VISVA-BHARATI

DEPARTMENT of CHEMISTRY

M. Sc. SEMESTER-WISE COURSE and CREDIT STRUCTURE

New Syllabus for M. Sc. from the Session 2019-2020 onwards

Convention of new paper codes: In **Paper Code MCH41-I M stands for M Sc, CH stands for Chemistry, 4 for 4th Semester, 1 for 1st paper, I for Inorganic.**

M. Sc. First Year, Semester I (5T+1P), (Total Marks: 300)

Original Course Code	Proposed Course Code	Subject	Marks	CP	No. of Lectures
CH 701	MCH11-I	Inorganic Chemistry (core)	50 (40 + 10)	4	50 L
CH 702	MCH12-I	Inorganic Chemistry (core)	50 (40 + 10)	4	50 L
CH 703	MCH13-O	Organic Chemistry (core)	50 (40 + 10)	4	50 L
CH 704	MCH14-O	Organic Chemistry (core)	50 (40 + 10)	4	50 L
CH 705	MCH15-P	Physical Chemistry (core)	50 (40 + 10)	4	50 L
CH 706	MCH16-PP	Physical Practical (core)	50 (40 + 10)	4	

M. Sc. First Year, Semester II (4T+2P), (Total Marks: 300)

Course No.	Proposed Course Code	Subject	Marks	CP	No. of Lectures
CH 807	MCH21-I	Inorganic Chemistry (core)	50 (40 + 10)	4	50 L
CH 808	MCH22-O	Organic Chemistry (core)	50 (40 + 10)	4	50 L
CH 809	MCH23-P	Physical Chemistry (core)	50 (40 + 10)	4	50 L
CH 810	MCH24-P	Physical Chemistry (core)	50 (40 + 10)	4	50 L
CH 811	MCH25-IP	Inorganic Practical (core)	50 (40 + 10)	4	
CH 812	MCH26-OP	Organic Practical(core)	50 (40 + 10)	4	

M. Sc. Second Year, Semester III (2ET + 3OT +1OP), (Total Marks: 300)

Course No.	Proposed Course Code	Subject	Marks	CP	No. of Lectures
CH 913	MCH31-E1	Elective-1	50 (40 + 10)	4	50 L
CH 914	MCH32-E2	Elective-2	50 (40 + 10)	4	50 L
CH 915	MCH33-I MCH33-O MCH33-P	Optional	50 (40 + 10)	4	50 L
CH 916	MCH34-I MCH34-O MCH 34-P	Optional	50 (40 + 10)	4	50 L
CH 917	MCH 35-I	Optional	50 (40 + 10)	4	50 L

	MCH 35-O MCH 35-P				
CH 918	MCH 36-IP MCH 36-OP MCH 36-PP	Optional (Practical)	50 (40 + 10)	4	

M. Sc. Second Year, Semester IV (4OT +1 Project), (Total Marks: 300)

Course No.	**Proposed Course Code**	**Subject**	**Marks**	**CP**	**No. of Lectures**
CH 1019	MCH41-I MCH41-O MCH41-P	Optional	50 (40 + 10)	4	50 L
CH 1020	MCH42-I MCH42-O MCH42-P	Optional	50 (40 + 10)	4	50 L
CH 1021	MCH43-I MCH43-O MCH43-P	Optional	50 (40 + 10)	4	50 L
CH 1022	MCH44-I MCH44-O MCH44-P	Optional	50 (40 + 10)	4	50 L
CH 1023	MCH45-PJ	Project*	100 (80 + 20)	8	

[N.B: (i) T = Theory; P= Practical; E= Elective; CP=Credit point; I/O/P = Inorganic/Organic/Physical; IP/OP/PP = Inorganic Practical/Organic Practical/Physical Practical; PJ = Project

(ii) *Project has to be executed from Semester-III and it will be evaluated in Semester-IV]

M. Sc. Semester-I

Theoretical

MCH11-I: Inorganic Chemistry (Core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Coordination Chemistry- Bonding, Stereochemistry and Structure: (13L)

Symmetry and Isomerism; ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, magnetic properties.

2. Complexes in Aqueous Solutions: (12L)

Metal ligand stability constant and its controlling factors, different tools of studying (pH-potentiometric, polarographic, spectrophotomectric, volumetric)and methods of measuring stability constants of complexes, Bjerrun half ň method, stability of mixed ligand complexes and calculations, determination of composition (Jobs, mole ratio and slope ratio methods), evaluation of thermodynamic parameters

3. Molecular Magnetism-I: (15L)

Basic concepts of magnetism, magnetization and magnetic susceptibility, types of magnetic behavior (dia-, para-, ferro-, ferri- and antiferro-) and their temperature dependence, Curie and Curie-Weiss laws, temperature independent paramagnetism, Pascal’s Constants and its utilities, determination of χ_M in solution, usefulness of μ_s and μ_j equation respectively for transition and inner transition series, van Vleck’s equation and its applications, spin-orbit coupling, zero-field splitting, quenching of orbital angular momentum, high-spin/low-spin equilibrium, types of exchange interactions, introduction to magnetic material: A systematic theoretical and experimental approach.

4. Electronic Spectra of Transition Metal Complexes: (10L)

Russel-Saunders (R-S) terms-Inter electronic repulsion parameters (B), splitting of R-S Terms in different Geometries, Orgel and Tanabe-Sugano diagram, selection rules for spectral transitions, calculation of Dq, B and β parameters, different types of d-d bands and their assignment, charge transfer bands.

LEARNING OBJECTIVES: (I) To introduce the various theories of coordination compounds; To study the origin of nephelauxetic effect; To gain knowledge about the impact of electronic, steric and Jahn-Teller effects; (ii) To introduce the metal ligand stability constant and its controlling factors; To gain knowledge about the methods of measuring stability constants of complexes: Bjerrun method; Able to determine the composition (Jobs, mole ratio and slope ratio methods) (iii) To introduce magnetism, followed by approach to the part of the topic; Preliminary discussions of different magnetic phenomenon e.g. Isolated and cooperative magnetism taking suitable molecules. (ix) Finally Interactions of different magnetic interactions pathways and their suitability of application part (x) Origin and importance of electronic spectral beheviour of transition metal compounds (xi) General nature of d-d, f-f (both Lanthanides and Actinides elements) of spectral properties with both theoretical and experimental viewpoints.

LEARNING OUTCOME: (i) Understanding theories of coordination compounds and capable of applying it (ii) Application of Bjerrun method in the determination of stability constants and Job's method in evaluating the composition of complexes (iii) To understand the importance of Molecular Magnetism in the present context (iv) Design approach of molecule towards applications and correlation between magnetic and spectral properties

M. Sc. Semester-I

Theoretical

MCH12-I: Inorganic Chemistry (Core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Cage, Metal Clusters and Ring Compounds: (13L)

Cage compounds- higher boron hydrides- structure and reactivity, equation of balance-styx numbers, Lipscomb topological diagrams, Wades rules, Jemmis' unifying electron counting rule, carboranes, metallocarborane, metalloborranes and heteroboranes, phosphorous cage compounds, metal clusters- cluster classification, skeletal electron counting, bonding in metal clusters, polyhedral skeleton electron pair theory (PSEPT),low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: application of isolobal and isoelectronic relationships, capping rules, Zintl ions.

2. Polymer Chemistry-1: (12L)

Basics: concepts of monomers, repeat units, degree of polymerization, classification of polymers, polymerization and kinetics of polymerization, polymer characterization- number, weight and viscosity average molecular weights, polydispersity index and molecular weight distribution, measurement of molecular weight, some inorganic polymers: synthesis, structural aspects and applications of silicones and siloxanes, borazine, silicates, phosphazenes, polyphosphates and polysulphates.

3. Organometallic Chemistry-1: (13L)

Alkyls and aryls of transition metals– types, routes of synthesis, stability and decomposition pathways, agostic interactions, organocopper in organic synthesis; compounds of transition metal-carbon multiple bonds: alkilidenes, alkylidynes, low-valent carbenes and carbynes-synthesis, nature of bonds, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis

4. Electro-analytical method-1: (12L)

Electrochemical cell, decomposition and discharge potential, current voltage diagram,electrodes, reversible and irreversible electrode processes, potentiometry & potentiometric titration, membrane electrodes, Donnan potential, ion-selective electrodes, Nikolskii-Eisenman equation, Cottrell Equation, Randles-Sevčik equation, excitation and switching potential, cyclic voltametry and its applications.

LEARNING OBJECTIVES: (i) To acquire knowledge on borones, carboranes, metallocarborane, metalloborranes and phosphorous cage compounds in the light of equation of balance, styx numbers, Lipscomb topological diagrams, Wades rules and Jemmis' unifying electron counting rule; Acquire knowledge of metal cluster in the light of polyhedral skeleton electron pair theory (PSEPT); (ii) Learn basic concepts of polymer and polymerization; Create interest in gaining knowledge regarding various average molecular weights of polymer and glass transition temperature; Exposure of various functional polymers-such as fire retarding polymers, electrically conducting polymers, biomedical polymers (contact lens, dental polymers, artificial heart, kidney, skin and blood cells) and self-healing polymers (iii) To gain knowledge about the nature of bonding in alkilidenes and alkylidynes; To gain knowledge on the chemical reactivity of 'Fischer and Schrock' carbenes and carbynes; (iv) Restatement of electrochemical cell to introduce decomposition potential, current-voltage diagram, potentiometric titration with special reference to inorganic systems, concept of ion-selective electrodes and their application in analytical chemistry, Donnan potential and Nikolskii-Eisenman equation along with their utility in analytical methods, votametry and polarography, analytical implications of dropping mercury electrode, Cottrell Equation and Randles-Sevčik equation, Heyrovsky-Ilkovic equation and plot, and cyclic voltametry and its analytical applications

LEARNING OUTCOME: (I) Understanding and prediction of structure and bonding of inorganic cage, metal cluster and ring compounds & able to correlate the structure and property of inorganic cage, cluster and ring compounds; (ii) Understanding the institute-industry interaction in the field of polymer science and search job opportunity through this course; (iii) Gaining intrest in the field of organometallic chemistry; (iv) Gaining keen interest to perform experimental research based on electroanalytical method.

M. Sc. Semester-I

Theoretical

MCH13-O: Organic Chemistry (Core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Static Stereochemistry: (12L)

Molecular symmetry and chirality, Conformation of acyclic and cyclic systems (3 to 5 and 7 to 8 membered ring), conformation of rings with single and multiple double bond, conformation of 3 to 6 membered heterocycles, stereoelectronic effects in heterocycles, optically active compounds with no asymmetric carbon, Baldwin's rule, stereochemistry of fused ring and bridged ring compounds (with special reference to decalin and phenanthrene systems).

2. Dynamic Stereochemistry: (12L)

Conformation and reactivity, Curtin-Hammett principle and Wenstein-Eliel equations, conformation reactivity and mechanism of acyclic and cyclic system (nucleophilic substitution reaction, formation and cleavage of epoxide ring, addition reactions to double bonds, elimination reactions, pyrolytic syn-elimination, oxidation of cyclohexanols, neighbouring group participation reactions), stereoelectronic effects, elementary idea about asymmetric synthesis.

3. Reactions Mechanism I: (13L)

Substitution reactions: Aliphatic nucleophilic substitution — S_N1, S_N2, mixed S_N1 and S_N2, SET mechanisms;neighbouring group participation by *pi*- and *sigma*-bonds, anchimeric assistance; S_Ni mechanism; nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon; effect of substrate structureson reactivity, nucleophiles, leaving group and reaction medium; phase transfer catalysis, regioselectivity; Aromatic nucleophilic substitution — S_NAr, benzyne and $S_{RN}1$ mechanisms; effect of substrate structureson reactivity, leaving group and attacking nucleophile; Aliphatic electrophilic substitution — S_E1, S_E2, and S_E^i mechanisms; electrophilic substitution accompanied by double bond shifts; effects of substrates, leaving group and solvent polarity on the reactivity, Aromatic electrophilic substitution — the arenium ion mechanism; orientation and reactivity; energy profile diagrams; the *ortho*/*para*ratio; orientation in other ring systems; *ipso* attack; *Free radical reactions*: types of free radical reactions; free radical substitution mechanism; mechanism at an aromatic substrate; neighbouring group assistance; reactivity for aliphatic and aromatic substrates at a bridgehead; reactivity in the attacking radicals; effects of solvents on reactivity; allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids; auto-oxidation; free radical rearrangements

Elimination reactions: E1, E2 and E1cB mechanisms; product stereochemistry; effects of substrate structures, attacking base, leaving group and the medium on reactivity; mechanism and orientation in pyrolytic elimination

4. Reaction Mechanism II: (13L)

Addition reactions: Addition to carbon–carbon multiple bonds — mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals; region- and chemoselectivity; orientation and reactivity; addition to carbon–hetero multiple bonds — mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles; addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds; Mechanism of condensation reactions involving enolates — Aldol, Knoevenagel, Claisen, Perkin and Stobbe reactions

Rearrangement reactions: Formation and stability of carbonium ions, carbanion, carbenes, nitrenes, radicals and arynes, rearrangement involving carbocation (Wagner-Meerwein, Pinacol-Pinacolone rearrangement), reaction involving acyl cation, PPA cyclization and Fries rearrangement, rearrangement of carbenes (Wolff &Arndst-Eistert synthesis), rearrangement of nitrenes (Hoffmann, Curtius, Schmidt, Lossen, Beckmann rearrangement); sigmatropic rearrangements

Metathesis and click chemistry: Definition, classes of reactions, catalysts used, mechanistic aspects and synthetic applications of methathesis reactions and click reactions in organic chemistry with suitable examples

LEARNING OBJECTIVES: Static and dynamic stereochemistry would provide the students enough opportunity to learn some advanced aspects of stereochemistry of organic compounds. Initially students will receive an idea on the correlation between molecular symmetry and chirality of organic molecules. Special emphasis would be given to conformational aspects of small to large ring sized asymmetric organic molecules. Subsequently stereochemistry of fused and bridged ring organic compounds would be discussed. Discussion on conformation and reactivity of various organic compounds on the basis of Curtin-Hammet principle is another important objective of the proposed topic. Stereochemical outcome in reactions like SN1, SN2, E1, E2, E1CB, epoxidation, NGP etc would be thoroughly discussed. Finally students will be familiarized with fundamental of asymmetric synthesis. Advanced knowledge on the reaction mechanism will also be acquired by the student in this course. Starting from basic steps the students will learn the intricate cases of reaction mechanism. In addition to fundamental steps they will learn the metathesis and click chemistry.

LEARNING OUTCOME: At the end of this course the students will be able to analyze and predict the stereochemistry of organic product molecules after a certain reaction. They shall be able to design synthetic strategy to obtain a target organic compound of practical importance with optically enriched form. Moreover the students will have a solid background on fundamental steps of organic chemistry. On the basis of this fundamental knowledge they can analyze any type of organic problems related to the reactions.

