Syllabi of the Courses

In

M.Sc. IV Semester (Chemistry)

Effective from September – 2013

Specialization Courses in Inorganic Chemistry

Course No: CHM-401
Title: Organo-Transition Metal Chemistry

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit-I **(12 hrs)**
Sigma Bonded Organometallic Compounds:

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 **(12 hrs)**
Pi-bonded Organometallic Compounds:

Classification, Structure and bonding in Metal- alkene, alkyne, allyl, 1,3-butadiene and Cyclobutadiene Complexes.
Sandwich Compounds: Characteristics; Classification, Synthesis, Reactions, Structure and bonding of Ferrocene.
Compounds with Transition Metal to Carbon multiple bonds: Alkylidene (Schrock and Fischer) Synthesis; Structural characteristics; Nature of bonding. Reactions and their synthetic applications.

Unit—III **(12 hrs)**
Catalytic Processes involving Transition Metal Organometallic Compounds:

Mechanistic aspects: Oxidative addition, Insertion reactions Reductive elimination and water gas shift reaction (WGSR).
Catalytic mechanism of Hydrogenation, Hydroformylation, Oxidation and Isomerization of alkenes; Olefin metathesis.
Fischer-Tropsch Synthesis and Ziegler Natta polymerization of alkenes.
Asymmeteric and supported Organometallic Catalysis (brief idea)

Unit—IV **(14 hrs)**

Fluxional Organometallic Compounds and Synthetic Reactions involving Organo-metallics:

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:

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

Course No. CHM-402
Title: Bio-Inorganic Chemistry.

Maximum Marks: 100 ***Total Duration-50 hrs.***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit-I **(14hrs)**
Iron Storage, Transport and Oxygen carriers:

Structure and Coordinating sites in biologically important ligands: Proteins, Nucleotides and Lipids.
The transport mechanism: uniport, symport and antiport.
Ferritin and Transferrin: Structure, Metal binding sites; incorporation and release of iron.
Porphyrins: Introduction, characteristic absorption spectrum and salient characteristics.
Haemoglobin and Myoglobin: Structure, oxygen saturation curves; Mechanism of oxygen transport and storage.Bohr effect and cooperativity in haemoglobin.
Hemerythrin and Hemocyanin: Structure, Metal binding groups and Dioxygen binding. Synthetic oxygen carrier model compounds: Vaska's iridium complex: Cobalt complexes with micro and macrocyclic ligands and Schiff base ligands.

Unit-II **(12hrs)**
Metallo-enzymes and Electron Carriers:

Enzyme, Apoenzyme, Coenzyme, Prosthetic group and Metalloenzymes, Mechanism of enzyme action.
Zinc enzymes:- Carboxypeptadiase, Carbonic Anhydrase and Alcohol. Dehydrogenase: Introduction, Structure, Mechanism of action and their model compounds.
Molybednum enzymes: An overview of the major molybdenum enzymes.
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 **(14hrs)**

Metal-Ion Induced Toxicity and Chelation Therapy:

Toxic levels of different metals. Sources of metal ion poisoning (external sources and internal disorders).
Mechanism of metal ion induced toxicity:- Toxicity of Pb, Cd, Hg, As, and CN^-
Metal ion promoted Carcinogenesis and probable mechanism of action.
Therapeutic Aspects of Chelating Drugs :- Conditional stability constant , Stereochemistry, Lipophilicity. HSAB theory and Plasma mobilizing index(PMI).
Types of Chelation Therapy: Single, Double, Synergistic and Mixed ligand chelation therapy.
Therapeutic index of different chelating drugs in metal ion detoxification. Radio protective chelating drugs.
Limitations and Hazards of Chelation therapy

Unit-IV **(10hrs)**

Metal Salts and Metal Complexes in Therapeutics:

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

Gold compounds and Rhematoid arthiritis.

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:

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

Course No: CHM-403
Title: Photo-Inorganic Chemistry

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit-1

(I5hrs)

Basics of Photo-Chemistry:

Absorption; mechanism of absorption of light

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

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

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

(I5hrs)

The Chemistry of Excited State Molecules:

Photochemical laws & quantum yield. Kinetics & quantum yield of photo-physical (radiative) and photo-chemical processes. Photochemical processes: primary, secondary, adiabatic & non- adiabatic. Properties of 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: (10hrs)

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: (10hrs)

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:

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

Course No. CHM-404
Title: Seminar lecture in Inorganic Chemistry

Max. Marks: 50

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

Part A : **Marks: 25**

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

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

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

Course No: CHM-405L
Title: Laboratory Course in Inorganic Chemistry.

