Cotton University, Guwahati
Department of Chemistry

PG (M. Sc.) CBCS Syllabus
for
Core, Laboratory and Elective Courses

Programme Learning Objectives (PLOs):

PLO1 To educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic laboratories.

PLO2 To provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on qualitative and quantitative technique.

PLO3 To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of all branches of chemistry involving applied organic, inorganic, physical, analytical, quantum, industrial, pharmaceutical, polymer, Nanoscience & technology.

PLO4 The department would like to attain worldwide recognition in Chemistry research and teaching.

PLO5 To expose the students to a breadth of experimental techniques using modern instrumentation.

PLO6 To focus on encouraging students to familiar with various academic activities like midterm tests, online tests, tutorial, surprise test, oral, seminar, assignments and seminar presentation.

PROGRAMME SPECIFIC OUTCOMES (PSOs)

On completion of M.Sc. Chemistry programme, graduates will be able to

PSO-1 Acquire knowledge about the basic concepts, fundamental principles, and the scientific theories related to various chemical phenomena and their relevance in the day-to-day life.

PSO-2 Design experiments, generate, analyze and interpret data to provide solutions to different scientific and industrial problems by working in pure and inter-disciplinary areas of chemical sciences.

PSO-3 Apply their knowledge of chemistry to solve different real-life problems.

PSO-4 Become familiar with the different branches of chemistry such as organic, inorganic, physical, analytical, computational, green, environmental, polymer and biochemistry.

PSO-5 Gain a thorough knowledge in the subject to be able to work in projects at different research as well as academic institutions.

PSO-6 Independently carry out research/investigation to solve practical problems and write/present a substantial technical report/document.

PSO-7 Operate sophisticated instruments (FT-IR, UV-Vis, Fluorescence, Cyclic Voltammetry, GC-MS, TGA-DSC etc.)

Mapping of PLO and Chemistry Courses

Table 1 CHEMISTRY COURSES

	Inorganic Chemistry I	Organic Chemistry I	Physical Chemistry I	Group Theory and Molecular Spectroscopy	Organic and Physical Chemistry Practical	Chemistry of Environmental Pollution	Inorganic Chemistry II	Organic Chemistry II	Physical Chemistry II	Quantum Chemistry and Molecular Spectroscopy	Inorganic and Physical Chemistry Practical	Computational Representation of Molecules
PSO	Core-1	Core-2	Core-3	Core-4	LAB 1	SEC 1	Core-5	Core-6	Core-7	Core-8	LAB 2	SEC 2
PSO 1	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
PSO 2	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
PSO 3	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
PSO 4	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
PSO 5	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
PSO 6					✓						✓	✓
PSO 7				✓	✓					✓	✓	

[Note: SEC - Skill Enhancement Course, SPL – Special Paper, OPE- Open Elective

Table 2 CHEMISTRY COURSES

PSO	Inorganic Chemistry III	Organic Chemistry III	Advanced Quantum Chemistry	Organometallics and Photo Inorganic Chemistry	Advanced Organic Synthesis	Chemical Kinetics and Electrochemistry	Nanostructures and Nanomaterials	Dissertation/Project Work	Analytical Methods in Chemistry	Dissertation/Project Work	Advanced Bioinorganic Chemistry	Natural Products and Medicinal Chemistry	Heterogeneous Catalysis	Chemistry in Human Life
	Core-9	Core-10	Core-11		SPL1		OPE1	Project	Core-12	DPW		SPL2		OPE2
PSO 1	✓	✓	✓		✓		✓	✓	✓	✓		✓		✓
PSO 2	✓	✓	✓		✓		✓	✓	✓	✓		✓		✓
PSO 3	✓	✓	✓		✓		✓	✓	✓	✓		✓		✓
PSO 4	✓	✓	✓		✓		✓	✓	✓	✓		✓		✓
PSO 5	✓	✓	✓		✓		✓	✓	✓	✓		✓		✓
PSO 6								✓	✓	✓				
PSO 7							✓	✓	✓	✓				