M. Sc. Semester-I

Theoretical

MCH14-O: Organic Chemistry (Core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Heterocyclic Chemistry of Fused Ring System: (12L)

indole, isoindole, tryptophan, quinoline, isoquinoline, carbazole, acridine, 1,8-naphthyridine, benzazepine, xanthene; synthesis/reactions/applications.

2. Green Chemistry:(13L)

the need of green chemistry, principles of green chemistry, concept of atom economy, tools of green chemistry – microwaves, ultrasound, ionic liquids, supercritical H_2O and CO_2 as solvents etc., green chemistry in real world cases and planning green synthesis in chemical laboratory.

3. Some Selective Name Reactions (Part-A): (12L)

Shapiro reactions, Mitsunobu reaction, Hofmann-Loffler-Freytag reaction, Barton reaction, ene reaction, Mannich reaction, Stork enamine reaction, Michael addition, Robinson annulations, Barton decarboxylation and deoxygenation, Sharpless asymmetric epoxidation.

4.Some Selective Name Reactions (Part-B): (13L)

Birch reduction, aldol condensation, Wittig reaction, Prevost reaction, Simmons-Smith cyclopropanation, Nef reaction, Favorskii reaction, Baeyer-Villigeroxidation, Claisen rearrangement, Beckmann rearrangement etc.

LEARNING OBJECTIVES: Heterocyclic chemistry is one of the most applied branches of organic chemistry and of utmost practical and theoretical importance. As a result, a great deal of research carried out in chemistry is devoted to heterocyclic chemistry. The aim of the present paper is to make the students know about some important simple heterocyclic ring systems containing heteroatom and their nomenclature and numbering. They will also know the synthesis, reactivity and the occurrence of these heterocycles. Students will learn proper applications of Name reaction for useful transformations and their mechanistic pathway. The objective of Green chemistry is to evaluate and design the new chemical products and processes that minimize adverse impacts on human and environmental issues. Conceptual Topics Green chemistry leverages chemists' ability to design new beneficial/sustainable substances and processes while taking into account the interconnectedness with local and global systems. This approach, called systems thinking, is a problem-solving strategy that identifies and understands the key components of a system, in contrast to an isolated part, then investigates solutions based on the system interactions. Teaching a systems approach challenges students to apply scientific principles to solve real-world problems, demonstrates chemistry's role as an essential science in finding solutions, and prepares future scientists for the collaborative interdisciplinary work required.

LEARNING OUTCOME: At the end of this course the students will have a basic background on the structure, synthesis and reactivity of several heterocyclic molecules. After learning the green chemistry course, students will gain the skills and vision that will enable them to contribute to a sustainable future through chemistry. With the full inclusion of Green Chemistry concepts, students of all disciplines, not just the chemical sciences, will have the ability to relate chemical concepts to the "real world" and to their chosen career path. Moreover, the students will be able to use several name reactions for achieving a target for synthesis.

M. Sc. Semester-I

Theoretical

MCH15-P: Physical Chemistry (core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Introductory Quantum Mechanics Revisited and Operator Algebra: (13L)

Wave-particle duality, uncertainty principle, postulates of quantum mechanics, Schrodinger waveequation and its solution, wave function and its probabilistic interpretation, orthogonality and normalization, eigenvalues and eigenfunctions, definition of various operators e.g. linear operator, Hermitian operator, inverse operator etc., theorems of quantum mechanics, eigenvalue equation, Commutation relationand its physical significance, Operators and observables, Matrix formulation of quantum mechanics.

2. Quantum Mechanics of Model Systems: (12L)

a) Free Particle & Particle-in-a-box:

Free Particle, particle-in-a-1d/2d/3d box with discussions on energy quantization, selection rules, Bohr's correspondence principleetc., checking the validity of Schrodinger wave equation based oncorrespondence principle and Heisenberg's uncertainty principle, tunneling.

b) Harmonic Oscillator:

Solution of Schrodinger equation by operator method as well as by solving the differential equation, selection rules, checking the validity of Schrodinger wave equation based on correspondence principle and Heisenberg's uncertainty principle, tunneling.

LEARNING OBJECTIVES OF UNIT 1 AND 2: The objective of this course is to introduce the basic principles of Quantum mechanics and to solve few model problems using those principles.

LEARNING OUTCOME: A student will have knowledge of postulates of quantum mechanics, operator algebra, commutation relations, uncertainty principles. Students will also learn the techniques how to solve Schrodinger equation for simple model systems. By the end of this course the student should get prepared for taking more advanced course on quantum chemistry in the coming semesters.

3. Ion-ion Interaction: (12L)

Ion association, Symmetric and asymmetric ion-pair formation, Bjerrum theory, the fraction of ion-pair, triple ion formation, determination of ion-association constant, activity coefficient of electrolytes, extended Debye-Hückel theory, Pitzer equation for activity coefficient, experimental determination of mean ionic activity coefficient.

4. Ion-Solvent Interaction: (13L)

Solvation of ions, solvation number, Frank-Wien model of ionic solvation, Born model, thermodynamics of ionic solvation, enthalpy and free energy of solvation of ions, experimental determination of solvation of ion.

LEARNING OBJECTIVES OF UNIT-3 AND 4: The objectives of this course are to know the behavior of the electrolytes in terms of the ionic aspects of electrochemistry in details.

LEARNING OUTCOME: True electrolytes are completely dissociated into ions when the parent salts are dissolved in water. The dependence of many of their properties on the concentration is determined by the interactions between the ions. Ion-ion interactions help to understand their thermodynamic and chemical properties. When an ionic crystals breaks into free ions in solution, they are stabilized by the solvent sheaths. So, there are number of models which establish this phenomenon of the interactions of an ion with the neighboring solvent molecules. Ion-solvent interactions are an essential part of the electrolytic solution which affects the equilibrium properties of the ionic solution. So unit-4 helps the students to get the clear picture of the ion-solvent interactions which regulate the different properties of electrolyte solutions.

M. Sc. Semester-I

Practical (core)

MCH16-PP: Physical Chemistry

Full Marks: 50 (40 + 10); Credit point: 4

1. To determine the rate constant of a reaction in a micellar media by conductometric method.
2. To verify Ostwald dilution law and determine the K_a of a weak acid by conductometric method.
3. To determine the composition of a mixture of acetic acid, sodium acetate and ammonium acetate by conductometry.
4. To study the formation of charge transfer complex and determination of stoichiometry of the complex conductometrically.
5. To determine the rate constant and salt effect on the rate constant of decomposition of $K_2S_2O_8$ by KI using spectrophotometric method.
6. To determine the dissociation constant of an indicator by spectrophotometry.
7. To study the kinetics of alkaline hydrolysis of crystal violet by spectrophotometry.
8. To determine the pK_avalue of a poly-basic acid by pHmetry and preparation of buffer solution of desired pH range.

LEARNING OBJECTIVES: In this course the students will get the benefit to know how one can determine experimentally physical quantities like the rate constant, dissociation constant of a weak electrolyte, determination of stoichiometry of the complex and composition of mixture of acids based on their theoretical study on chemical kinetics, conductance of an electrolytic solutions, ionic equilibrium and spectroscopy, respectively.

LEARNING OUTCOME: The students will enrich their understanding on the physical chemistry through the practical classes. It is expected to be a very good opportunity for a student to talk with the nature based on the demand from the class room teaching or elsewhere. Here a student can check his/her level of common sense in basic science by which he/she can gossip with other. At the same time the students will be read to do more sophisticated experiments in the coming semesters.

M. Sc. Semester-II

Theoretical

MCH21-I: Inorganic Chemistry (Core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Inorganic Reaction Mechanism-I: (13L)

Energy profile of a reaction, application of different reaction parameters in understanding reaction mechanism-linear free energy relationship, effect of leaving group, non-leaving group, entering group, steric hindrance and acceleration, solvent exchange reaction, importance in suggesting reaction mechanism, derivation of some important rate laws, kinetically indistinguishable schemes, techniques of fast kinetics, classification of ligand substitution reaction mechanism, associative, dissociative, interchange, etc., Eigen mechanism, proton ambiguity, internal conjugate base formation

2. Bioinorganic Chemistry-I: (12L)

Metal ions in biology, myoglobin, hemoglobin, heamocyanin, hemeerythrin, cytochromes, rubredoxin, feredoxins; biological fixation of nitrogen, chlorophyll and photosynthesis; PS-I, PS-II, bioenergetics and ATP cycle, glucose storage, Na^+/K^+ ion pump, ionophores

3. Structure and Properties of Solids: (13L)

Structure of mixed oxides-spinel, inverse spinel, ilmenite, perovskite, OSSE; crystal defects-intrinsic and extrinsic, thermodynamics of crystal defects, Schottkey and Frenkel defects; color centers, dislocations, Burger vectors and Burger circuits, non-stoichometric compounds; electronic properties of solids-conductors, semiconductors, insulators, superconductors; ferroelectricity, anti-ferroelectricity, piezoelectricity, pyroelectricity, cooperative magnetism, quantum theory of paramagnetism, photoconductivity.

4. Thermo-analytical Methods (12L)

Introduction to thermal analysis: thermo-gravimetric analysis (TGA), differential thermo-gravimetric analysis (DTGA), differential thermal analysis (DTA) – principles and methods, presentation of thermal data, differential scanning calorimetry (DSC): a brief outline and a comparative discussion of DSC with DTA, thermal degradation, laws governing nucleation and growth of nuclei, applications of thermal methods of analysis with special reference to solid state reactions, decomposition of inorganic compounds.

LEARNING OBJECTIVES: (i) The objective of first unit is to highlight the kinetics and mechanism of ligand substitution reactions of transition Metal Complexes. It aims to understand the different factors specially, the crystal field effect on the reaction pathways, lability and inertness of the metal complexes; (ii) The interdisciplinary subject of unit-2 has developed through the cross-fertilization of the knowledge emerged from the studies in different areas like Chemistry, Biochemistry, Physics, Biology, Medicine, etc. The main objective to introduce the studies of Bioinorganic Chemistry is to project the role of trace elements (both metals and non-metals) and inorganic chemistry in the biological system. The students are expected to know the important metallobiomolecules including the metalloenzymes functioning in our system; (iii) while going through unit-3 students will learn the method for looking at structural features of complex oxides like spinels, ilmenite, perovskites and related systems in detail. Broad discussion of all possible defects, dislocations, Burger vectors and Burger circuits will be conducted. The dielectric properties like ferroelectricity, anti-ferroelectricity, piezoelectricity, pyroelectricity with specific examples will he discussed; (iv) In unit-4 the learners will be introduced to the thermal analysis techniques and their importance in analytical methods and reaction kinetics of decomposition of inorganic compounds. A broad discussion on TGA, DTA and DSC will be presented followed by a precise comparison between them and their utilization. A brief introduction to the laws of nucleation and growth of nuclei with simple mathematical approach will be highlighted.

LEARNING OUTCOME: (i) After learning the subject, the students will be able to compare the organic reaction mechanism (taught from the very beginning of Chemistry Honours Course) and inorganic reaction mechanism. The students will also be able to realise the role of crystal field theory in controlling the reactivity of inorganic meal complexes; (ii) Moreover the students will be able to understand the importance of the inorganic elements besides the carbon, hydrogen, oxygen and nitrogen in the biological system. The students will also be able to understand the role of metal ions in the basic biological processes like photosynthesis, respiration, nitrogen fixation, etc.

M. Sc. Semester-II

Theoretical

MCH22-O: Organic Chemistry (Core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Natural Products with Special Reference to Biosynthesis: (12L)

Natural products: biosynthesis of a) non-nitrogenous secondary metabolites from shikimic acid, flavonoids and related polyphenolics, b) mono and diterpenoids from mevalonic acid c) triterpenoids from geranylpyrophosphate.

2. Structure and Functions of Proteins and Lipids: (13L)

Structure and functions of proteins: chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, Ramachandran diagram, forces responsible for holding of secondary structures, □-helix, □-sheet, tertiary structure of protein folding, quaternary structure, biosynthesis of peptide chain, lipids: fatty acids, structure and functions of triacylglycerols, glycerophospholipids, properties of lipid bilayers, biological membranes, fluid-mosaic models of membrane structure.

3. Enzymes, Receptors and Nucleic Acids: (12L)

Enzymes: chemical and biological catalysis, properties of enzymes like catalytic power, specificity and regulation, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site directed mutagenesis, mechanism of enzyme action: transition state theory, example of some typical enzyme mechanisms, e.g. chymotrypsin, ribonuclease, concept of receptors, nucleic acids: purine and pyrimidine bases of nucleic acids, base pairing via H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it, structure of different RNAs, and biosynthesis of peptide chain.

4. Coenzyme Chemistry: (13L)

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, structure of pyridoxal phosphate (PLP), PLP dependant enzymes, reactions catalyzed by PLP dependant enzymes, racemisation, decarboxylation, transamination, structure of NAD^+, $NADP^+$, interconversion between acetaldehyde and enthanolcatalyzed by yeast alcohol dehydrogenase, stereospecificity of the reduction of aldehyde by NAD-dependant enzyme, FMN, FAD, mechanism of reactions catalyzed by falvoprotein.

LEARNING OBJECTIVES: The aim of the present paper is to make the student acquainted with the structure and function of proteins, genetic materials and other secondary metabolites. Detailed knowledge on these small and macromolecules gives them the abiliy to correlate the important biological processes with sructures of carbohydrates, amino acids, lipids and nucleic acids. They can understand the importance of several classes of protein molecules like enzyme, receptors in terms of their chemical structure and can understand the controlling processes of life in biological cell. Together with the knowledge on conenzyme structure and mechanism of action it will be prossible for them to correlate the importance of vitamins in several biological processes.

LEARNING OUTCOME: At the end of the course the students will be able to explain several biological processes in terms of chemical structure and function of the macromolecules. They will also be able to diagonize the activity of life in terms of molecular properties.

M. Sc. Semester-II

Theoretical

MCH23-P: Physical Chemistry (core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Group Theory-I: (10L)

Introduction to symmetry, symmetry elements and symmetry operations, definition of a group, point symmetry groups, group multiplication tables, theorems of groups, conjugate elements and class, symmetry operators and their matrix representations, function space, reducible and irreducible representations, equivalent representations, characters of representations.

2. Group Theory-II: (14L)

Great orthogonality theorem: statement and interpretation, proof of its corollaries, character table and its construction, number of times an irreducible representation occurs in a reducible one, the reduction of reducible representations, notation of irreducible representations, representations andquantum mechanics, the invariance of Hamiltonian operator under symmetry transformations, direct product representation, molecular vibrations, symmetry species of the vibrational mode, selection rules for infra-red and Raman spectra, crystal field splitting, SALC of atomic orbitals.

LEARNING OBJECTIVES OF UNIT-1 AND 2: The objective of this course is to introduce the idea of symmetry and Group theory and the connecting link between chemistry and group theory. The role of symmetry in understanding the bonding, reactivity, spectroscopic activities of different molecules will also be explored in this course.