Maximum Marks: 150 ***Total Duration-150 hrs***
External Examination Marks: 120 ***Internal Assessment Marks: 30***

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 $[Co(NH_3)_5Cl]Cl_2$ 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 $I^- \backslash I2$ 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: (5 Experiments)

- Determination of Iron (II) with 1,10-Phenanthroline.
- Determination of Phosphate by Molybdenum blue method.
- Determination of formula of Iron (III) thiocyanate complex by Job's Continuous variation method.
- Determination of composition of Iron (II)—2,2-bipyridyl complex by Mole ratio method.
- Determination of rate of Aquation of complex $[Co(NH_3)_5Cl]Cl_2$ 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:

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

Elective Course in Inorganic Chemistry
Course No: CHM – EC-01
Title: Inorganic Polymers

Maximum Examination Marks: 50 ***Total Duration: 25 hours***
External Marks: 40 ***Internal Assessment Marks: 10***

Unit-I **(05 hours)**
Introduction to Inorganic Polymers:

Definition, Classification and Comparison with organic polymers.
Inorganic Polymeric Reactions: Condensation, addition and coordination.
Applications and characterization of Inorganic polymers.

Unit-II **(08 hours)**
Boron-Nitrogen and Sulphur-Nitrogen Compounds:

Bonding in higher boranes: Types of bonds, empirical rules for bonding in boron clusters, a detailed account of carboranes and metallocarboranes.
Boron-Nitrogen and Sulphur-Nitrogen: Properties, structure, bonding and uses of Borazines, Boron nitride, Polythiazyls and Sulphur Nitrides.

Unit-III **(07 hours)**
Phosphorus Nitrogen Polymers and Polyphosphates:

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

Unit-IV **(05 hours)**
Silicon-Oxygen Polymers:

Silicates: Classification, structure and bonding.
Zeolites: Potential applications as ion exchangers, adsorption agents, catalysts and gas separators.
Silicones and Polysiloxanes: Preparation, properties, bonding and uses.

Books

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

Specialization Courses in Organic Chemistry

Course No: CHM-406
Title: Heterocyclic Chemistry

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit I
Structure and Nomenclature of Heterocyclic compounds: 13 hrs
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: 13 hrs
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: 12 hrs
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: 12 hrs
Structure, Synthesis and reactions of Benzo- fused heterocycles like Benzo-pyrrole, Benzo-furan,Benzo-thiophene, Quinoline, Isoquinoline, Chromones, Coumarins, Iso-Coumarins, 2 and 4-benzopyrones, Benzopyryllium salts and purines.

Recommended Books:

1. Heterocyclic Chemistry, 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. CHM-407
Title: Chemistry of Natural Products

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit-I

Terpenoids and Carotenoids: **(12 hrs)**
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-terpineol, abietic acid and β-carotene.

Unit-II

Alkaloids: **(13 hrs)**
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: **(15 hrs)**
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: **(10hrs)**
Introduction, classification, physical, chemical, degradative and spectral methods of structure determination and biosynthesis (Acetate and Shikimic acid pathway)
Flavonoids: Isolation, separation and quantification. Antioxidant activity of flavonoids. Robinson's synthesis, Baker Venketraman synthesis, Kostanecki synthesis of flavanone and Flavanol.
Isolation, structure determination and synthesis of Cyanidin, Chrysin, Quercitin & Genestein.
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. CHM-408
Title: Bio-Organic and Medicinal Chemistry

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit-I **(12 hrs)**

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

Prostaglandins : Introduction and nomenclature, approaches to prostaglandin synthesis, cyclo-hexane, precursors-Woodward synthesis of PGF_{2a}. Cyclo-heptane precursors -Corey's synthesis of prostoglandin's E & F.Their relationship with oxygenase I and II.

