1. 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. Bokris 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: CH15409CR
Title: Advanced Laboratory Course in Physical Chemistry
(04 Credits)

Max. Marks: *100* ***Duration:*** *128 Contact hours*
External Exam: *80 Marks* ***Internal Assessment****: 20 Marks*

A. Tensiometry

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

B. Cryoscopy

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

C. Spectrophotometry

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

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. Estimate the surface area of a working electrode through chronoamperometry and chronocoulometry.
2. Using Cyclic Voltammetry 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 (Polyvinyl alcohol) using viscosity method.
2. Explore the nature of chemical bonding (head-head and Head tail linkage of monomers) in polyvinyl alcohol using Viscometry.
3. Determination of partial molar volume of sodium chloride solutions as a function of concentration from density measurements.

Books Recommended

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

Course No. CH15410DCE
Title: Bio-Inorganic Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

Unit-I Iron Storage, Transport and Oxygen carriers (08 Contact hours)

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.

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 (08 Contact hours)

Zinc enzymes:- Carboxypeptadiase and Carbonic Anhydrase- introduction, structure, mechanism of action and their model compounds.

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 Chelation Therapy (08 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.

Unit-IV Metal Salts and Metal Complexes in Therapeutics (08 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; Clarenden; 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: CH15411DCE
Title: Acid Base, Non-Aqueous & Inorganic Polymer Chemistry
(02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

Unit-I Acids and Bases (08 Contact Hours)

Acid-Base Theories: Lowry Bronsted, Lewis, Lux Flood & Usonavich.

Super acids: Introduction, Hammet Acidity Function, Details of HF, H_2SO_4, HSO_3F based super acid systems and & their uses.

HSAB: Concept, Classification, Parameters, Pearson-Pauling paradox.

Applications of HSAB concept in Geochemical differentiation of chemical elements. Qualitative analyses of metallic cations, Redox chemistry, Drug designing and Chelation theory.

Unit-II Reaction in Non-aqueous Solvents (08 Contact Hours)

Properties of a solvent: Classification of Non-aqueous solvents; Comparison of aqueous and non-aqueous solvents, details of important chemical reactions in liquid H_2SO_4, NH_3, SO_2, BrF_3 and N_2O_4.

Unit-III Inorganic Polymers-I (08 Contact Hours)

Classification, and reasons for delayed introduction of Inorganic Polymers.

Inorganic Polymeric Reactions: Condensation, Addition, and Coordination. Types and Significance of Coordination polymers.

Boron Nitrides: Carboranes & Metallocarboranes and Fluorocarbons: Introduction, Preparation, Properties, Structure-Bonding and Uses.

Unit-IV Inorganic Polymers –II (08 Contact Hours)

Polymeric Sulfur and Sulfur Nitrides: Preparations, properties, Structure-Bonding and Uses.

Polyphosphates: Preparation, Reactions, Properties, Structure-Bonding and Uses.

Silicates: Classification, Properties, Structure and Uses.

Silicones: Preparation, Reactions, Properties, Structure-Bonding and Uses.

Books Recommended

1. Inorganic Chemistry Gary Wulfsberg; Viva Books, 2002.
2. Inorganic Chemistry; 4th edn; Huheey, Keiter and Keiter, Pearson Education ; 1983.
3. Chemistry of Elements; 2nd edn; Greenwood , Earnshaw; ButterworthHeinemann;1998.
4. Advanced Inorganic Chemistry, 5th edn ; F.A.Cotton & G.Wilikinson; Wiley;1988.
5. The Chemistry of Non aqueous solvents; Vols II & III Lagowski; Academic Press.
6. Development of Inorganic Polymer Chemistry; Lappert& Leigh; Elsevier; 1962. Fluoropolymers; Wall; Wiley; 1972.
7. Inorganic Polymers NJLRay; Academic Press; 1978.
8. Inorganic Porymers James. E.Mark, HarryAllock & Roberta West; Prentice Hall.
9. Inorganic Porymers F.G-A-Stone & W. A. Graham; Academic Press.

Course No: CH15412DCE

Title: Medicinal Chemistry (02 Credits)

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

External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

Unit-I **(08 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.