LEARNING OUTCOME: By the end of this course, students will be able to identify the point group a molecule belongs, symmetry species of the normal modes of vibration and their spectroscopic activities. The student will learn how to generate molecular orbitals by symmetry adapted linear combination of atomic orbitals (SALC) which will help one doing quantum chemistry calculation with more ease.

3. Quantum Mechanics of Rotational Motion: (12L)

Angular momentum operators and their commutation relations, operator algebra and ladder operators for rotational motion, solution of Schrodinger equation using the operator method as well as the technique for solution of differential equation, quantum Mechanics of rigid rotor and its application.

4. Hydrogen-like Atoms: (14L)

Separation of translational and internal motion of a two-body problem, determination of radial part of the wavefunction, relation among principal, azimuthal and magnetic quantum number, nodal properties of angular part as well as the radial part of the hydrogen atom wavefunction, shape of the orbitals, space quantization, selection rules for hydrogen atom.

LEARNING OBJECTIVES OF UNIT-3 AND 4: To provide the students idea of how rotational motion of microscopic particles can be treated quantum mechanically giving rise to important concepts of space quantization, quantization of angular momentum and various selection rules associated with rotational motion. They will also learn the use of transformation of coordinate from Cartesian to spherical polar and use of Relative and COM coordinates. Study of Hydrogen atom will provide the technique of exact solution of the Schrödinger equation and acquaintance with some important differential equations like Legendre and Laguerre.

LEARNING OUTCOME: Clear conception of quantization of rotational motion will help the students pursue research works in the difficult field of quantum mechanics. The knowledge acquired will help the students able to work in the field of opto-electronic devices which has tremendous engineering and technological applications.

M. Sc. Semester-II

Theoretical

MCH24-P: Physical Chemistry (core)

Full Marks: 50 (40 + 10); Credit point: 4

1. Statistical Thermodynamics: (13L)

Motivation for study, entropy and probability, Stirling's approximations, Maxwell-Boltzmann distribution, Gibbs paradox, Sackur-Tetrode equation, concept of partition functions, translational, rotational, vibrational and electronic partition functions, thermodynamic properties in terms of partition functions, equilibrium constant , equipartition principle, Einsteinand Debye theory of specific heat capacity of solids.

LEARNING OBJECTIVES OF UNIT-1 : Through this course the students will learn the connection between the macroscopic properties of a thermodynamic system and the dynamics associated with the microscopic constituents. Here they may surprise to know that all the thermodynamical properties can be connected with the partition function which is the central quantity in the subject, statistical thermodynamics. The function carries the information of the mechanical behavior of the system from the microscopic point of view through the energy spectrum of the system.

LEARNING OUTCOME: During this course student will able to explain thermodynamics phenomena such as spontaneity, temperature dependence of the heat capacity, equitation partition of energy from the microscopic point of view. At the same they will feel easy to explain the enhancement of the rate processes such vaporization chemical reaction etc. with increase in temperature.

2. Biophysical Chemistry: (12L)

Hydrophobic hydration, micelle formation, hydrophobic interaction, stabilization and denaturation of protein, water structure alternation theory of denaturation of protein, protein–lipid interaction, transport of ions and small molecules through membranes, ion channels

LEARNING OBJECTIVES OF UNIT-2: Biophysical chemistry is an interdisciplinary field of study in which biological systems are meant to understand by carefully investing the essentials of its physical properties. Biophysical chemistry deals with bio-macromolecules and their physical interactions. The inside and outside of a living cell is full of biomolecules, from simple ones to sophisticated complex machineries, of which the collective interplay control the biological processes, such as cellular growth and differentiation. Unit-2 helps to understand the interplay of the biomolecules at the molecular level.

LEARNING OUTCOME: Unit-2 includes the structure and dynamics of enzymes and membrane-associated proteins; the structure of the protein, the assemblies that are responsible for energy and signal transduction processes such as transportation; studies of protein-ligand binding interactions, and protein denaturation pathways. These detailed studies come in aid to understand the essential and natural biological processes.

3. Interface and Colloidal Stability: (13L)

Colloidal aggregates, nanoparticles, stability of colloids and nanoparticles in solution, surface charge of colloidal particles, electrical double layer and theories of electrical double layer, Helmholtz- Perrin model, Gouy-Chapman model, Stern model, zeta-potential, determination of zeta potential, streaming potential, sedimentation potential, DLVO theory, optical properties of colloids and nanoparticles.

LEARNING OBJECTIVES OF UNIT-3: Colloid and surface chemistry is a core subject of physical chemistry. It is an interesting and interdisciplinary topic to realize diverse fields of science (pharmaceuticals, food, cosmetics, detergents, medicine and biology, up to materials and microelectronics). Study of colloids and interfaces is crucial to acquire the knowledge of the forces between the molecules and the particles or surfaces to know the structure and stability of the colloid particles and the character of the electrified interface.

LEARNING OUTCOME: Colloids have many important and exciting properties of which stability is possibly the most important factor. Electrified interfaces are of vital importance in many aspects of everyday life. Structure and property of the electrified interface helps to understand the many phenomena like the stability of colloid, movement of colloid particles in presence of electrical field, corrosion and the transport phenomena of biological molecule through cell membrane.

4. Advanced Experimental Instruments:Basic principles and applications (12L)

Electron Microscopy: transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), fluorescence confocal microscopy, fluorescence correlation spectroscopy, UV-VIS absorption spectrometry, fluorimetry, FTIR spectrometry, atomic absorption spectrometry, excited state lifetime measurement techniques: TCSPC, transient absorption, up-conversion etc.

LEARNING OBJECTIVES OF UNIT-4: Through this unit the students will introduce into the working principles of modern instruments (which recognize the status of a scientific department) applying the knowledge on basic science.

LEARNING OUTCOME: Here the students may have the necessary background for the working at any experimental laboratory.

M. Sc. Semester-II

Practical (Core)

MCH25-IP: Inorganic Chemistry

Full Marks: 50 (40 + 10); Credit point: 4

1. Analysis of some ores and alloys.
2. Preparation of some complex salts and their characterization.
3. Determination of composition and formation constant of a few selected systems by pH and spectrophotometric method.
4. Magnetic susceptibility measurements

LEARNING OBJECTIVES: Analysis of some ores and alloys; Preparation of some complex salts and their characterization; Determination of composition and formation constant of a few selected systems by pH and spectrophotometric method; Magnetic susceptibility measurements

LEARNING OUTCOME: Students will acquire skill in analyzing alloys, complexes, spectroscopic data and magnetic susceptibility parameters

M. Sc. Semester-II

Practical (Core)

MCH26-OP: Organic Chemistry

Full Marks: 50 (40 + 10); Credit point: 4

I. Separation of components from a mixture of organic compounds followed by their characterization

a. Chemical Separation

b. Chromatographic Separation

LEARNING OBJECTIVES: One of the critical problem of practical organic chemistry is to separate a mixture of organic compounds. For characterization and property elucidation of an organic compound, the sample should be available at its pure state. Several techniques of separation are available to get a pure organic compound. As a first step the students will be trained to separate a binary mixture of organic compounds using chemical and chromatographic methods. During their learning process they will also understand the limitations of the technique used for separation.

LEARNING OUTCOME: Students will acquire the skill to separate binary mixture of organic compounds using chemical and chromatographic procedures.

M. Sc. Semester-III

Theoretical

MCH31-E1: Elective-1 (Physical and Inorganic Chemistry)

Full Marks: 50 (40 + 10); Credit point: 4

Group A (20 +5)

1. Alternative Energy Studies: (12L)

Natural solar energy conversion process (reactions of photosynthesis), photolysis of water, modeling and mimicking of photosynthesis process, photophysical and photochemical process of semiconductor based materials and dye sensitized photo-galvanic cells in solar energy conversion, theoretical aspects of this conversion process.

LEARNING OBJECTIVES OF UNIT-1: Harnessing environmentally sustainable energy supplies is one of the key challenges the society facing. There are intense research activities towards the goal of harnessing energy from the sun. The concept of making fuels using sunlight is on the basis of natural photosynthesis where plants use sunlight to covert water and CO2 to O2 and sugars. The objective of this course is first to introduce the students the mechanism of natural photosynthesis and introduce how the scientists have mimicked this in the laboratory for the purpose of generating fuels.

LEARNING OUTCOME: After finishing the course the student will learn the basics of natural photosynthesis and operational principles of different photovoltaic systems including the recent advances in this growing field such as dye-sensitized solar cell, quantum dot sensitized solar cell, nanohybrid systems.

2. Physical Chemistry of Polymers: (13L)

Polymerization reaction, kinetics of free radical and condensation polymer, graft polymerization, morphology and crystallinity of polymer by TGA and SEM analysis, molecular weight determination of polymer by light scattering method and GPC method, criteria for polymer solubility, thermodynamics of polymer solutions, good and bad solvents, theta temperature, Flory-Huggins model, dilute polymer solution, excluded volume.

LEARNING OBJECTIVES OF UNIT-2: The use of polymeric materials is increasing rapidly as they are replacing the usage of the conventional materials, such as metals, wood and natural fibers. They have many industrial applications too. Thus, this unit approaches to the science of polymer from a view point of physical chemistry and is concerned with the relationships between structures and properties.

LEARNING OUTCOME: The proposed syllabus provides a through coverage of the fundamental aspects of the polymer synthesis and its characterization. A detailed and in-depth knowledge of important polymers, their synthetic procedures, structures and molecular and bulk properties can be obtained from the curriculum.

Group B (20 + 5)

3. Inorganic Photochemistry-1: (13L)

Basics of photochemistry- absorption, excitation, photochemical laws, quantum yield, lifetime of excited states, flash photolysis, stopped flow techniques, energy dissipation by radiative and non-radiative process, absorption spectra, Franck-Condon principles, photochemical stages- primary and secondary process; properties of excited states- structure, dipole moment, acid-base strength, reactivity; photochemical kinetics- calculation of rates of radiative process; bimolecular deactivation - quenching; excited states of metal complexes- comparison with organic compounds, electronically excited states of metal complexes, charge transfer excitation.

4. Supramolecular Chemistry-I: (12L)

Basic concepts and principles, molecular recognition and host-guest interactions, anion coordination and recognition of anionic substrates, organometallic receptors and their host-guest complexes, spherical recognition, podand, podate, cyrptand, cryptate, coronand, coronate, molecular devices and supramolecular assemblies, supramolecular orbital, supramolecular arrays: ribbon. Ladder, rack, braded, grid; harnessing non-covalent forces to design functional materials

LEARNING OBJECTIVES: (i) In the first unit the relationship between nuclear properties and its structure are to be discussed in details; (ii) Various types of nuclear reactions and the theory involved are to be introduced in the second unit; (iii) In the unit three, the basics of photochemistry are taught. The photochemical laws are to be discussed in this regard. The quantum yield, lifetime of excited states, Flash photolysis and stopped flow techniques are important parts of this unit. The knowledge about the photochemical kinetics and calculation of rate laws of radiative process are to be taught in this field. Excited states of metal complexes- comparison with organic compounds, electronically excited states of metal complexes, charge transfer excitation and different photochemical properties are needful parts of this unit which are to be taught carefully to students to fulfill their learning aptitude; (iv) Background, importance and origin of the topic of supramolecular Chemistry, defining the terms and significance attached to supramolecular chemistry, recognition all types, Host-Guest complex, molecular and supramolecular devices, and molecular assemblies are studied.

LEARNING OUTCOME: (i) The students will be eligible to teach Inorganic photochemistry in future in M. Sc. level. On the other hand, the students will gain interest to perform experimental as well as theoretical research on this area having basic and technological importance of science. (ii) A Simpler approach to understand and importance of Supramolecular Chemistry as well as application e.g. devices such as electronic, photonic and ionic; numerous assemblies and significance.

M. Sc. Semester-III

Theoretical

MCH32-E2: Elective-2 (Organic Chemistry)

Full Marks: 50 (40 + 10); Credit point: 4

1. NMR Part-A (13L)

Nuclear magnetic resonance (NMR spectroscopy): general introduction and definition: chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurements, chemical shift values and correlation of proton bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohol, phenols, enols, carboxylic acids, amines, amides and mercapto): chemical exchange; effect of deuteration, complex spin-spin interaction between two, three, four, five nuclei (first order spectra), virtual coupling, stereo chemistry; hindered rotation; Karplus curve-variation of coupling constant with dihedral angles; specification of complex spectra-nuclear magnetic double resonance, contact of shift reagent, solvent effect; Fourier transformation technique; nuclear overhauser effect (NOE); resonance of other nuclei – F, P;

2. NMR Part-B: (12L)

Carbon-13 NMR spectroscopy- general considerations; chemical shift values (aliphatic, olefinic, alkyne, heteroaromatic and carbonyl carbon); coupling constant; two dimensional NMR spectroscopy – COSY, NOESY, DEPT, INEPT, APT, INADEQUATE technique.

3. Mass Spectroscopy: (12L)

Introduction; ion production – EI, CI, FD and FAB; factors affecting fragmentation; ion analysis; ion abundance; mass spectral fragmentation of organic compounds; common functional groups;

molecular ion peak; metastable peak; McLafferty rearrangement; nitrogen rule; high resolution mass spectroscopy; example of mass spectral fragmentation of organic compounds with respect to their structure determination.

4. Identification of Organic Compounds by Spectroscopic Technique: (13L)

Application of spectroscopic technique (UV, FT-IR, NMR and Mass) in a combined manner to solve structural problems of unknown organic compounds.

LEARNING OBJECTIVES: Spectroscopic tools are the most important devices that are routinely used for the determination of structure of organic molecules. Two important sub-branches of spectroscopy are NMR and Mass. The aim of the present paper is to make the students acquainted with the basic and advanced NMR and Mass spectroscopic techniques for solving simple and complex chemical structures and to make them analyze a spectral outputs. They will be able to predict the fragmentation patterns expected to arise in the mass spectrum of alkanes, alkyl halides, ethers, alcohols, ketones, amines etc.

LEARNING OUTCOME: At the end of this course students will be able to determine structure of a molecule using the output of NMR and Mass spectral data. They can solve the problems related to the determination of unknown structure of organic molecules using the combination of various spectroscopic methods.

M. Sc. Semester-III

Theoretical

MCH33-I: Optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Metal Ion Promoted Reactions: (13L)

Important reactions-oxidative addition, reductive elimination, oxidative coupling, insertion, electrophilic and nucleophilic attack on the ligand; catalytic cycle, Tolman catalytic loop; homogeneous/heterogeneous catalysis: hydrogenation by Wilkinson's catalyst, water gas shift reaction, Fisher-Tropsch synthesis, isomerization, alkene polymerization, Wacker-Smidt synthesis, hydroformylation, hydrosilation, hydrophosphylation, hydroamination, hydrocyanation and hydroboration reactions, Monsanto acetic acid synthesis, Heck reaction, oxopalladation reactions, mobil process, synthesis of methanol,photo-dehydrogenation catalyst (platinum POP).