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

Unit-II **(13 hrs)**

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 **(13 hrs)**

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 **(12 hrs)**

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. CHM-409
Title: Seminar lecture in Organic Chemistry

Max. Marks: 50

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

Part A: **Marks: 25**

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

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

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

Course No: CHM- 410L
Title: Laboratory Course in Organic Chemistry

Maximum Marks: 150 ***Total Duration-150 hrs***
External Examination Marks: 120 ***Internal Assessment Marks: 30***

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 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.

4. Spcctrophotomctric estimation (UV/visible)

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

5. Elcctrophoresis/ Paper chromato^raphy

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 V

Elective Course in Organic Chemistry
Course No: CHM-EC-02
Title: Organic synthesis

Maximum Marks: 50 ***Total Duration-25 hrs***
External Examination Marks: 40 ***Internal Assessment Marks: 10***

Unit-I
Oxidative and Reductive Processes in Organic Synthesis: 7 hrs

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: 6 hrs

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: 6 hrs

The disconnection approach: Introduction to synthons, their types and equivalent reagents. Reversal of Polarity(umpolung). One group, two group and Reteroelectrocyclic disconnections. Reterosynthetic Analysis involving connections and rearrangements. Guidelines for good disconnections.
Reterosynthetic analysis of alcohols, amines (aliphatic and aromatic), alkenes, carbonyl compounds, carboxylic acids and their derivatives using one group disconnecitons and FGIs. Use of acetylenes in the syntheses of above mentioned compounds.

Unit-IV
Designing Organic Synthesis-II: 6 hrs

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

Specialization Courses in Physical Chemistry

Course NO: CHM- 411
Title: Computational and Quantum Chemistry

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit-I

Numerical Methods: (13 hrs)

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

a. Solution of Equations:

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

b. Numerical calculus and interpolation

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

Newton-Cotes formulae, errors in integration formulae. Lagrange's interpolation, piece-wise interpolation and Cubic splines.

c. Eigenvalues and Matrix Diagonalization:

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

Unit-II

Electronic Structure Theory, Hartree-Fock Method: (13 hrs)

Review of Hartree-FockMethod, HF Equation, Fock, Coulomb and exchange operators and integrals, restricted and unrestricted Hartree-Fock formalism, Roothaan equation,. The Fock matrix elements, Koopman's theorem, Slater-Condon rules. Matrix form of Roothaan equation, the SCF procedure. ….5 hrs

Slatter-type orbitals, Gaussian basis sets. Model SCF calculations on H_2/HeH^+. 3 hrs

Configuration Interaction: Electron correlation, configuration interaction (CI), configuration state functions, Brillouin theorem, full and truncated CI theories- CID, CISD, CISDTQ, Size consistency problem. Moller-Plesset and Coupled Cluster methods. ….5 hrs

Unit-III

Density Functional and Semi-Empirical Methods: (12 hrs)

Density Functional Theory: Electron probability density. Hohenberg-Kohn theorems, Kohn-Sham formulation, n- and v- representabilities, the local density approximation, E_x&$E_c$functionals. …5hrs

Semiempirical methods: The ZDO approximation. Detailed treatment of CNDO, INDO and NDDO theories.Introduction to MNDO, AM1 and PM3 methods.
Molecular mechanics methods, force fields. …5 hrs

Molecular Properties: Basic ideas about molecular geometry, Optimization of molecular geometry: quasi_newton, steepest descent and conjugate gradient methods. Molecular vibrational frequencies, thermodynamic properties. …3 hrs

Unit- IV

Quantum Chemistry Software Packages: (12 hrs)

A. A quick tour of GAUSSIAN Interface. Input to Gaussian. Model calculations illustrating various features of the package**..(** The book '**Exploring Chemistry with Electronic Structure Methods**' by Forseman and Frichwill be used for these experiments**)** ….10hrs

1. A single point energy calculation: HCHO /CH_3.CO.CH_3, HCHO MOs
2. Geometry Optimization: Input and Output for ethene, fluoroethene- comparison. Transition state optimization($H_3CO \rightarrow H_2COH$)
3. Optimization and NMR chemical shift for methane and benzene
4. Frequency calculations: Input, Formaldehede frequencies, Normal modes, zero point energy, polarizability, heperpolaraziability.
5. Stationary points characterization –C_3H_5F, 1, 3 hydrogen shift on C_3H_5F PES
6. Model Chemistries: Basis set effect on HF bond length. Periodic trends in transition metal-complexes ($M(CO)_6$, M= Cr, Mo, W)
7. Selecting an appropriate theoretical method:
   a) Semi-empirical methods: AM1 calculation on TTP (tretraphenylporphin)
   b) Post SCF methods, Electron correlation , MP and CC methods: HF bond energy, Optimization of O_3.
   c) Density Functional Theory: CO_2 structure and atomization energy.
   d) Butane / Isobutaneismerization energy, acetaldehyde –ethylene oxide isomerization barrier.