[Note: SEC - Skill Enhancement Course, SPL – Special Paper, OPE- Open Elective

Cotton University: M.Sc. Syllabus – Chemistry
Overview of Courses for Chemistry Students

Semester I:

Core Courses: C01 – Inorganic Chemistry I (Cr 3+1+0 = 4)
C02 – Organic Chemistry I (Cr 3+1+0 = 4)
C03 – Physical Chemistry I (Cr 3+1+0 = 4)
C04 – Group Theory and Molecular Spectroscopy (Cr 3+1+0 = 4)

Laboratory Courses: LAB 1 – Organic and Physical Chemistry Practical (Cr 0+0+4 = 4)

Elective Courses: SEC 1 – Offered by same or other department (Cr 2+0+0 = 2)

Semester II:

Core Courses: C05 – Inorganic Chemistry II (Cr 3+1+0 = 4)
C06 – Organic Chemistry II (Cr 3+1+0 = 4)
C07 – Physical Chemistry II (Cr 3+1+0 = 4)
C08 – Quantum Chemistry and Molecular Spectroscopy (Cr 3+1+0 = 4)

Laboratory Courses: LAB 2 – Inorganic and Physical Chemistry Practical (Cr 0+0+4 = 4)

Elective Courses: SEC 2 – Offered by same or other department (Cr 2+0+0 = 2)

Semester III:

Core Courses: C09 – Inorganic Chemistry III (Cr 3+1+0 = 4)
C10 – Organic Chemistry III (Cr 3+1+0 = 4)
C11 – Advanced Quantum Chemistry (Cr 3+1+0 = 4)

Elective Courses: SPL 1 – Choose any one SPL 1 from the list (Cr 4+1+0 = 5)
OPE 1 – Offered by same or other department (Cr 3+1+0 = 4)

Semester IV:

Core Courses: C12 – Analytical Methods in Chemistry (Cr 3+1+0 = 4)
DPW – Dissertation/Project Work (Cr 0+0+6 = 6)

Elective Courses: SPL 2 – Choose any one SPL 2 from the list (Cr 4+1+0 = 5)
OPE 2 – Offered by same or other department (Cr 3+1+0 = 4)

[Note: SEC - Skill Enhancement Course, SPL – Special Paper, OPE- Open Elective]

List of Skill Enhancement Courses (SEC) offered by Dept. of Chemistry

1. SEC 1: Chemistry of Environmental Pollution (Cr 2+0+0 = 2)

2. SEC 2: Computational Representations of Molecules (Cr 2+0+0 = 2)

   OR

   Computer Programming for Science Students (Cr 2+0+0 = 2)

List of Special Paper Courses (SPLs) offered by Dept. of Chemistry

1. SPL 1: Organometallics and Photo-Inorganic Chemistry (Cr 4+1+0 = 5)

   OR

   Advanced Organic Synthesis (Cr 4+1+0 = 5)

   OR

   Chemical Kinetics and Electrochemistry (Cr 4+1+0 = 5)

2. SPL 2: Advanced Bioinorganic Chemistry (Cr 4+1+0 = 5)

   OR

   Natural products and Medicinal Chemistry (Cr 4+1+0 = 5)

   OR

   Heterogeneous Catalysis (Cr 4+1+0 = 5)

List of Open Elective Courses (OPEs) offered by Dept. of Chemistry

1. OPE 1: Nanostructures and Nanomaterials (Cr 3+1+0 = 4)

2. OPE 2: Chemistry in Human Life (Cr 3+1+0 = 4)

CORE COURSES: SEMESTER I

C01 – Inorganic Chemistry I — Credits: 3+1+0=4

Theory: 60 Lectures

Learning Objectives:

LO1 To provide basic principles of chemical bonding in polyatomic molecules, bonding theories, shapes of molecules and study of effect of various chemical forces on the physical properties of molecules.
LO2 To introduce the structures of various inorganic solids/crystals and their thermal stability and solubility.
LO3 To enhance the knowledge of acid-base and redox chemistry of inorganic compounds.
LO4 To study lanthanide and actinide chemistry.
LO5 To know about the bonding in coordination compounds, understanding of magnetic properties of transition metal complexes with different geometries.