2. Physical Characterization of Inorganic Compounds by Spectral Analysis-I: (12L)

Electron spin resonance spectroscopy (ESR) - basic principle and spectral display, standard material for ESPR spectroscopy (dpph), detailed understanding of hyperfine coupling constant, significance of g-tensors, application to detect free radicals (H, CH_3, C_6H_5, NH_2, CD_3, PH_4, F_2^-,

$[BH_3]^-$, etc) and various transition metal complexes having one unpaired electron, charge transfer spectra and its application

3. Organometallic Chemistry-II: (13L)

Transition metal pi complexes-transition metal complexes with alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes: preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on the ligands and to organic synthesis; transmetallation and cyclization reactions, fluxional organometallic compounds.

3. Nuclear Detection Techniques and Spectroscopy: (12L)

Mossbauer spectroscopy: Mossbauer effect, nuclear recoil, Doppler effect, instrumentation, chemical shift-examples, quadruple effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds, application of Mossbauer spectroscopy-nature of metal-ligand bond, coordination number, structure, oxidation state; NQR.

LEARNING OBJECTIVES: (i) Acquire knowledge about various important organo metallic reactions as mentioned in the syllabus (Unit-1); to introduce homogeneous/heterogeneous catalysis as mentioned (Unit-1); (ii) acquire knowledge about the characterization of different known and unknown synthetic inorganic samples. The students will get the idea to unveil the structure and property relationship through the spectroscopic investigations. Specially, the ideas of EPR study will be exclusive one to understand the reaction mechanism particularly the radical mediated reaction pathway and this will motivate the students to enhance their knowledge about the anti-oxidant ingredient based research works for the advancement in chemical and pharmaceutical industries; (iii) The different transition metal pi-complexes are subject of this unit which are taught to enlighten the students. The transition metal complexes with ligands like alkenes, alkynes, allyl, diene, dienyl, arene and trienyl are involved in this part. The preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on the ligands in complexes are taught here. The utility in organic synthesis is also relevant for applications. The transmetallation and cyclization reactions are discussed in this regard. The fluxional organometallic compounds are needful to discuss here; (iv) To study Mossbauer spectroscopy: Mossbauer effect, nuclear recoil, Doppler effect, instrumentation, chemical shift-examples, quadruple effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds, application of Mossbauer spectroscopy-nature of metal ligand bond, coordination number, structure, oxidation state.

LEARNING OUTCOME: (i) To understand the role of transition metal ions in various industrially important organo-metallic reactions; (ii) the students will be able to apply ESR in characterizing inorganic compounds; (iii) The students will gain knowledge to teach organo-metallic chemistry in future in M. Sc. level. Also, the students will gain high enthusiasm to perform experimental research on this area having basic and technological importance of science; (iv) students will be able to understand the basic principle of nuclear quadruple resonance spectroscopy (NQR) and and apply it in analysing various metal complexes

M. Sc. Semester-III

Theoretical

MCH33-O: Optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Concept of MO: (12L)

Molecular orbitals of hydrogen molecule, derivation of secular equations and determinant, introduction to Hückel molecular orbital (MO) method as a mean to explain modern theoretical methods, molecular orbitals of allyl, butadiene and other longer conjugated systems, resonance energy, bond order and charge density, aromaticity and antiaromaticity cyclopropenyl, cyclobutadienyl, cyclopentadienyl systems, pictorial Representation of MOs for molecules with sigma bonds, methane, methylene, qualitative application of MO theory to reactivity, potential energy diagrams to represent the reaction pathway.

2. Structural Effects on Reactivity: (13L)

Linear free energy relationships (LFER), Hammett equation, substituent constants (σ), theories of substituent effects, interpretation of σ values, reaction constant ρ, significance of the sign and magnitude of reaction constant, deviations from Hammett equation, through conjugation effect, introduction of parameters like σ, σ^+, σ^-in Hammett plot, concave upward deviation, concave downward deviations, dual parameter correlations, inductive substituent constant, the Taft equation.

3. Supramolecular Chemistry: (12L)

Basic Concept: definitions of supramolecular chemistry, host-guest chemistry, chelate and macrocyclic effects, preorganisation, thermodynamic and kinetic selectivity, supramolecular interactions (i.e., cation-π, π–π etc.), cation, anion and neutral molecular binding, crown ethers, podands/lariat ethers, spherands, cryptands, complexation of organic cations, calixarenes, cation host to anion host, shape selectivity guanidinium receptors, coordination interactions, cavitands: cyclodextrins and molecular tweezers, molecular switches.

4. Supramolecular Chemistry: Applications: (13L)

Catenanes, rotaxanes and molecular knots, self assembly and templates, strict self assembly and self assembly with covalent modification, electrostatic and H-bonding effects in templating catenanes/catenands/catenates/rotaxanes/pseudo-rotaxanes, metal templates for catenanes (Sanvage) π stacking in catenane and rotaxane formation (Stoddart), helicates and molecular knots, molecular devices, history and future of nanoscale machines, relation to host-guest chemistry (definition of supramolecular device), supramolecular photochemistry, photo- and electro-chemical sensors, dendrimers, molecular device components, machines based on catenanes/ rotaxanes, chemically assembled electronic nanocomputing.

LEARNING OBJECTIVES: The first two units of this course directs the student to understand what do we mean by quantitative organic chemistry. The discussion on the historically important Hammett equation gives them a sense on how to correlate quantitatively the structure and the reactivity of the functional groups. Understanding on two constant terms guides them to analyze the reaction mechanism in a more precise way to get more insight on the energy barriers associated with the process. Together with the concept of molecular orbital theory they can understand the chemical properties and reaction mechanisms in terms of the spatial distribution of electrons in atoms and molecules. Finally they will gain the concept of potential energy surface.

While progressing through the second part of the paper, students will be introduced to the field of Supramolecular Chemistry, its development and recent advances. Definition and concepts of Supramolecular Chemistry will be discussed. Supramolecular architectures found in nature and their functional purposes as well as concepts of self-assembly and nanochemistry will be built up during this course. Synthetic utility of covalent and non-covalent interactions in Supramolecular Chemistry, the concept of supramolecular synthon and how these can be used in supramolecular synthesis will also be focused in this course. Synthesis and applications of Cation, Anion, and Neutral molecule binding receptors, Catenanes, rotaxanes, Molecular knots, Molecular devices will be explained.

LEARNING OUTCOME: After finishing the course the students will gain sufficient knowledge to understand and preidct some important observables, characteristic to organic molecules and reactions in terms of some parameters associated to the functional groups and reactions. With the concept of potential energy surface they can get the entry point to the modern theoretical research in organic chemistry. Moreover, students will be familiar with the principles, perspectives, applications of Supramolecular Chemistry based on recent research as well as developments in this multidisciplinary field which has grown tremendously in the last few decades.

M. Sc. Semester-III

Theoretical

MCH33-P: Optional (Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Classical Mechanics-I: (20L)

Description of motion, definition of velocity, revisit of basic calculus, acceleration, central problem of mechanics, Newton’s prescription to solve the problem, laws of motion: law ofinertia, law of causality, definition of mass, law of reciprocity, superposition principle of force,introduction to the idea of law of force for motion, application of Newton’s prescription totranslation, rotation and vibrational motion, time-reversal symmetry, work-energy theoremand definition of kinetic energy, conservative and non-conservative forces, definition ofpotential energy, conservation of total mechanical energy for conservative system and its implication in the context of first law of thermodynamics, potential energy and stability of motion, energy diagram, bounded and unbounded motion, principle for the determination offorce constant of a chemical bond.

2. Classical Mechanics-II: (08L)

Newton's equation of motion in the Lagrangian form, generalized coordinate systems, invariance of the equation of motion in Lagrangian form, application of the Lagrangian equation of motion to the isotropic harmonic oscillator, definition of generalized momentum, the Legendre dualtransformation and its applications, the Hamiltonian function, Hamiltonian system and Hamilton's equation of motion, correspondence between total mechanical energy and the Hamiltonian function, definition of phase space, non-Hamiltonian systems.

LEARNING OBJECTIVES OF UNIT-1 AND 2: The behavior of a microscopic particle is drastically deferent from our everyday experience, i. e., deterministic nature of the motion of a macroscopic object. The wave-particle duality is compounded in the behavior of microscopic particles. Thus formulation of the dynamics of this class was developed in an imaginary and abstract fashion. To understand this one may need the background in depth on the classical physics. Part of this has been included in the present course. Here the students will learn the philosophy of the Newtonian mechanics and related aspects with the revisit of kinematics and calculus. They also will learn here the extension of the Newtonian mechanics to the Hamiltonian description of motion for a system with many degrees of freedom.

LEARNING OUTCOME: Making use **of** the present knowledge the student will realize that the law of causality for the microscopic world must be different from the classical mechanics as a consequence of the complimentary principle. In other words, the dynamical equation of state cannot be expressed in terms of force.

Finally, using the Hamiltonian equation of motion for the many particles a student can learn the statistical mechanics based on the phase space description.

3. The Langevin Description of the Brownian Motion: (12L)

History of Brownian motion and its significance in basic science, the Einstein’s model on the Brownian motion, Einstein’s theory: the diffusion equation, revisit of the Fourier series and the Fourier transformation, application of the series and the transformation, the Dirac delta function and its properties, irregular movement of particles suspended in a liquid and its relation to diffusion, diffusion and mobility, determination of Avogadro number, experimental confirmation, theoretical observation on Brownian motion and the existence of a random force, Langevin description of Brownian motion: general expression for mean square displacement (i) short time limit and (ii) long time limit, relation between random and viscous force: the fluctuation-dissipation theorem.

4. Probabilistic Description of the Brownian Motion: (10L)

Brownian motion in velocity space: Fokker-Planck equation, calculation of M_1 (v), calculation of M_2 (v), Brownian motion in phase space (motion in a force field): Kramers’ equation, Kramers’ equation as a generalization of Liouville equation and connection to equilibrium statistical mechanics, Kramer’s theory of activated process (i) calculation of j and (ii) calculation of n_a, a simple connection to transition state theory, overdamped motion: Smoluchowski equation and diffusion over a barrier, the master equation: applications in (i) unidirectional random walk, and (ii) quantized harmonic oscillator interacting with a radiation field.

LEARNING OBJECTIVES OF UNIT-3 AND 4: Here the students will go through an introductory course on the Brownian motion with the formulation of stochastic processes based on the Langevin description of motion and its equivalent representation i. e. the Fokker-Planck equation.

LEARNING OUTCOME: Through the course on the Brownian the students will learn the Einstein's picture on the Brownian motion. Based on this they will identify the diffusion coefficient and its relation with the mobility. Here a student may surprise to know that how Einstein indirectly confirmed that matter is discrete which was claimed by chemists from long back. In addition to that the students will learn the microscopic theory of barrier crossing dynamics with help of the Fokker-Planck description of the Brownian motion. It would put a huge impact in the mind of a chemistry student who frequently deals with the thermal reactions.

M. Sc. Semester-III

Theoretical

MCH34-I: Optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Bioinorganic Chemistry-II: (12L)

Metal-proteininteraction-storage, transfer and activity; study of metalloprotein and metalloenzyme-catalase, peroxidase, ceruloplasmin, cytochrome c oxidase, carbonic anhydrase, carboxypeptidase, metallothionine, xanthine oxidase, sulphite oxidase, nitrate reductase, superoxide dismutase, chemistry of respiration; Vitamin B_{12} and B_{12} co-enzyme; metal deficiency and diseases, toxic effects of metals, detoxification of metal ions.

2. Inorganic Reaction Mechanism-II: (13L)

Ligand substitution reaction of octahedral complexes-different types, isomerization and racemization; substitution reactions of square planar complexes-different theories of trans and cis effects, nucleophilicity scale, kinetics of chelate formation; substitution reaction of tetrahedral complexes, studies of fast reactions, kinetic and activation parameters-tools to propose plausible mechanism; stereochemical changes: racemisation in octahedral complexes, types of ligand rearrangements, isomerization in 4, 5 and 6 coordinated complexes; reactions of coordinated ligands; template reactions.

3. Molecular Magnetism-II: (13L)

Magnetic orbital and exchange pathways in polynuclear systems, quantitative approach to exchange interactions, Bleaney-Bower's equation, orthogonality and accidental orthogonality phenomenon, deliberate synthetic approaches to ferromagnetically coupled systems, magnetization versus field studies, calculation of ground state and spin manifold, canting/hidden canting and weak ferromagnetism, spin frustration, polynuclear transition metal complexes: magneto-structural correlations, magnetism without metals and magnetic materials, advanced magnetic materials and its recent developments.

4. Supramolecular Chemistry-II: (12L)

Receptors and receptor-substrate complexes, co-receptor molecules and multiple recognition, supramolecular reactivity and catalysis, supramolecular electronic, ionic and photonic devices, catenanes and rotaxanes, systematic approach towards supramolecular architecture, self-assembly and self-processes.

LEARNING OBJECTIVES: (i) Unit-1 is the continuation of the syllabus present in Sem. II. This portion aims to explore the mechanistic paths of reactivity of different metalloenzymes and metalloproteins including the transport and storage proteins in an advanced level (ii) The objective of unit-2 is to highlight the kinetics and mechanisms of ligand substitution reactions of square planar and tetrahedral metal complexes. This section will highlight the trans-effect and its origin; isomerisation and racemisation of metal complexes. This section will also give the chemistry behind the change of reactivity of the ligands through coordination. (iii) In unit-3 Mechanisms of magnetic exchange of different paramagnetic partners, systematic approach both theoretical and experimental design synthesis of suitable molecules and materials, Single Molecule Magnets (SMM), Single Chain Magnets (SCN) etc will be discussed (iv) In unit-4 advancement on Supramolecular Chemistry and some applications will be discussed.

LEARNING OUTCOMES: (i) After completion of the given course content, the students will be able to understand the role of metal ions in the biological functions of different mealloenzymes and metalloproteins This understanding will help the students rationalise the different biochemical processes (ii) The students will be able to rationalise the reaction pathways of different types of reactions of metal complexes like ligand substitution in octahedral, tetrahedral and square planar complexes. The knowledge on the reactivity of coordinated ligand s can be exploited in the activation different organic molecules (iii) Students will gain knowledges on molecules to materials on the basis of magnetic properties, recent discoveries of numerous magnetic phenomenon and their scope of future research; (iv) Students will be able to undertake research on supremolecular chemistry.

M. Sc. Semester-III

Theoretical

MCH34-O: Optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. **Protection and Deprotection:** **(13L)**

The role of protective groups in organic synthesis, principle of protection and deprotection, different procedures for protection and deprotection of hydroxyl (including 1,2- and 1,3-dihydroxy),phenols, amines, carbonyls and carboxylic groups.