Unit II **(08 Contact hours)**

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 III **(08 Contact hours)**

Antibiotics: Classifications-structural and mechanistic, cell wall biosynthesis inhibitors, protein synthesis inhibitors. Pencillins-classification and structures. Synthesis of Pencillins, V, G, chloramphenicol.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 anticancer agents (Taxol) role of alkylative agents and antimetabolites in treatment of cancer, mitotic inhibitors (elementary idea).

Unit IV **(08 Contact hours)**

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

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

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. Medicinal Chemistry- V. K. Ahluwalia 2009, Ane Books Pvt.Ltd
5. Foye's Principles of Medicinal Chemistry 5th Ed. David A Williams 2002. Lippincott Williams and Williams.
6. The Organic Chemistry of Drug Design and Action 2nd Ed 2004, Richard B Silverman

Course No: CH15413DCE

Title: Designing Organic Synthesis (02 Credits)

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

External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

Unit-I 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.

Unit-II 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-III Designing Organic Synthesis-I (8 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.

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.

Unit-IV Designing Organic Synthesis-II (8 Contact hours)

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).

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, 6lh Ed., J. March,; Wiley; 2012.
9. Organic Synthesis- The disconnection Approach; Sturat Warren; Wiley; 2013

Course No: CH15414DCE
Title: Chemistry of Materials (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

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

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

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

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

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

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

Unit-III Optical materials (8 Contact hours)

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

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

Unit- IV Solid electrolytes and High Tc Superconductors (8 Contact hours)

Ionic Conductors: Introduction to ionic conduction, types of ionic conductors, mechanism of ionic conduction- interstitial jumps (Frenkel) and vacancy mechanism. Super-ionic conductors: Diffusion and transition superionic conductors. Examples and applications of ionic conductors.

High T_c superconductors: Superconductors: Properties and types. high Tc superconductivity in cuprates: Structure and preparation of 1-2-3 materials, mechanism of high Tc superconductivity, Applications of High Tc materials.

Books Recommended

1. Introduction to Solids, Azaroff, Tata McGraw, 1993.
2. Solid State Chemistry and its Applications, West, Wiley, 2014.
3. The Physical Chemistry of Solids, Borg, Biens, Academic press, 1992.
4. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders college, 2001
5. Principles of Solid State, H. V. Keer, Wiley Eastern; 2008.
6. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
7. The Physics and Chemistry of materials, J.I. Gersten, F.W. Smith, John Wiley and sons, Inc. 2001.
8. New directions in solid state chemistry, C.N.R. Rao and J. Gopalakrishnan, Cambridge University Press, 2nd ed. 1997.
9. Introduction to superconductivity, Micheal Tinkham, Dover books, 2nded. 2004.

Course No: CH15415DCE
Title: Computational Chemistry (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

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

Unit- II 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 Runga-Kutta methods.
Numerical integration: Newton-Cotes formulae, Romberg integration, errors in integration formulae.

Unit- III 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, piecewise interpolation.
Least squares approximation, linear and quadratic.

Unit-IV Use of Mathematica 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: CH15416 DCE

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: CH15417GE
Title: Synthetic Polymers and Applications (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
External Exam: *40 Marks* ***Internal Assessment****: 10 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: CH15418GE
Title: Basic Organic Reactions- The Biological Connection
(02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

Unit-I Substitutions Reactions (08 Contact hours)

Introduction to Organic substitution reactions.

Nucleophilic substitutions: Chemical and enzymatic hydrolyses of glycosidic bonds - An example of S_N reaction. Mustard gas and treatment of neoplastic disease. Benzo [a] pyrene and nitrosoamines and cancer. Biological S_N1 reaction involving allyl cations. Biosynthesis of glycosides via UDP sugars - A S_N2 process. N - Acetylation of amino sugars.

Esterificaiton in oils and fats. Transesterification: Prohibition of biosynthesis of prostaglandins by Aspirin. Transesterification of triglycerides with ethanol to get biodiesel.

Unit-II Addition Reactions (08 Contact hours)

Introduction to Organic Addition Reactions.