Unit 1: Chemical Bonding

Molecular Orbital Theory: Introduction, qualitative molecular orbital treatment for homonuclear and heteronuclear diatomic molecules (N_2, O_2, CO, NO, HF), Bonding in polyatomic molecules (H_2O, BeH_2, H_2O, CO_2, NO_2, NH_3) based on the concept of hybridization and LCAO-MO. Molecular shape in terms of molecular orbitals – Walsh diagrams.

Correlations in Bond properties- Bond length, Bond Order and Bond Strength. Hydrogen bonding interactions. Effect of hydrogen bonding and other chemical forces on melting and boiling points and solubility.

(14 lectures)

Unit 2: Structure of Simple Solids

Packing of spheres – hexagonal and cubic close packing, tetrahedral and octahedral holes in close-packed structures- metals and alloys, solid solutions. The ionic model for the description of bonding in ionic solids. Characteristic structures of ionic solids- the NaCl and CsCl types, the sphalerite and wurtzite types of ZnS, the NiAs structure type, The perovskite and spinel structure types of mixed-metal oxides- importance ionic radii and the radius ratios in determining structure type among ionic solids. Lattice energy considerations, Thermal stability and solubility of inorganic solids.

(12 lectures)

Unit 3: Acid Base and Redox Chemistry

Hard and soft acid-base (HSAB) concept and its applications. Strength of oxo acids and halo acids, strength of inorganic bases- periodic trends in acidity and basicity of hydrides, oxides, oxyacids of non-transition elements. Relevance of acidity and basicity in catalysis. Nonaqueous solvents.

Standard electrode potentials, pH dependence of electrode potentials. Redox stability of metal ions in water, oxidation by atmospheric oxygen. Applications of Latimer and Frost diagrams,Rredox behaviour of non-transition elements based on electrode potential data.

(12 lectures)

Unit 4: Chemistry of Inner Transition Elements

Lanthanides and Actinides: Extraction and separation, periodic properties, redox Chemistry, magnetic and spectral properties, analytical applications (Lanthanide Shift Reagents).

(10 lectures)

Unit 5: Coordination Chemistry: Bonding and Magnetic properties

Crystal field theory of bonding in octahedral, tetrahedral and square planar transition metal complexes. Factors affecting crystal field splitting, Crystal field stabilization energy, Spectrochemical series. Jahn Teller Distortion, Ligand field theory of metal complexes.

Magnetic properties of transition metal complexes.

(12 lectures)

Course Outcomes:

After the completion of the course, the students will acquire knowledge of

CO1 chemical bonding theories, molecular shapes and effect of various chemical forces on the properties of molecules.

CO2 structure of inorganic solids and their thermal stability and solubility.

CO3 acid-base and redox chemistry of inorganic compounds

CO4 the chemistry of inner transition elements.

CO5 bonding in coordination compounds and magnetic properties of coordination compounds.

C02 – Organic Chemistry I   Credits: 3 + 1 + 0 = 4

Theory: 60 Lectures

Learning objectives:

The students will be able to understand
LO1 Application of kinetics and energetics in elucidation of organic reaction mechanism.
LO2 Stereogenic center and stereochemistry of organic molecules without chiral enter.
LO3 Stereoselective reactions and effect of structure on stereoselectivity.
LO4 Description of aromaticity in benzenoid, polycyclic systems and annulenes.
LO5 Structure and reactivity of heterocycles with more than one heteroatom.

Unit :1 Kinetics and Energetics of Reaction Mechanism

TST theory of reaction rates: kinetics & thermodynamics of activation. Reaction profiles for multistep reactions, Hammond postulate, Curtin-Hammett Principle; kinetic and thermodynamic control.

Linear free energy relationships (LFER): Hammett equation - substituent and reaction constants; the Taft treatment of polar and steric effects in aliphatic compounds; kinetic isotope effects in organic reactions.

Effects of conformation on reactivity: anomeric effect, stereoelectronic effects, neighbouring group participation.