2. **Organic Synthesis-I:** **(12L)**

The disconnection approach, basic principles, guidelines for disconnection with special emphasis on chemoselective, regioselective, stereoselective and stereospecific reactions, functional group inter conversion, synthon and reagent, synthetic equivalent, illogical electrophile and illogical nucleophile, umpolung synthesis.

3. **Organic Synthesis-II:** **(12L)**

Designing synthesis of some target molecules with proper retrosynthetic analysis, e.g., menthol, taxol, penicillin, reserpine, progesterone, estrone, periplanone B, L-Hexoses etc.

4. **Special Techniques in Organic Synthesis:** **(13L)**

The background of organic synthesis, reactions with solid-supported reagents and catalyst, solid phase synthesis, phase transfer reactions, sonochemistry, microwave in organic synthesis, ionic liquid in organic synthesis, electro-organic synthesis, concept of organocatalyst.

LEARNING OBJECTIVES: The protection and deprotection techniques are the useful tools in synthetic organic chemistry. The students will be acquainted with the use of these teniques to achieve their target synthesis. The primary goal of retrosynthesis in organic chemistry is to help chemists to synthesize the desired molecules by reverse approach. Generally, retrosynthesis is considered as input the structure of a target molecule and returns a sequence of feasible reactions linking the target to commercially available starting materials. The number of possible synthesis plans is often astronomical, and it is therefore desirable to identify the plan(s) that minimize some user-specified objective like reaction steps, available reagents, reaction conditions etc. The challenge of identifying these optimal syntheses can be framed as a one-player game—the retrosynthesis game—to allow for useful analogies with chess and Go, for which powerful solutions based on deep reinforcement learning now exist.

LEARNING OUTCOME: The concept of retrosynthesis has very useful outcome. At the end of the course student will gather a knowledge to design the synthesis of a target molecule terminating in buyable substrates. The proper planning and knowledge of several possible routes for a particular target molecule makes them possible to design and synthesise several naturally occurring substrate.

M. Sc. Semester-III

Theoretical

MCH34-P: Optional (Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Approximate Methods and their Applications: (10L)

Variation theorem, Linear variation method, applicability of variation method to excited states, time-independent perturbation theory for non-degenerate states, perturbation of a two-level system, many level systems, degenerate perturbation theory and their applications, Eckert's theorem, hydrogen and helium atoms, Hellman-Feynman and virial Theorems.

2. Theory of Many Electron Wavefunctions: (15L)

Introduction to spin, operator algebra for spin, construction of matrix representation of spin operators, eigenvalues and eigenfunctions of spin operators, non-relativistic wave function for hydrogen atom, many-electron wave functions: examples with two and three electron systems, Slater determinants, projection operators, parity operator and Pauli principle, the Pauli exclusion principle, introduction of core, Coulomb, and exchange integrals with their properties: example of *He* atom, Hartree self-consistent method for many-electron systems, Coulomb operators, exchange operators, Coulomb and Fermi hole, restricted and unrestricted Hartree-Fock calculations.

LEARNING OBJECTIVES OF UNIT-1 AND 2: To introduce different approximate methods of quantum chemistry. Different methods for solving many body systems such as Hartree-Fock self-consistent field method, Post Hartree-Fock-methods, Several semi-empirical methods. In this course student will get introduced the basics of density functional theory , useful tool to characterize the properties of molecules and materials.

LEARNING OUTCOME: At the end of this course, students will have advanced level understanding of methods of treating many body systems. This course will make in turn, prepare students for doing Ph. D. in Computational Chemistry

3. Photophysics of Electronically Excited Molecules: (18L)

Physical properties of the electronically excited molecules, nature of changes on electronic excitation, potential energy diagram , shapes of absorption band and Franck-Condon principle, emission spectra, environmental effect on absorption and emission spectra, excited state dipole moment, excited state acidity constants-pK* values, excited state redox potential, emission of polarized luminescence and photophysical processes in electronically excited molecules, types of photophysical pathways, radiationless transition-internal conversion and intersystem crossing, fluorescence emission, fluorescence and structure, triplet states and phosphorescence emission, emission property andthe electronic configuration, photophysical kinetics of unimolecular processes, state diagrams, delayed fluorescence, the effect of temperature on emission processes,photophysical kinetics of bimolecular processes, kinetic collisions and optical collision, bimolecular collisions in gases and vapours and the mechanism of fluorescence quenching, collisions in solution, kinetics of collisional quenching: Stern-Volmer equation, concentration dependence of quenching and excimer formation, quenching by foreign substances.

4. Rotational, Vibrational and Raman Spectroscopy: (07L)

Rigid & non-rigid rotors, vibrational spectroscopy: harmonic and anharmonic oscillators, normal coordinates, effects of anharmonicity, vibration-rotation transitions, Raman and Rayleigh scattering: classical and quantum mechanical treatments, polarization of scattered light, rotational and vibrational Raman spectroscopy, resonance Raman effect, selection rules of rotational, vibrational and Raman spectroscopy.

LEARNING OBJECTIVES OF UNIT 3 AND 4: Here the students will learn features of electronically excited molecules from various perspectives such as dipole moment, acidity and the chemical activity in terms of redox potential. At the same time they will address the release of energy through the use of phenomenological rate laws for the physical kinetics which may lead to identify the possible routes of the relaxation process.

In the next part, the student will learn the principle to determine the force constant and bond length , respectively. At the same time they will introduce into the Raman Spectroscopy is a peculiar one to recognize the symmetry of a molecule.

LEARNING OUTCOME: The student will learn to compare distribution of electrons in the molecule between ground and excited states. Through this he/she may be strongly motivate to study molecular physics at electronically excited state theoretically which is now at early stage in the field of theoretical chemistry. The students may find another important way to apply their knowledge to instrumentation for the investigation of biosystem.

M. Sc. Semester-III

Theoretical

MCH35-I: Optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Errors and Evaluation: (12L)

Precision-standard deviation, relative standard deviation; accuracy- absolute error, relative error; types of error in experimental data- systematic (determinants), random (indeterminate) and gross; source of errors and the effects upon the analytical results; methods of reporting analytical data, statistical evaluation of data.

2. Inorganic Photochemistry-II: (13L)

Ligand field photochemistry- photosubstitution, photooxidation and photoreduction, ground state and excited state, energy content of the excited state, development of redox potentials of the excited states; redox reactions by excited metal complexes- energy transfer, exciplex formation, conditions of the excited states to be useful redox reactants, excited electron transfer, photochemical reactions of Cr, Fe and Ru complexes, role of spin-orbit coupling in the lifetime of the complexes, application of redox process for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light; sensitization and metal complex sensitizers; inorganic photochemistry in biological process and their model studies, solar-energy conservation and storage.

3. Electro-Analytical Methods-II: (12L)

Fundamentals, electrode-solution interface layer, electrolytic process, three-electrode system; supporting electrolyte, DME; Ilkovic equation, Ilkovic-Heyrolsky equation, test of reversibility, current-voltage diagram, DC and AC polarography, stripping voltametry

4. Physical Characterization of Inorganic Compounds by Spectral Analysis-II: (13L)

Application NMR spectroscopy-fundamentals, the contact and pseudo-contact shifts, factors affecting nuclear relaxation, application of H-1, C-13, P-31 and F-19 NMR towards the structural elucidation of metal-organic complexes, an overview of metal nucleides with emphasis on Pt-195 and Sn-119 NMR

LEARNING OBJECTIVES: (i) Studies on precision- standard deviation, relative standard deviation (ii) Understanding on accuracy- absolute error, relative error; Types of error in experimental data- systematic (determinants), random (indeterminate) and gross; Source of errors and the effects upon the analytical results; Methods of reporting analytical data, Statistical evaluation of data (iii) Understanding of errors in the analytical evaluation (iv) Understanding on Ligand field photochemistry with emphasis on photo-substitution, photo-oxidation and photo-reduction (iv) Understanding on the characteristics of ground state and excited state, the energy content of the excited state, development of red-ox potentials of the excited states, Red-ox reactions by excited metal complexes- energy transfer, exciplex formation, conditions of the excited states to be useful redox reactants, excited electron transfer, photochemical reactions of Cr, Fe and Ru complexes, role of spin-orbit coupling in the lifetime of the complexes. (v) Understanding on the application of red-ox process for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light (vi) Understanding on sensitization and metal complex sensitizers, inorganic photochemistry in biological process, Solar-energy conservation and storage (vii) The students will acquire knowledge about the characterization of different known and unknown synthetic inorganic samples. The students will get the idea structure determination pathway. This course content helps them to explore different functionality of the inorganic complexes towards the practical and industrial applications. The students will earn the interest to judge the role of inorganic complexes in organic synthesis and that will help them to apply the inorganic materials towards the chemical and pharmaceutical industrial purposes in future.

LEARNING OUTCOME: The outcome of the learning is highly significant in modern field of science. The students will be eligible to teach Inorganic photochemistry thoroughly in future in M. Sc. level. On the other hand, the students will gain capability to perform experimental as well as theoretical research on this area having basic and technological importance of science.

M. Sc. Semester-III

Theoretical

MCH35-O: Optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Oxidation Reactions in Organic Synthesis: (12L)

Fundamental concepts of redox reactions in organic chemistry, oxidation of alcohols: by chromium and manganese reagents, silver carbonate, oxidation via alkoxysulphonium salts and other methods, oxidation of carbon-carbon double bonds,dihydroxylation, epoxidation, Sharpless epoxidation, diastereoselective epoxidation of homoallylic alcohols, ozonolysis, photosensitized oxidation of alkenes, Pd-catalyzed oxidation of alkenes, oxidation of carbonyl compounds, Baeyer-Villiger oxidation of ketones and related reactions, conversion to a,b-unsaturated ketones, other methods, use of ruthenium tetraoxide and thallium (III) nitrate as oxidizing agents for organic substrate, other oxidizing agents.

2. Reduction Reactions in Organic Synthesis: (13L)

Catalytic hydrogenation: concept of hydrogenation and hydrogenolysis, hetereogeneous and homogeneous catalytic hydrogenation (the catalyst used, selectivity of the reduction, reduction of the functional groups, stereochemistry and mechanism), transfer hydrogenation.

Reduction by dissolving metals: reduction with metal and acid (reduction of carbonyl compounds), reduction with metal in liquid ammonia, reductive fission of alcohols and halides; reduction by hydride transfer reagents: aluminium alkoxide, lithium aluminium hydride and sodium borohydride and their modified reagents (selectivity of the reduction, reduction of functional groups, stereochemistry and mechanism), reduction with boranes and dialkyl boranes.

Wolf-Kishner reduction, desulphurisation of thioacetals, reduction of organic compounds by di-imide, low-valent titanium reagents, trialkyl-tin-hydrides, trialkyl-silanes and other reagents.

3. Organometallic Chemistry, Part-A: (12L)

Preparation, properties and reactions of organomagnesium, organolithium and organozinc, reagents in synthesis, the role of boron, silicon, sulphur and phosphorus in organic synthesis.

4. Organometallic Chemistry, Part-B: (13L)

Principle, preparation, properties and applications of some transition metals in organic synthesis with special reference to copper, palladium, cobalt, titanium and nickel.

LEARNING OBJECTIVES: Importance and concepts of reductions and oxidation reactions will be discussed. To built up the concepts of organic reduction and oxidation reactions or organic redox reactions is one of the goals of this course. Applications of organic redox reactions in multistep organic sysnthesis of bioactive molecules, drugs and other molecules with potentials technological applications will also be taught in this course. Recent developments and applications of organic redox reactions will also be discussed in this course. Organometallic chemistry is the disciple dealing with compounds containing at least one direct metal-carbon bond. Organometallic compounds are widely used in research and industrial chemical reactions. Students will learn how to prepare the organometallic reagents and their application in organic synthesis.

LEARNING OUTCOME: During this course, students will be acquainted with the principles and perspectives of organic redox reactions and applications in multistep organic syntheses. They can outline the synthesis of several organometallic reagents. They will also be familiar with the recent research and developments regarding organic redox reactions and orgaometallic chemistry.

M. Sc. Semester-III

Theoretical

MCH35-P: Optional (Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Connection between Thermodynamics and Statistical Mechanics: (12L)

Definition of microstates and macrostates, Boltzmann's definition of entropy, formula for calculation of thermodynamic properties in terms of number of microstates, determination of number of microstates for classical ideal gas, connection among the properties of ideal gas, Gibbs paradox, Sackur-Tetrode equation.

2. Ensemble Method and its Application: (13L)

Definition of ensemble, a priori probability, Gibbs postulate in statistical mechanics, ergodic hypothesis, prescription for studying of thermodynamic systems based on ensemble method, preparation of equilibrium ensemble corresponding to given thermodynamic system (isolated, closed and open), determination of distribution function, partition function, calculation of thermodynamic properties in terms of partition function, theory of fluctuations, calculation of fluctuation in energy, number of particles, density, entropy, volume, temperature etc.

3. Boltzmann, Fermi-Dirac and Bose-Einstein Statistics: (13L)

Canonical partition functions for non-interacting distinguishable and non-identical particles, Boltzmann statistics, grand canonical partition function for non-interacting identical particles, Fermi-Dirac and Bose-Einstein statistics and their limiting behavior, ideal monoatomic gas, the translational partition function, the electric and nuclear partition function, thermodynamic function, ideal diatomic gases, the rigid rotor-harmonic oscillator approximation, the vibrational partition function, the rotational partition function of a heteronuclear molecule, the symmetry requirement of the total wave function of a homonuclear diatomic molecule, the rotational partition function of a homonuclear diatomic molecule, thermodynamic function.

4. Classical and Quantum Statistics: (12L)

The classical partition function, phase space and the Liouville equation, equipartition of energy, ideal polyatomic gas, the vibrational and the rotational partition functions, thermodynamic function, hindered rotation, a weakly degenerate ideal Fermi-Dirac gas, a strongly degenerate ideal Fermi-Dirac gas, a weakly degenerate ideal Bose-Einstein gas, a strongly degenerate ideal

Bose-Einstein gas, an ideal gas of photons, the density matrix, the classical limit from the quantum mechanical expression for Q.

LEARNING OBJECTIVES: To provide the students with important concepts of Statistical Mechanics and its connection with Thermodynamics. To introduce the elegant concepts of ensemble and consequently Maxwell-Boltzmann (MB), Bose-Einstein (BE) and Fermi-Dirac (FD) statistics. The students are also taught when and how one needs to switch from classical to quantum statistics and vice versa.

LEARNING OUTCOME: It is expected that upon completing the course the students will have considerable knowledge in the field of statistical mechanics/thermodynamics which will help them pursue research works in diverse fields of physics and chemistry as statistical mechanics is a ubiquitous topic. The topics covered in the course also bear huge relevance in designing devices with great technological and engineering applications.

M. Sc. Semester-III

Practical

MCH36-IP: Optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Separation by chromatographic techniques.