8. 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)
    $CH_2O \rightarrow H_2 + CO$
    d) Isodesmic reactions: Modellingthe $\Delta_f H$ of CO_2 via an isodesmic reaction.

B. Semi-empirical/Dynamics package MOPAC (general Introduction) …2hrs

Books Recommended:

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

Course NO: CHM- 412

Title: Self Assembling in Colloidal systems and Advanced Electrochemistry

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit- I

Self-assembly of surfactants and its consequences: (13 hrs)

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

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

Unit- II

Self assembly of block copolymers and polymer-surfactant mixtures: (12 hrs)

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

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

Unit-III

Instrumental Methods in Electrochemistry: (12 Hrs)

Fundamentals: Electrode potential and its measurement, Standard and formal electrode potentials, three electrode measurements, uncompensated resistance. Overview of Electrode Processes-Faradaic and Nonfaradaic processes, factors affecting electrode reaction rate. Mass transfer: Convection, migration, diffusion, Fick's 1^{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: (13 Hrs)

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. D. Fennell Evans, H. Wennerstrom, "The Colloidal Domain where physics, chemistry, biology and technology meet" VCH, New York, 1994.
2. Robert J. Hunter, "Foundations of Colloid Science", Oxford University Press, New York, 2007.
3. P.C. Heimenz, "Principles of Colloid and Surface Chemistry", Marcel Dekker Inc. New York, 1986.
4. M. J. Rosen, "Surfactants and Interfacial Phenomena", John Wiley & Sons, New York, 2004.
5. R. D. Vold and M. J. Vold, "Colloid and Interface Chemistry", Addison-wesley, 1982.
6. D. Y. Meyer, "Surfaces, Interfaces and Colloid", VCH Publishers, Inc. 1991.
7. Jonsson, Lindmann, Homberg and Kronberg, "Surfactants and polymers in aqueous solution", John Wiley and sons, 1998
8. Colloids and Interfaces with Surfactants and Polymers – An Introduction J. W. Goodwin, 2004, John Wiley & Sons Ltd, ISBN: 0-470-84142-7 (HB) ISBN: 0-470-84143-5 (PB).
9. Frederik Wurm, Holger Frey: Linear–dendritic block copolymers: The state of the art and exciting, perspectives, *Progress in Polymer Science* 36 (2011) 1–52
10. M.J.Lawrence & G.D.Rees,Advanced Drug Delivery Reviews,Vol,45,p 898,2000.
11. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
12. I. W. Hamley, The Physics of Block Copolymers (Oxford University Press, Oxford, 1998.
13. P. Alexandridis and J. F. Holzwarth, Curr. Opin. Colloid Interface Sci. 5, 312 (2000).
14. N. Hadijichristidis, S. Pispas and G. A. Floudas Block Copolymers (Wiley, New York, 2003).
15. Electrochemical Methods Fundamentals and Applications, 2nd Edition, Allen J. Bard, Larry R. Faulkner, John Wiley and Sons, INC.
16. Physical Electrochemistry-Principles, Methods and Applications, Israel Rubinstein (Ed.) Marcel Dekker, Inc. New York.
17. Understanding Voltammetry, 2nd Edition, Imperial College Press.
18. Elements of Molecular and Biomolecular Electrochemistry, Jean-Michel Saveant, Wiley-Interscience.
19. Electrochemistry, 2nd Edition, Carl H. Hamann, Andrew Hammett, Wolf Vielstich, Wiley-VCH.
20. Modern Electrochemistry 2B, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.
21. Handbook of Electrochemistry, C. G. Zoski (Ed.) Elsevier.