(12 Lectures)

Unit 2: Stereochemistry

Classification of organic molecules into different Point Groups, R/S, E/Z nomenclature in C, N, S, P containing compounds; concept of absolute and relative configuration; chirality in molecules devoid of chiral centers- allenes, spiranes and biphenyls (atropisomerism), binaphthyls.

Concepts of stereogenic center – chirotopic and achirotopic center; homotopic and heterotopic ligands and faces (prostereoisomerism and prochirality etc.); optical purity and enantiomeric excess; conformation of acyclic organic molecules, chirality of conformers, cyclohexane (di- and tri- substituted), cyclohexanone and decalins.

(16 Lectures)

Unit 3: Stereodifferentiating reactions

Stereospecific and Stereoselective synthesis; classification of stereoselective synthesis, diastereoselective, enantioselective and double stereo-differentiating reactions, nucleophilic addition to aldehyde and acyclic ketones– Cram, Felkin and Felkin-Anh model, Prelog's rule, Stereoselective nucleophilic addition to cyclic ketones (Cram and Felkin-Anh models).

Acyclic stereoselection: reactions at α-and β-positions of a chiral center.

(11 Lectures)

Unit 4: Aromaticity

Aromaticity of benzenoid and non-benzenoid compounds including monocyclic and fused ring systems, molecular orbital description, Frost's model, non-aromatic and antiaromatic compounds, molecular stability and reactivity, aromaticity driven reactions including acid-base reactions; aromaticity of higher annulenes; Homoaromatic compounds.

(8 Lectures)

Unit 5: Heterocyclic chemistry

Heterocyclic compounds containing two or more hetero atoms: Synthetic methods of preparation, properties and applications in medicinal chemistry e.g., azoles (pyrazole, imidazole, oxazole and thiazole derivatives), diazines (pyrazine, pyrimidine and pyridazine derivatives), benzo-diazines, heterocyclic compounds containing one nitrogen atom and an oxygen or sulphur atom (oxazine, phenoxazine and thiazine derivatives), triazines and tetrazines.

(13 Lectures)

Course outcomes:

After completion of the course, the students will be able to-
CO1 derive mechanism of unknown organic reaction based on energetic.
CO2 assign different stereo chemical descriptors in organic compounds.
CO3 predict stereoselectivity in organic reactions.
CO4 identify and understand the properties of aromatic compounds.
CO5 work out the synthetic route for various heterocycles and understanding their chemical properties.

C03 – Physical Chemistry I   Credits: 3 + 1 + 0 = 4

Theory: 60 Lectures

Learning Objectives:

LO1

1. To introduce students with the basic concepts of thermodynamics of non-ideal gases and non-ideal solutions.
2. To understand about the three-component phase equilibrium.
3. To make students familiar with the basic principles of non-equilibrium (irreversible) thermodynamics and its various concepts such as internal entropy production, generalised forces and flows, non-equilibrium stationary states etc.

LO2

1. Introduction of statistical thermodynamics and its various concepts such as distribution, macrostate, microstate, ensemble, partition function etc.
2. Different types of statistics such as Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein.
3. Maxwell-Boltzmann statistics in details along with partition function for various types of gases.
4. To give basic idea about obtaining thermodynamic functions and equilibrium aspects from partition functions for gases.

LO3

1. To give basic concepts about polymer chemistry along with various classification of polymers.
2. To introduce the concepts of dispersity and various average molecular weights of polymers and their determination techniques.
3. To know about the chain configuration of polymers in solution.
4. Introduction of various polymerization techniques along with their kinetics.

Unit 1: Equilibrium and Non-Equilibrium Thermodynamics

Non-ideal systems: Fugacity and fugacity coefficients for gases, activity and activity coefficients for non-ideal solutions – the different scales of activity and activity coefficients.

Phase equilibrium: Application of Gibbs phase rule to three component systems, triangular plots, water-acetic acid chloroform and ammonium chloride-ammonium sulphate water system.