2. Colorimetric estimation of some metal ions.

3. Measurement of some water quality parameters.

4. Green synthesis of some inorganic compounds

LEARNING OBJECTIVES: (i) Separation by chromatographic techniques, (ii) colorimetric estimation of some metal ions (iii) measurement of some water quality parameters (iv) green synthesis of some inorganic compounds

LEARNING OUTCOME: Achievement of skill in chromatographic techniques and colorimetric estimations

M. Sc. Semester-III

Practical

MCH36-OP: Optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Preparation of organic compounds by conventional and green chemical methods followed by purification and characterization by spectroscopic technique

2. Quantitative estimation of:
   a. Sugars (Glucose, Cane sugar)
   b. Phenol
   c. Aniline
   d. Nitrogen by Kjeldhal method
   e. Saponification and iodine value
   f. Carboxylic acids
   g. Olefinic double bonds

LEARNING OBJECTIVES: The students will learn how to prepare and detect a target organic molecule. They will also learn the procedure of quantitative estimation of several organic compounds.

LEARNING OUTCOME: At the end of this practical course the students will gain the skill for preparing and detecting target organic structure. They will also learn how to estimate quantitatively several common organic molecules.

M. Sc. Semester-III

Practical

MCH36-PP: Optional (Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Determination of surface excess of different surface active molecules.

2. Simultaneous determination of the ionization constant and the solubility of sparingly soluble drug molecules (Potentiometric titration method).

3. Determination of the stability constants of complexby pH metric titration.

4. Spectroscopic determination of ternary Phase Diagrams.

5. Determination of the effect of solvent polarity on absorption spectra by using solvatochromic dyes.

6. Spectroscopic determination of binding constant of charge transfer /host- guest molecular complex by Benesi-Hildebrand method .

7. Determination of CMC of surfactants and study the effect of salt on CMC by spectrophotometry .

8. The spectroscopic determination of pKa valuesof photoacids and determination of pH of unknown solution.

LEARNING OBJECTIVES: In this course the students will get another opportunity to know how one can determine surface excess of different surface active molecules, the stability constants of a complex, the solubility of sparingly soluble drug molecules, a ternary phase diagram, the effect of solvent polarity on absorption spectra, binding constant of charge transfer /host- guest molecular complex, of CMC of surfactants and study the effect of salt on CMC etc. based on their theoretical study on Galvanic cells, ionic equilibrium and spectroscopy, respectively.

LEARNING OUTCOME: A promising student will be excited here to enter into the modern research laboratory on bio physical chemistry or material science.

M. Sc. Semester-IV

Theoretical

MCH41-I: Optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Selected Topics of Coordination Chemistry: (12L)

Introduction, ligand-field spectra of octahedral complexes, complexes of lower symmetry, charge transfer bands, circular dicroism and optical rotatory dispersion, pictorial molecular orbital description of bonding, effects of pi-bonding, group theoretical treatment, comparison between different approaches to bonding in coordination compounds

2. Selected Topics on the Chemistry of p Block Elements: (13L)

Major landmark discoveries in the chemistry of p-block elements, the concept of hypervalency in p-block compounds, participation of d-orbital in bonding of p-block compounds: current status, resurgence of dative bonds in p-block compounds, recent development in carbon and silicon chemistry: intercalation, graphene, carbon molecular sieves and silicon quantum dots, recent development in phosphorus chemistry: phosphorus stabilized in zero oxidation state, frustrated Lewis pair (FLP) and oxyacids of phosphorus, fluorine in inorganic, organic and medicinal chemistry and fluorinated polymers, noble gas elements and compounds as ligand.

3. Selected Topics of Chemical Bonding: (12L)

Valence bond and molecular orbital theories – comparative account; Heitler-London theory of hydrogen molecule, group orbital in molecular orbital approach; bonding in di, tri and tetra atomic molecules, Walsh diagram; evidence of MO pictures from spectra and reactivity; explanation of spectrochemical and nephelauxetic series; molecular term symbols.

4. Enthalpy and Entropy Driven Inorganic Reactions: (13L)

Basics of enthalpy and entropy, spontaneity and thermodynamics, thermodynamics of electronic acid-base interaction: $E_AE_B + C_AC_B$, molecular basis for electron transfer, reduction potentials and free energies, redox reactions in aqueous systems, reduction process for metal ores, redox reactions in the gas phase and in the atmosphere, role of entropy changes in free energy, energy and entropy in noble-gas chemistry, explosives.

LEARNING OBJECTIVES: Unit-1: Students will learn some selected topics in coordination chemistry such as ligand-field spectra, complexes of lower symmetry, charge transfer bands, circular dicroism and optical rotatory dispersion. Molecular orbital description of bonding, effects of pi-bonding, group theoretical treatment, comparison between different approaches to bonding in coordination compounds will taught. Unit-II: Students acquire knowledge about some selected topics on the chemistry of p block elements. Unit III: Student will learn about selected topics of chemical bonding based on valence bond and molecular orbital theories. Unit IV: Student will be taught enthalpy and entropy driven inorganic reactions.

LEARNING OUTCOME: Students will understand ligand-field spectra, complexes of lower symmetry, charge transfer bands, circular dicroism, optical rotatory dispersion, and molecular orbital description of bonding, effects of pi-bonding and group theoretical treatment of complexes. Students will be familiar the utility of enthalpy and entropy driven inorganic reactions.

M. Sc. Semester-IV

Theoretical

MCH41-O: Optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Concept on Pharmacodynamics: (12L)

Drug targets: enzymes, receptors, concept on pharmacokinetics: drug absorption, distribution, metabolism and excretion, structure activity relationship (SAR), cardiovascular drugs: introduction to cardiovascular disease, synthesis and mode of action of amylnitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa.

2. Local Anti-Infective Drugs and Antibiotics: (13L)

Synthesis and mode of action of sulphonamides, nalidixic acid, norfloxacin, aminosalicylic acid, ethinamide, fluconazole, chloroquin and primaquin; antibiotics: cell wall biosynthesis, inhibitors, β-lactam rings, synthesis and bioactivity of penicillin and cephalosporin.

3. Asymmetric Synthesis, Part A: (12L)

Introduction, kinetic and thermodynamic principles to asymmetric synthesis, diastereoselective and enantioselective synthesis; methods of asymmetric synthesis: resolution, use of chiral pool, chiral auxiliaries, use of stoichiometric chiral reagents, asymmetric catalysis.

4. Asymmetric Synthesis, Part B: (13L)

Asymmetric hydrogenation with special reference to Ru-BINAP catalyst, asymmetric reduction of prochiral ketones with Baker’s yeast and CBS catalyst, asymmetric epoxidation with special reference to Sharpless and Jacobsen epoxidation, asymmetric diethyl zinc addition to carbonyl compound, asymmetric aldol reactions, asymmetric Michael reaction; few important industrial application of asymmetric synthesis.

LEARNING OBJECTIVES: This course contains two parts. In the first two units they gain the knowledge on the processes for drug design. Moreover they acquire knowledge on the synthesis and usage of several chemotherapeutic agents. In the second part students will gain the knowledge on asymmetric synthesis. Asymmetric synthesis part-A and part-B aim to provide the students information on various methods of synthesis of optically active organic compounds. Basically three types of asymmetric synthetic strategies would be discussed. These includes chiral resolution techniques, chiral auxiliary method, asymmetric catalysis method. Asymmetric catalysis again would be divided into chiral metal complex catalysis, organocatalysis and biocatalysis. All these strategies would deal with formation of C-C bond forming reactions like asymmetric aldol reaction, Michael addition reaction, Diels-Alder reaction, Hydrogenation reaction, prochiral ketone reduction enough examples. Finally synthesis of few industrially important chiral compounds would be performed employing the above discussed asymmetric reactions.

LEARNING OUTCOME: At the end of this course students will have a basic background on medicinal chemistry and pharmacology. Moreover students will be able to design optically pure organic compounds of industrial importance in cost effective, environmentally friendly way. The shall be able to modify the hazardous synthetic method with green methods to obtain chiral drug molecules.

M. Sc. Semester-IV

Theoretical

MCH41-P: Optional(Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Formulation for the Mechanical Wave: (06L)

Examples and classification of waves, definition of a traveling wave and its mathematical representation, derivation of the wave equation for the mechanical wave, the Sinusoidal waves and the dispersion relation, intensity and the energy transport by the wave motion.

2. Formulation for the Electromagnetic Wave: (20L)

Electrostatics, the superposition principle, Coulomb' s law of force, definition of the electric field, field lines, flux of the field lines, the Gauss's law, revisit of the curl and the divergence of a vector, gradient of a scalar, correspondence between the Cartesian and the spherical polar coordinates, correspondence between the Cartesian and the cylindrical coordinates, divergence of an electric field, curl of an electric field due to static source charges, definition of the electric potential, super position of potential, the Poisson's equation, the work done to move a charge,

The Lorentz force, current and magnetic force, continuity equation for the current density, steady current, magnetostatics and the Biot-Savart law, the Ampere's law, the curl of the magnetic field in magnetostatics, divergence of the magnetic field, the Ohm's law, microscopic view of the Ohmic resistance, electromotive force, motional electromotive force, the Faraday's law, the Maxwell's equation, wave equation for the electromagnetic wave and its solution, electromagnetic wave in vacuum, conductor and in dielectric medium, dielectric constant, oscillating dipole, polarization of waves, LCR and RCR waves, superposition of waves, standing wave and its relevance in quantum mechanics, the Young's double-slit experiment.

LEARNING OBJECTIVES OF UNIT-1 AND 2: For the necessary remaining background for the formulation of the matter wave, in the binging of the present course the student will learn the formulation of both mechanical and electro- magnetic waves through the visit with electro statics, magneto statics and electrodynamics. Here a student may surprise to know several things (i) atomic or molecular Hamiltonian can be written with the Coulomb potential (ii) electric field without charge (Faraday's law which brought revolution in the industry) and magnetic field without current (Maxell's correction (to the Ampere's law) which was among the two top cited discoveries in the Nineteenth century, why?) (iii) the existence of the dispersion relation and its implication with the wave equation which is very important to speculate the wave equation for the matter wave. In addition to those the student will learn the interference of waves which is the precursor to address the first principle of the quantum mechanics as a demand of the self interference of a microscopic particle. Finally, a student will learn here the formulation of standing wave which is quite amazing to correlate it with the stationary states of a quantum system (which confine in a finite space) and understand the quantization of energy qualitatively.

LEARNING OUTCOME: Through this unit the students will have necessary background for the study on the formulation on the quantum mechanics.

3. Revisit of Birth of Quantum Mechanics: (10L)

Thermal and non-thermal radiations, black body radiation, characteristics of the radiation, necessity of new fundamental constant, formulation of the black body radiation, calculation of the number of modes, Raleigh-Jeans law and ultraviolet catastrophe, Plank's hypothesis: birth of the quantum mechanics, quantization of energy of oscillating dipole and electric field, Plank's distribution, Wein's distribution and its hints to Planck, justification of the Planck's distribution and determination of the Plank' constant, comparison of the action of a classical system with the Plank's constant and determination of the condition to apply the quantum mechanics to a system, temperature dependence of heat capacity of solids, Einstein's theory of heat capacity of solids,photoelectric effect and bizarre behavior of the radiation, Compton effect and the particle behavior of the radiation, Bohr's theory and its limitation, quantum classical correspondence, Franck-Hertz experiment, Stern-Gerlach experiment and spin angular momentum, de Broglie hypothesis and its genesis.

LEARNING OBJECTIVES OF UNIT-3: In the next step, through the study on the formulation of the black body radiation student will learn how Planck realized that the energy of an oscillating dipole as well as cavity mode is quantized. Here student will feel that It was a revolutionary discovery in the history of science and Planck was rewarded by the Nobel Prize. After that students will note how Einstein extend this concept for the microscopic mechanical oscillator to explain the temperature dependence of the heat capacity. Here they also will note how Debye contributed to attend the correct description. Then student may surprise to note that how Einstein gave the formulation on the photo electric effect (radiation behaves as a particle) borrowing the quantization concept as proposed by Planck. It was an revolutionary discovery in the history of science and Einstein was rewarded by the Nobel Prize. Student would note here how history of science is important in the progress of it. Here student may surprise to know, Einstein was not happy for the reward since he believed that world would recognize him through his revolutionary concept on space and time which are not absolute quantities. Anyway, theory of the photoelectric effect was corroborated by another independent experiment carried out by Compton and he was rewarded by the Nobel prize. Then student will learn how Bhor introduced the quantization of energy of electron to explain atomic line spectrum. He was awarded by the Nobel prize for this work. Then the student may surprise to recognize the formulation proposed by Goudsmit and Uhlenbeck which claimed existence of intrinsic spin angular(which has no classical analogue). They were awarded by the Nobel Prize. In the next step student may excite highly through the introduce of the de Broglie's hypothesis which claimed (based on the wave packet dynamics) that the wave-particle duality is a universal feature of the nature. The hypothesis was checked immediate experimentally by two independent experiments with electron by Davisson and his coworker, Germer and G.P. Thomson (here I mention for the first time name of a scientist along with his surname, why?), respectively. After confirmation of the wave nature of the particle, three Nobel prizes were given to recognize the revolutionary discovery in the history of science (why?) to de Broglie, Davisson and his coworker, Germer, and G. P. Thomson

(son of J. J. Thomson who got the Nobel prize for the discovery of fundamental particle, electron), respectively. Shortly student will learn as the answer of the question, why?. If there was no de Broglie or like him still all the above mentioned Nobel Prize winning work will remain mystery to us!!! In other words, the quantum mechanics proposed independently by Schrödinger and Hisenberg as a law of causality for the dual nature of the microscopic world.

LEARNING OUTCOME: The study on the experimental observations as well as the old quantum theory may serve an important background to propose the formulation of the quantum mechanics.

4. Formulation of Quantum Mechanics (Matter Wave): (14L)

Double slit experiment with bullet, thought experiment with the electron, self-interference of a particle, the superposition principle, the Heisenberg's uncertainty principle, the first principle of quantum mechanics, the complimentary principle and its implication, postulate of the state function, genesis of the Schrodinger's postulate, interpretation of the wave function, logical acceptance of the interpretation, the continuity equation from the Schrödinger equation, definition of the probability current density in quantum mechanics, postulate on the momentum operator, genesis of the postulatefor the expectation value of an operator, experimental interpretation of this and eigenvalue equation, postulate on the operator corresponding to a classical observable, normalization of the wave function, understanding the energy eigenvalues for one-dimensional motion, wave packet formalism, Dirac representation of state, properties of the Bra and Ket vectors, Hilbert space, the Schrodinger's picture and the Heisenberg's picture, quantum-classical correspondence, understanding tunneling and genesis of selection rule.

LEARNING OBJECTIVES OF UNIT-4: Then student should realize certainly that we have to tackle the mystery of the microscopic world in an imaginary and abstract fashion as the dual nature does not correspond to our everyday experience. With this such kind of demand the student will recognize the first principle of quantum mechanics (probabilistic description of motion of a single particle which is strange to our everyday experience) through the double slits experiments with water waves or light waves and bullets (thought experiment to avoid un necessary complicacy) and electrons (thought experiment and but its outcome would correspond certainly to the experimental results at the relevant scale for the system). Based on this and the experimental results, the students will be embedded in the philosophy of quantum mechanics with the notes how one can address all the postulates as well as the formulation of the quantum mechanics. Finally, the students will finish his/her present course with two generic signature of quantum mechanics, tunneling and selection rules, respectively.