Electrophilic additions: Electrophilic addition to carbocations in Terpenes. Alkylation of steroidal side chain during biosynthesis of Lanosterol to Ergosterol, Stigmasterol and β-Sitosterol. Nucleophilic addition to carbonyl group. Amide formation during synthesis of peptides and proteins. Unique structure of amide bond.

Addition of alcohols to carbonyl group**:** Hemiacetal and Acetal formation in sugars. Formation of glycoside**:** Chemistry and Stereochemistry.

Enzyme catalysed addition to α, β-unsaturated carbonyl compound. Michael acceptors as Carcinogens. Pericyclic reactions in biological systems.

Unit-III Condensation Reactions (08 Contact hours)

Introduction to condensation reactions.

Aldol reaction between formaldehyde and glycoaldehyde and formation of glycoaldehyde through benzoin condensation between formaldehyde and HCN during biosynthesis of carbohydrates.

Claisen and Aldol reactions in nature.

(a) HMG-CoA and Mevalonic acid.
(b) In biosynthesis of phenols.
(c) Claisen reaction involving Acetyl Coenzyme A and Malonyl Coenzyme A
(d) Reverse Claisen reaction: β-oxidation of fatty acids.
(e) Aldol and reverse aldol reactions during carbohydrate-metabolic pathway.
(f) Reactions at α-carbon atom in biological systems.
(g) Enzymatic aldol reaction through involvement of enamines.
(h) Nature's enolates: The lysine enamines and coenzyme A.

Biological Transamination

Unit-IV Biological Oxidation –Reductions (08 Contact hours)

Introduction to redox reactions.

Oxidations in biological systems: Autooxidation in fats and oils – The origin of rancidity. Natural antioxidants Antioxidants-mechanism of action Radical oxidation in prostaglandins. Oxidative phenol coupling in biosynthesis of morphine / thyroxine. Biological oxidation of pregnelonone to progesterone and cholesterol to choles-4-ene-2-one. Mechanism of oxidations by FMN and FAD. Oxidation of alcohols by NAD^+.

Reduction in biological systems: NADH and NADPH - The biological equivalents of $NaBH_4$. Reductions by $FADH_2$ and $FMNH_2$. Reductive amination in nature.

Books Recommended

1. Foundation of Inorganic, Organic and Biological Chemistry; Cavet, Denniston and Topping; W.C Brown Publicaiton; 1995.
2. Organic and Biological Chemistry; John R. Holum; Wiley; 2001.
3. Essential of Organic Chemistry; Paul M. Dewick; Wiley; 2006.
4. Paula Bruice; Organic Chemistry; Paula Y. Bruice; Pearson; 2012.
5. Organic Chemistry; F.A Carey and Robert Giuliano; Tata McGraw Hill; 8th Ed. 2012.
6. Organic Chemistry; Clayden, Greeves, Warren and Wolthers, Oxford University Press; 2012.

Course No: CH15419GE
Title: Novel Materials (02 Credits)

Max. Marks: *50* ***Duration:*** *32 Contact hours*
External Exam: *40 Marks* ***Internal Assessment****: 10 Marks*

Unit-I Block Co-Polymers and Langmuir Blodgett Films (08 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.

Unit- II Organic Solids and Molecular Devices (08 Contact hours)

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

Molecular devices: Molecular rectifiers and transistors, switches and sensors.

Unit-III Optical materials: (08 Contact hours)

Luminesence and phosphors. Lasers - general principle of lasing action, Ruby laser, semiconducing 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.

Unit- IV Nanomaterials and composites (8 Contact hours)

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: CH15420OE
Title: Food Chemistry (02 Credits)

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

Unit-I Food Components (08 Contact hours)

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

Unit-II The Chemistry of Food Colours and flavours (08 Contact hours)

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-III The Chemistry of Food Preservatives: (08 Contact hours)

Introduction. Basis of Food Preservation. Food additives: Sodium Chloride, Nitrites, Smoke, SO_2, Benzoates and other Organic acids.

Unit-IV The Undesirables in Food Stuff (08 Contact hours)

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.