Non-equilibrium thermodynamics: Concept of internal entropy production in irreversible processes. Generalised forces and flows, coupled forces and flows, phenomenological relations, statement of Onsager's reciprocal relation. Non-equilibrium stationary states in some open systems – statement of Prigogine's principle of minimum entropy production, the explanation of sustenance of highly ordered biological organisms in spite of continual increase of entropy.

(18 Lectures)

Unit 2: Statistical Thermodynamics

Statistical thermodynamics: Molecular energy levels and concept of distribution of gas molecules in energy levels. Concept of macrostate, microstate and thermodynamic probability. Concept of ensembles – micro-canonical, canonical and grand canonical ensembles, definition of canonical ensemble partition function Q. Ideas of Maxwell-Boltzmann, Fermi-Dirac, Bose-Einstein and the corrected-Boltzmann statistics, question of indistinguishability of particles.

Boltzmann distribution in a pure gaseous system, the molecular partition function q and its significance, relation between Q and q for a pure gas. Molecular significance of heat and work. Translational, electronic, nuclear, rotational and vibrational partition functions of gas molecules. Thermodynamic functions of monatomic, diatomic and polyatomic gases – calculation of equilibrium constants of gaseous reactions, residual entropy calculations.

(20 Lectures)

Unit 3: Polymer Chemistry

Some basic concepts: Monomers, repeat units, degree of polymerization, concepts of linear, branched and network polymers with examples. Classifications of polymers with examples: natural and synthetic polymers, thermoplastic and thermosetting polymers, classification on the basis of use as fibres, elastomers and plastics.

Polydispersity and average molecular weight concept. Number, weight and viscosity average molecular weights – numerical calculations, polydispersity index. Determination of molecular weights: viscosity, osmotic pressure and light scattering methods.

Polymers in solutions: Chain configuration of macromolecules – root mean square end to end distance and radius of gyration; random flight model and chain stiffness concept, short range and long range effects, average dimension of polymer chains, concept of theta solvent.

Chain and step polymerisation, introductory concepts of cationic, anionic and coordination chain polymerisation and ring-scission step polymerisation. Review of free-radical chain polymerisation kinetics, kinetics of step polymerisation and of chain copolymerisation.

(22 Lectures)

Course Outcomes:

After completion of the course, students will acquire knowledge of

CO1 The fundamentals of non-ideal gases and non-ideal solutions, three component phases equilibrium and non-equilibrium (irreversible) thermodynamics with its various concepts.

CO2 The basic principles of statistical thermodynamics along with thermodynamic functions and equilibrium aspects.

CO3 (i) The polymerization procedures, classifications, various molecular weights and kinetics. (ii) The configurations of polymers in solution using Random flight model.

C04 – Group Theory and Molecular Spectroscopy Credits: 3 + 1 + 0 = 4

Theory: 60 Lectures

(Note: Separate answer-scripts to be supplied for Part A and Part B during examination.)

Learning Objectives:

LO1 To make students familiar with shapes of different molecules in their most stable state and to make them capable of visualizing molecules in 3-D space and to quantify them.
LO2 To introduce students with the fundamental principles and techniques of spectroscopy and to make them familiar with basic and advanced techniques
LO3 To make the students familiar with the basic principles of rotational, vibrational and Raman spectroscopic techniques
LO4 To understand and acquire knowledge on the application of these techniques

Part A: Group Theory

Unit 1: Molecular symmetry and symmetry groups

Concept of group theory, Symmetry elements and symmetry operations, Classes of symmetry operation, Symmetry point groups, Assignment of point groups to simple molecules, Structure and symmetry of Inorganic complexes (coordination number 2-6), Shapes and Symmetry of s, p and d orbitals.

(8 lectures)

Unit 2: Representation of groups

Matrix representation of symmetry operations, The Great Orthogonality Theorem Reducible and Irreducible representation of groups, Features and Construction of Character tables (C_{2v}, C_{3v} and C_{2h}).

(8 lectures)

Unit 3: Applications of Group Theory and Symmetry

Molecular Vibrations- determining symmetry types of normal modes of vibrations with selected examples, Selection rules for Fundamental Vibrational Transition (IR and Raman).