LEARNING OUTCOME: This course may be considered as a very fundamental one for the study on the microscopic world. The students would be able to explain in detail the properties of the model systems such as free particle, particle in a box, harmonic oscillator, rotational motion and H-atom, respectively. At the same they will use the LCAO (which is used frequently in the chemistry class) knowing the origin of the principle. Finally, the present study may be helpful for the course with quantum mechanical treatment of many electron system and to understand the spectroscopic phenomena.

M. Sc. Semester-IV

Theoretical

MCH42-I: Optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Environmental Chemistry: (12L)

Biochemical effects of As, Pb, Cd, Hg, Cr, and their chemical speciation, monitoring and remedial measures; eutrophication, wastewater treatment, control of air pollution: different methods, role of plants, various source of soil pollution; noise pollution, Agricultural and industrial pollution, Green solution to various environmental hazards.

2. Lanthanides, Actinides and Super-heavy Elements:(13L)

Coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, Organolanthanides and actinides, separation of lanthanides and actinides, analytical application of lanthanides and actinides-lanthanides as shift reagents and high temperature super conductors, manmade elements-theoretical background, production, separation and predicted properties.

3. Nanomaterials: (12L)

Theoretical aspectsnanostructured materials, 0D, 1D and 2D nanostructures, concept of quantum confinement: quantum dot, quantum wire, quantum well; quantum transport: Ballistic conduction, Coulomb blockade and tunneling conduction; effect of quantum confinement on optical properties, optical properties of metallic nanoparticles, core-shell nanostructure; magnetic properties of nanostructured materials, fullerenes and carbon nanotubes, basic characterization tools for nanomaterials, applications of nanomaterials.

4. Physical Characterization of Inorganic Compounds by Spectral Analysis-III: (13L)

Basic concept of Raman Spectroscopy, application of vibration spectroscopy- symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, mode of bonding of ambident ligands, ethylenediamine and diketo complexes, resonance Raman spectroscopy, surface enhanced Raman spectroscopy (SERS).

LEARNING OBJECTIVES: (i) Study biochemical effects of As, Pb, Cd, Hg, Cr, and their chemical speciation, monitoring and remedial measures; eutrophication, wastewater treatment, control of air pollution: different methods, role of plants, various source of soil pollution; noise pollution, Agricultural and industrial pollution, Green solution to various environmental hazards; (ii) Study coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, Organo lanthanides and actinides, separation of lanthanides and actinides, analytical application of lanthanides and actinides-lanthanides as shift reagents and high temperature super conductors, manmade elements-theoretical background, production, separation and predicted properties; (iii) Students will be able to characterization of inorganic compounds by Raman Spectroscopy and SERS. The students will get the idea of structure, symmetry and reactivity of inorganic complexes. The course content will help them to explore the idea of Raman Spectroscopic technique for environmental sample analysis. This course will eventually help them to obtain the clear understanding of the uses of Raman Spectroscopy for the investigations and studies of the inorganic material-based systems in the domain of scientific research and industrial applications.

LEARNING OUTCOME: (i) Understanding the impact of various metals on environments; (ii) The PG students will get information about the characterization and uses of different Lanthanide and Actinide complexes. The students will aware about the role of these complexes in catalysis of organic synthesis. The students will acquire the idea about the different properties specially magnetism and spectral behaviour of the complexes. The students will get the idea of the uses of the complexes in the electrochemical purposes. The students will be able to investigate different known and unknown synthetic inorganic samples of Ln and Ac. The students will enrich their knowledge about the structure determination pathway. Ultimately, this course content helps them to explore different functionality of Ln and Ac based inorganic complexes towards the practical and industrial applications.

M. Sc. Semester-IV

Theoretical

MCH42-O: Optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. General Considerations on Pericyclic Reactions: (12L)

Introduction, construction of π-molecular of simple and complex conjugated system, phase and symmetry of orbitals, construction of molecular orbitals of conjugated ions and radicals, frontier molecular orbitals (FMO), excited states, theory of pericyclic reactions, types of pericyclic reactions;cycloaddition reactions: definition FMO approach, correlation diagram

2. Electrocyclic reactions: (13L)

Definition, conrotatory and disrotatory motions in ring opening and ring closing reactions, open chain conjugated system having 4nπ and (4n+2)π conjugated electrons, thermal-induced and photo-induced cyclization, Nazarov cyclization, Woodward-Hoffmann selection rules and microscopic reversibility, correlation diagram, FMO approach, Huckel-Mobius method for electrocyclic reactions, stereochemical effect.

3. Cycloaddition reactions: (12L)

Theory of cycloaddition reactions, thermal and photo-induced cycloaddition reaction, [2+2] cycloaddition reaction, Diels-Alder reaction, stereochemistry involved in cycloaddition process, endo and exo selectivity, secondary orbital interaction, orientation effects in Diels-Alder reaction, regioselectivity, intramolecular Diels-Alder reaction, Lewis acid catalyzed cycloaddition, frontier Orbital description, correlation diagrams, Huckel-Mobius method for [2+2] and [4+2] cycloaddition, cycloreversion/retrocycloaddition reaction, cycloaddition involving ketene. chelotropic cycloaddition and elimination, 1,3-dipolar cycloadditions, periselectivity.

4. Sigmatropic Rearrangement: (13L)

Classification of Sigmatropic rearrangements, hydrogen shifts and carbon shifts ([1,j] and [i,j]), FMO approach, Woodward-Hoffmann selection rule, Huckel-Mobius method, Claisen and Cope rearrangements, fluxional molecules, ene reaction and other group transfer reactions: definition, FMO approach, effects of Lewis acid.

LEARNING OBJECTIVES: This course aims to provide the students knowledge on fundamentals of pericyclic reactions. Basic difference between pericyclic reactions and ionic-free radical reactions would be point of discussion. Frontier molecular orbital theory would be applied to pericyclic reactions like electrocyclic reactions, cycloaddition reactions, sigmatropic reactions.

LEARNING OUTCOME: At the end of the course, students will be able to predict the outcome of the pericyclic reaction. They can predict the product stereochemistry, will be able to judiciously select reaction condition either as thermal or photochemical way. Most importantly, students will be able to design and synthesize complex organic compounds of practical importance employing pericyclic reaction strategies in simple and green way.

M. Sc. Semester-IV

Theoretical

MCH42-P: Optional (Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Molecular Reaction Dynamics (MRD): (13L)

Motivation, important vocabularies of MRD, energy partitioning, a simple model of energypartitioning, molecular collisions and free path phenomena, collision cross-section and the inter
molecular potential, dynamics of elastic molecular collisions, the reaction cross-section, the reaction probability, elastic scattering as a probe of the interaction potential, intermolecularpotential from experiment and theory, angular distribution in direct reactive collisions.

LEARNING OBJECTIVES OF UNIT-1 : Molecular reaction dynamics is a modern branch of Chemical kinetics. The traditional approach is to consider the elementary step of a chemical reaction and determine their rate constant and activation energies. The aim of the subject Molecular reaction dynamics is to understand the individual collisional event carrying out a chemical reactions under controlled conditions to measure such quantities product angular distributions and product internal energy state distributions and how the reactivity depends on the different internal states of reactant molecules and to relate this information to the detailed interplay of forces responsible for the reactions.

LEARNING OUTCOME: After the completion of the course the student will have an idea about different experimental techniques to study the molecular collisions, introduced terminologies of MRD. The student will learn how to use experimental data to generate PES of an underlying reaction and for a given PES, how to interpret experimental product angular distributions. The first step in interpreting the experimental results is to deduce the nature of forces at work. The student will learn how to get idea about forces from the experimental data or other way around, how to predict experimental results for a given force.

2. Solid State Chemistry: (12L)

Crystalline and amorphous structures, lattice vector and reciprocal lattice vector, defects in the solid state, band theory of solids, band theory: quantum mechanical aspect, Brillouin zone, free-electron gas theory of metal, Fermi energy, electrical and thermal conductivity of metals, semiconductor Hall effect and Hall co-efficient.

LEARNING OBJECTIVES OF UNIT-2: The objective of this course is to introduce the basics of solid state physics so that student will enable to employ classical and quantum mechanical theories needed to understand the physical properties of solids.

LEARNING OUTCOME: At the end of the course student will be able to understand the characteristic physical properties of different categories of solid materials, with an emphasis on the crystalline state and will have knowledge of a wide spectrum of theoretical approaches to model the mechanical, thermal and electrical properties of solid materials. Student will understand the origin of bands, know the concepts of phonons and how the dispersion relation appears for different crystal structure. Student will understand how, electrons and holes behave in semiconductors and how they conduct.

3. Electrode Kinetics: **(12L)**

Butler-Volmer equation and its application, Tafel equation from Volmer equation, equilibrium exchange current density and its determination, current potential reaction for reversible electrode, Doss rectification, electrokinetics of corrosion reaction, Pourbaix diagrams, corrosion current and corrosion potential, Evans diagrams.

4. Semiconductor–Electrolyte Interface: **(13L)**

The structure of the semiconductor–electrolyte interface, analogies between semiconductors and electrolytic solutions, the Garrett-Brattain space charge, differential capacity, Mott-Schottky equation, flat band potential, application of semiconductor electrode in photoelectric device.

LEARNING OBJECTIVES OF UNIT-3 AND 4: The study of semiconductor-electrolyte interface has both fundamental and practical incentives. The course is designed to make the students understand the similarities and the differences with the metal-electrolyte ounterparts. The knowledge of this topic is particularly useful in the fields of electrochemistry and solid-state physics.

LEARNING OUTCOME: The knowledge acquired will be extremely useful in many technologies including microelectronics, environmental remediation, sensors, solar cells and energy storage.

M. Sc. Semester-IV

Theoretical

MCH43-I: optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Polymer Chemistry-II: **(12L)**

Inorganic polymers-coordination polymers including metal organic frame work (MOF), homopoly and heteropoly acids and salts; synthesis, structure, reactions and bonding as applicable in respect of molybdenum blue, tungsten blue, ruthenium blue, Creutz–Taube complex, platinum blue, tungsten bronze, ruthenium red, Wolfram’s red salt, Krogmann’s salts, organometallic polymers-different types; olefin metathesis and metathesis polymerization, ring opening metathesis polymerization (ROMP), acyclic diene metathesis polymerization (ADMP), carborane polymers, Zieglar-Natta catalysts and green catalysts.

2. Redox Reactions and its Mechanism: (13L)

Classification, kinetics and mechanism, outer-sphere electron transfer reactions-controlling factors, self-exchange rate, electron tunneling hypothesis, hetero-nuclear redox reaction and simplified Marcus theory; Marcus cross relationship and its application, solvated electron; inner-sphere electron transfer reaction-characteristics and controlling factors, ligand transfer, role of bridging ligand, chemical mechanism of electron transfer, complementary and non-complimentary redox reactions.

3. Physical Characterization of Inorganic Compounds by Spectral Analysis-IV: (13L)

Electron paramagnetic resonance - zero field splitting factor and its importance in napthyl radical and various metal centers having more than one odd/even number unpaired electrons, spin polarization for atoms and transition metal ions, spin-orbit coupling, EPR activity and application to metal-ligand complex with paramagnetic metal ions and paramagnetic ligands, isotropic and anisotropic EPR spectra of metal complexes, electronic spectra for chemical analysis (ESCA)-basic principle and applications.

4. Advanced Inorganic Materials: (12L)

Beyond band theory of solids, functional oxide materials, magnetoresistance, colossal magnetoresistive materials (CMR), spin polaron, dynamic Jahn-Teller distortion, double exchange, superexchange, Goodenough-Kanamori-Anderson rules (GKA), phase separation: homogeneous, inhomogeneous, structural and electronic, charge ordering (CO), orbital ordering (OO), effect of ionic radius on the physical properties of these functional materials, chemical pressure, size disorder, photonic crystal.

LEARNING OBJECTIVES: (i) Study various inorganic polymers such as coordination polymers, polyphosphazenes, silicones, inorganic rubber, sulfur-nitrogen polymers, polyatomic ions of Sn, Pb, S, Se and Te, homopoly and heteropoly acids and salts; Acquire knowledge about Organo-metallic Polymers; Learning about Polymerization: Metal ion initiated polymerization and coordination polymerization, olefin metathesis and metathesis polymerization, ring opening polymerization (ROP), Zieglar-Natta catalysts and green catalysts; Polymer metal complexes and their role in analytical chemistry; (ii) The objective of this section is to highlight the pathways (i.e. outer sphere and inner sphere) of electron transfer reactions; (iii) Students will be able to characterize inorganic compounds by EPR and ESCA. The PG students may acquire knowledge about the characterization of different known and unknown synthetic inorganic samples. The students will get the knowledge of EPR active inorganic complexes with unpaired multi-electronic systems; (iv) In this special topic on advanced inorganic materials students will be introduced to a part of the frontier area of materials chemistry. The discussion will start from the failure of band theory to explain the electronic properties of several metal oxide systems. The concept of electron correlation will be introduced. Students will get familiar to the Mott and Mott-Hubbard insulator, charge transfer insulator and their genesis. A general introduction to the functional oxide materials will be provided with their potential technological prospect. Several features of the electronically correlated functional oxides like interplay between spin, charge, orbital and lattice degree freedom, and thus evolved properties like magnetoresistance, negative colossal magnetoresistive materials (CMR), spin polaron, dynamic Jahn-Teller distortion, double exchange, superexchange, charge ordering (CO), orbital ordering (OO), and phase separation will be highlighted. Introduction to Goodenough-Kanamori-Anderson rules (GKA) to predict the magnetic ground state of the interacting magnetic ions via superexchange will be discussed with suitable examples. The effect of ionic radius, size disorder parameter and chemical pressure on the physical properties of these functional materials will be discussed with proper examples.

LEARNING OUTCOME: (i) Understanding of up-to-date knowledge of inorganic polymers and their applications, (ii) The understanding of the subject will benefit the students to realise the different factors controlling the electron transfer reactions including the biochemical redox processes. This knowledge may also find applications in the redox reactions industrially important. (iii) The students will get the idea to unveil the structure and properties relationship through the spectroscopic investigations. Specially, the ideas of EPR study will be exclusive one to get the idea of reaction mechanism particularly the radical mediated reaction pathway and this will give motivate the student to enhance their knowledge about the anti-oxidant ingredient based research work relevant for chemical and pharmaceutical industries. This course will also help the students to get the notion of the redox-reaction mediated chemical processes. The students will get the idea regarding the isotope related EPR based studies through the course.