Course NO: CHM- 413

Title: Non-Equilibrium and Statistical Thermodynamics

Maximum Marks: 100 ***Total Duration-50 hrs***
External Examination Marks: 80 ***Internal Assessment Marks: 20***

Unit- I

Non-equilibrium Thermodynamics: (12 hrs)

Irreversible processes and uncompensated heat, degree of advancement, reaction rate & affinity. Gibb's equation, entropy production, entropy production due to matter flow, heat flow, charge flow & chemical reactions. …6 hrs

Concept of forces & fluxes, Onsager's theory of irreversible processes-phenomenological laws, their domain of validity. Chemical reactions near equilibrium. Transformation properties of forces and fluxes. Electrokinetic phenomena. …6 hrs

Unit-II

Classical Statistical Mechanics and Ensembles: (12 hrs)

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 …7 hrs

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. …5 hrs

Unit-III

Quantum Statistics: (12 hrs)

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 …5 hrs

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 ..6 hrs

Unit- IV

Statistical Thermodynamics of Interacting Systems: (14 hrs)

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

Statistical Mechanical treatment of imperfect gases. Virial equation of state from grand partition function, virial coefficient in the classical limit, second and third virial coefficients. …5 hrs

Statistical thermodynamics of solutions: Lattice model, regular solution theory, Statistical Mechanics of polymer solution. …4 hrs

Books Recommended:

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

Course No: CHM- 414

Title: Seminar Lecture in Physical Chemistry

Max.Marks-50

Each student shall be attached with a particular teacher of Physical Chemistry section who in consultation with the student concerned will assign a topic of current/ general interest.

Part A : **25 Marks**

The student shall consult literature/internet and collect the relevant material. He/she will prepare a review on the topic and shall submit in a prescribed format (both hard and soft copies).

Part B : **25 Marks**

The candidate will deliver the seminar lecture on the date and time fixed for the purpose.

Both the components shall be evaluated internally by a group of teachers of the concerned branch, headed by the senior most teacher. The total marks of the course out of 50 shall be communicated to the controller of examination.

COURSE NO: CHM-415

Title: Laboratory Course in Physical Chemistry

Maximum Marks: 150 ***Total Duration-150 hrs***
External Examination Marks: 120 ***Internal Assessment Marks: 30***

A. Tensiometry

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

B. Cryoscopy

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

C. Spectrophotometry

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

D. Spectrofluorometry

1. To determine the rate constant for fluorescence quenching of anthracene or perylene by CCl_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 formation constant of Ag-NH_3 complex.
4. Determination of (a) Standard electrode potential & (b) Activity Coefficient.

F. Conductometry

1. Verification of Debye-Huckel-Onsagar law.
2. Precipitation titration of $BaCl_2$ 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 alchol) using viscosity method.
2. Explore the nature of chemical bonding 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).

Elective Course in Physical Chemistry
Course No: CHM-EC-03
Title: Chemistry of Materials

Maximum Marks: 50 ***Total Duration-25 hrs***
External Examination Marks: 40 ***Internal Assessment Marks: 10***

Unit-I

Langmuir Blodgett Films and Liquid crystals: (6 hrs)

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.

….3 hrs

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. ..3hrs

Unit- II

Organic Solids and Molecular Devices: (6 hrs)

Organic solids and fullerenes: Organics conductors, organic superconductors, magnetism in organic materials. Fullerenes- History, bonding, properties, doped fullerenes, fullerenes as superconductors and fullerene related compounds (carbon nanotubes) …4 hrs

Molecular devices: Molecular rectifiers and transistors, artificial photosynthetic devices, switches and sensors. ..2 hrs

Unit-III

Optical materials: (6 hrs)

Luminesence and phosphors. Lasers – general principle of lasing action, Ruby laser, Neodymium-YAG lasers, semiconducing lasers, quantum cascade and quantum dot lasers. …..4 hrs

Nonlinear optical effects, second and third order harmonic generation, nonlinear optical materials. ..…2 hrs

Unit- IV

Semiconductor electrodes: (7 hrs)

Review of Structure of seminconducting/electrolyte interface, Band bending. Kinetics of electron transfer reactions and fundamentals of photoelectrochemical phenomena across semiconductor/electrolyte interface; photoelectrochemical cells (photoelectrosynthesis and photogalvanic cells)., Photoelectrocatalysis-water splitting and electroreduction of CO_2.

Books Recommended:

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