M. Sc. Semester-IV

Theoretical

MCH43-O: optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Organic Photochemistry: (13L)

Basic principles, Jablonski diagram, excited state (S1, T1) of some organic molecules, quenching, photolytic cleavage, cis-, trans isomerization, mechanism, photochemical reactions of carbonyl compounds, olefins and conjugated carbonyl compounds, □-cleavage or Norrish type-I for cyclopentanones, cyclobutanones, □-cleavage reaction, Norrish type-II, formation of photoenols/photoenolisation, Paterno-Buchi reaction (Photocycloaddition reaction), addition to electron rich alkenes and electron deficient alkenes, oxetane formation with diene and alkynes, intramolecular Paterno-Buchi reaction, [2+2] cycloaddition reaction of enones with alkenes.

2. Photo Rearrangements: (12L)

Photo rearrangement of cyclopentenone, cyclohexanone, di-π-methane rearrangement, rearrangement of dienones, photo rearrangements of α,β-unsaturated ketones, aza-di-π-methane rearrangement, rearrangements in aromatic compounds, Barton reaction.

3. Photoredox Reactions in Organic Chemistry: (12L)

Photoreduction of carbonyl compounds, photo reduction of aromatic hydrocarbons, photochemical oxidations, photo-oxidation of alkenes and polyenes, substitution in aromatic system.

4. Radical Reactions in Organic Chemistry: (13L)

Definition, generation of free radicals, detection, shapes and stability, stable free radicals, example of addition, substitution, oxidation, cyclization and rearrangement involving radical reaction mechanism.

LEARNING OBJECTIVES: The aim of this course is to make the students acquainted with the fundamental concepts of free radical generation and organic photochemical reactions. The ideas of fundamental photochemical processes and photochemical transformations will be discussed. There will be a detailed coverage of a range of photochemical reactions and their synthetic utility will also be focused in this course. Free radicals are one of the most common intermediates generated in protochemical processes. Free radicals are unique and rare species. They are present only under special and limited conditions. Interestingly, some of the free radicals are familiar to us in our lives. Students will learn their reactivities and characteristic properties.

LEARNING OUTCOME: Students will be acquainted with the fundamental concepts of photochemical processes and transformations as well as organic photochemical reactions and various molecular events of organic photochemistry. Students will also be able learn the applications of photochemical reactions in various synthetic transformations and related mechanisctic pathway. Students will also get an exposure on the recent research and developments of organic photochemistry and its synthetic utility.

M. Sc. Semester-IV

Theoretical

MCH43-P: Optional (Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Computational Chemistry: (20L)

The Born-Oppenheimer approximation, post Hartree-Fock calculation, electronic correlation, ab initio calculation: Hartree-Fock-Roothan method, configuration interaction (CI) method, Condon-Slater rule, spin-orbit interaction, the concept of basis sets, concept of PES, geometry optimization, stationarypoints and normal modes of vibration, molecular orbital theory (MOT), valence bond theory (VBT), chemical bonding, semi-empirical MO treatments of planar conjugated molecules, thefree-electron MO method, the Hückeland extended Hückel MO method, the Pariser-Parr-Pople(PPP) method, general semi-empirical MO methods, molecular dynamics and molecular mechanics method, quantum Monte Carlo method , solvent effects introduction to density functional theory (DFT), Hohenberg-Kohn variation theorem, Kohn-Sham equations, exchange-correlation energy, local density approximation, generalized gradient approximation.

2. Molecular Interaction: (10L)

Intermolecular potential energy, intermolecular repulsion and attraction, electrostatic forces, inductive forces, quantum mechanical treatment for dispersion forces, Hellmann-Feynman theorem, electrostatic theorem, model potentials,non-covalent interactions.

LEARNING OBJECTIVES OF UNIT-1 AND 2: Through this unit the students will introduce into advanced theory on quantum chemistry to deal with a system having many electrons.

LEARNING OUTCOME: The unit may serve as an important background for the students who will join at computational chemistry laboratory for doing Ph.D

3. Irreversible Thermodynamics-I: (10L)

Thermodynamic criteria for non-equilibrium states, Clausius inequality, principle of local equilibrium, local parameters, dissipation function, affinity of chemical reaction, entropy production and entropy balance equations, generalized flux and forces, Prigogine equation, stationary states, linear phenomenological equations (LPE), cross effects between physical processes, cross effects in chemical reactions, Curie-Prigogine symmetry principle, fluctuation, microscopic reversibility and Onsager equation, regression of fluctuation, Knudsen effect, mechanocaloric effects, Soret effect, Dufour effect, principle of minimum entropy production.

4. Irreversible Thermodynamics-II: (10L)

Stability of steady state, Maxwell's demon, forbidden coupling, applications in physico-chemical and biological phenomena: reverse osmosis, membrane transport, carrier mediated transport (CMT), oscillatory reactions.

LEARNING OBJECTIVES OF UNIT-3 AND 4: To provide the students with the concepts of various transport processes and rates of chemical reactions. To make the students realize that almost all systems found in nature are not in thermodynamic equilibrium, for they are changing or can be triggered to change over time, and are continuously and discontinuously subject to flux of matter and energy to and from other systems and to chemical reactions. Some systems and processes are, however, in a useful sense, near enough to thermodynamic equilibrium to allow description with useful accuracy by currently known non-equilibrium thermodynamics.

LEARNING OUTCOME: Knowledge of irreversible thermodynamics can be successfully applied to describe biological processes such as protein folding/unfolding and transport through membranes. It is also used to give a description of the dynamics of nanoparticles, which can be out of equilibrium in systems where catalysis and electrochemical conversion are involved. Also, ideas from non-equilibrium thermodynamics and the information theory of entropy can adapted to describe general economic systems.

M. Sc. Semester-IV

Theoretical

MCH44-I: Optional (Inorganic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Nuclear Properties and Structure: (13L)

Nuclear stability–different factors, nuclear models- Fermi gas model, liquid drop model, nuclear shell model, nuclear magic number and its derivation from nuclear potential well, nuclear spin, nuclear configuration and parity, nuclear isomerization and non-optical transitions, nuclear temperature and entropy; models of disintegration-radiation emission (fluorescence) and electron emission (Auger effect), theory of radioactivity decay-golden rule and selection rule, radioactive equilibrium.

2. Nuclear Reactions: (12L)

General features, types of nuclear reactions, conservation laws, Q-value and cross-section of nuclear reaction, mechanism of nuclear reactions, resonance and non-resonance reaction, nuclear fission-discovery, characteristics, fission yields, reproduction factor, four factor formula, critical size, atom bomb; nuclear reactors, breeder reactor, natural fission reactor; calculation of fission probability from Bohr-Wheeler's theory; nuclear fusion- characteristics, hydrogen bomb, stellar energy, controlled fusion reaction. Szilard-Chalmer reaction, nuclear activation analysis.

3. Atomic Spectroscopy: (10L)

Basis principle, instrumentation and applications of atomic absorption spectroscopy (AAS), atomic emission spectroscopy (AES), flame emission spectroscopy (FES), inductively coupled plasma mass spectroscopy (ICPMS) and fluorimetry.

4. Separation Techniques: (15L)

Solvent extraction: principle, distribution ratio and partition coefficient, successive extraction and separation; different methods of extraction systems; Craig extraction and counter current distribution; problems; chromatography: general principle; classification, mathematical relations of capacity, selectivity factor, distribution constant and retention time; chromatogram, evaluation in column chromatography: band broadening and column efficiency; Van Deemeter equation; column resolution, numerical problems, GC, LC, TLC, PC, SEC.

LEARNING OBJECTIVES: (i) The PG students may acquire knowledge about the characterization of different known and unknown toxic inorganic samples. The students will get the idea to quantitatively determine the environmental samples. The students will acquire the knowledge of quantitative analyses of medicinal and biochemical samples. The students will learn about the different instrumentations techniques and its related advancements. The students will get the idea of quantitative analyses of diverse types of samples for practical uses including scientific research and industrial purposes; (ii) Study basis principle, instrumentation and applications of Atomic Absorption Spectroscopy (AAS), Atomic Emission Spectroscopy (AES), Flame Emission Spectroscopy (FES), Inductively Coupled Plasma Mass Spectroscopy (ICPMS) and Fluorometry; (iii) Study solvent extraction: principle, distribution ratio and partition coefficient, successive extraction and separation; different methods of extraction systems; Acquire knowledge about Craig extraction and counter current distribution; Introduce chromatography: general principle; mathematical relations of capacity, selectivity factor, distribution constant and retention time; chromatogram, evaluation in column chromatography: band broadening and column efficiency; Van Deemeter equation; column resolution

LEARNING OUTCOME: (i) Achieve the efficiency in analysing sample using AAS, AES, FES and ICPMS. (ii) Understanding and application of various advanced separation techniques

M. Sc. Semester-IV

Theoretical

MCH44-O: Optional (Organic)

Full Marks: 50 (40 + 10); Credit point: 4

1. Advanced Heterocyclic Chemistry, Part A: (13L)

Nomenclature of heterocycles – replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles; aromatic heterocycles – tautomerism in heterocyclic systems, reactivity of aromatic heterocycles, non-aromatic heterocycles – conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction, anomeric and related effects, hydrogen bonding and intermolecular nucleophilic-electrophilic interactions, meso-ionic systems – general classification, chemistry of some important meso-ionic heterocycles of type A and B and their applications.

2. Advanced Heterocyclic Chemistry: Part B: (12L)

Heterocyclic synthesis – principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions; synthesis and reactivity of 3-, 4-, 5-, 6-, & 7- membered heterocycles and one, two or more heteroatoms (aziridines, oxiranes, thiiranes, azetidines, oxetanes, thietanes, diazines, triazines, thiazines, azepines, oxepines); benzo-fused five and six-membered heterocycles – synthesis and reactions including medicinal applications of benzopyrroles, benzofurans, benzothiophenes, quinolizinium and benzopyrylium salt, coumarins and chromones, heterocycles and pharmaceutical industry.

3. Natural Products: (12L)

Structure and stereochemistry, Natural products: Structure and stereochemistry of alkaloids (yohimbine/quinine); terpenoids (citral, geraniol, linalool, caryophyllene), steroids (cholesterol).

4. Natural Products, Biosynthesis: (13L)

Biosynthesis of alkaloids like atropine, quinine, natural products: biosynthesis: terpenoids and steroids.

LEARNING OBJECTIVES: The heterocyclic chemistry is vast and expanding area of chemistry because of obvious application of compounds derived from heterocyclic rings in pharmacy, medicine, agriculture, plastic, polymer and other fields. Students will be able to synthesize, characterise and imply in the treatment of infectious diseases by virtue of the therapeutic properties of those compounds. Many heterocyclic compounds synthesized in laboratories have been successfully used as clinical agents. The objective of this course is to make the students understand the properties, reactivities and stabilities of hetero aromatic compounds of fused ring system. They will know the important synthetic routes and reactivity for fused ring hetero aromatic compounds. They will also learn about the applications of these hetero aromatic compounds in the synthesis of important industrial and pharmaceutical compounds. Moreover they will learn about the structure, properties and synthesis of natural products like alkaloids, terpenoids and steroids.

LEARNING OUTCOME: At the end of the course the students will have a strong background on heterocyclic chemistry and natural product chemistry.

M. Sc. Semester-IV

Theoretical

MCH44-P: Optional (Physical)

Full Marks: 50 (40 + 10); Credit point: 4

1. Radiation-matter Interaction: (15L)

Theory of electromagnetic radiation, interaction between matter and electromagnetic radiation: semiclassical treatment using time-dependent perturbation theory, absorption and emission of radiation, electric dipole transitions, Einstein's treatment of absorption and emission phenomena, Fermi golden rule, transition probabilities and rates, spectral shapes, correlation with experimental quantities, intensity of electronic transitions, theoretical absorption intensity, oscillator strength, selection rules, directional nature of light absorption, lifetimes of excited electronic states of atoms and molecules.

2. Electronic Spectroscopy, Atoms: (10L)

Atomic structure: Vector representation of momenta and vector coupling, Angular momenta and magnetic moments, coupling of angular momenta, Russell-Saunders coupling, atomic term symbols, spectra of alkali metal atoms, hydrogen atom, helium and alkaline earth metal ions.

3. Electronic Spectroscopy, Molecules: (15L)

Electronic energy and total energy- potential energy curve, resolution of total eigenfunction and total energy, vibrational structure of electronic transition, rotational structure of electronic bands, intensity in electronic bands, intensity distribution in the vibrational structure, Franck-Condon principle, wave-mechanical formulation of Franck-Condon principle, vibrational sum rule and vibrational temperature, classification of electronic states and electronic transitions, multiplet structure, symmetry properties of electronic wave functions, Hund's coupling cases, uncoupling phenomena, selection rules, allowed electronic transitions, forbidden electronic transitions, Zeeman effect and Stark effect.

4. Principle of Lasers and its Applications : (10L)

Two-level transition (absorption, induced and stimulated emission), Einstein model for two- level transition, principle of Maser and Laser action, population inversion (two/three/four level systems), basic element in laser (resonator, gain medium, pumping technique), characteristics of laser radiation (coherence: temporal/spatial; polarization, monochromaticity, intensity), single mode laser (solid/gas laser: Ruby, Nd:YAG,Ar-ion, CO2, excimer etc.), tunable laser (dye laser), harmonic generation, application of laser (chemical problem).

LEARNING OBJECTIVES: In the beginning of the course the students will understand the EMR radiation based on the Maxell's equation. Then they will explore basic theory for the radiation matter interaction considering the disturbance of a quantum system by a high intensity radiation(semi classical treatment of radiation matter interaction) based on the perturbation theory of the quantum mechanics. Using this the students will understand many spectroscopic phenomena.

Finally, the student will be introduced into the principle which is used to generate coherent radiation with high intensity.

LEARNING OUTCOME: The students will able to explain the fine structure of atomic and molecular spectra. At the same time they may surprise to know the principle for the determination of the molecular partition function (which is very important in statistical mechanics) experimentally using the energy spectrum. The students also know the principle for the determination of the electronic wave function experimentally which may be an important input for the theoretical study on the dynamics at the excited states. In addition to these the student will recognize how Einstein used the simple mind to determine the rate constant for the spontaneous emission (which is purely quantum mechanical origin) indirectly based on the concept of dynamic equilibrium. Finally, the student will learn the principle to produce and use of coherent radiation with high intensity.

M. Sc. Semester-IV

Project

MCH45-PJ: Optional (Project)

Full Marks: 100 (80 + 20); Credit point: 8

Topic selection in consultation with the teacher, literature search from different reference books and using internet search, typed written-up with proper tables, structures, figures and literature to be submitted, seminar lecture on this topic to be delivered in presence of external expert and sectional teachers.

LEARNING OBJECTIVES: Through a project work in a specialised branch under the supervision of a guide the student will gain the skill for running a scientific research work. They will have the ability to design, execute and present a complete research project in a laboratory.

LEARNING OUTCOME: The student will have an entry point to the research field and will have a good training to contribute his/her research work to the science community.