(8 lectures)

Part B: Molecular Spectroscopy

Unit 4: Introduction

Electromagnetic spectrum, Representation of spectra, Signal-to–noise ratio: Resolving power, The Width and Intensity of Spectral transitions, Fourier Transform Spectroscopy, Enhancement of Spectra: computer averaging.

(8 lectures)

Unit 5: Rotational (Microwave) Spectroscopy

Classification of molecules according to their moments of inertia, Rotational spectra of the rigid diatomic molecules (eg. HCl), selection rule, intensity and the effect of isotopic substitution, Rotational spectra of diatomic molecule as non rigid rotator, spectra of symmetric top molecules, asymmetric top molecules, Stark effect.

(12 lectures)

Unit 6: Infrared and Raman Spectroscopy

Harmonic and Anharmonic oscillators, The diatomic vibrating rotator, The vibration-rotation spectrum of diatomic molecules, fundamental vibration frequencies, overtone and combination frequencies, P, Q, R branches, Modes of vibrations in polyatomic molecules (e.g. CO_2, NH_3) and their symmetry, the influence of rotation on spectra of polyatomic molecules, the influence of Nuclear spin.

Molecular Polarizability, Pure Rotational Raman spectra of Linear, symmetric and asymmetric Top molecules, Raman activity of vibrations, Rule of Mutual Exclusion, Stokes' and Anti-Stokes' lines, Structure determination of selected molecules/ions from IR and Raman Spectroscopy (CO_2, SO_2, N_2O, NO_3^-, ClO_3^-, ClF_3).

(16 lectures)

Course Outcomes:

CO1 Symmetry is related to shape but group theory is the assignment of these shapes. This course will make the students assign a mathematical group to a particular shape and will also allow them to elucidate spectroscopic properties of molecules.
CO2 This course will also make the students capable to assign spectroscopic bands and to understand their underlying features.
CO3 Students will understand the fundamentals of spectroscopic technique.
CO4 Students will be able to solve problems relating to structure elucidation using the information obtained from rotational, vibrational and Raman spectroscopic techniques.

LAB COURSE: SEMESTER I

LAB 1 – Organic and Physical Chemistry Practical Credits: 0+0+4 = 4

Practical: 120 Hours

Learning objectives: **90 Hours**

LO1 Separation and identification of mixtures of organic compounds.
LO2 Introduction to multistep organic synthesis.
LO3 Estimation of organic compounds by titrimetric and gravimetric methods.
LO4 Chromatographic separation technique taking amino acids as an example.

Unit 1: Organic Chemistry Practical

A. Qualitative organic analysis

Binary mixtures of organic compounds, covering compounds with major functional groups, should be given with an objective to train students in

i. Qualitative separation by physico-chemical methods and
ii. Identifying the compounds by chemical analysis.

B. Organic estimation

i. Glycine by sodium hydroxide in the presence of formaldehyde
ii. Amino acid by colorimetric method using ninhydrin
iii. Glucose and sucrose in a mixture

C. Chromatographic application

Separation and identification of amino acids present in a ternary mixture by paper chromatography

D. Organic preparation: Two-step preparation

i. Benzanilide from benzophenone
ii. Benzilic acid from benzoin
iii. Anthranilic acid from phthalic anhydride

Unit 2: Physical Chemistry Practical **30 Hours**

(1) Study of the ternary phase equilibrium of acetic acid-chloroform-water at room temperature and construction the triangular plot phase diagram.

(2) Study of the complex formation between Cu^{2+} ion and ammonia by distribution method using water-chloroform mixtures and hence to find the composition of the complex.

(3) Study of the equilibrium between iodine, iodide ion and tri-iodide ion by distribution method and determination of the equilibrium constant of the reaction.

(4) Determination of the viscosity-average molar mass of a polymer by viscometric method.

(5) Determination of the dissociation constant of a weak acid using Hendersen's equation.

(Any new experiments may be added from time to time)

Course outcomes:

After completion of the course students will be able to-
CO1 Separate and identify unknown organic mixtures using traditional knowledge.
CO2 Understand the concepts behind a multistep synthesis.
CO3 Use concepts of organic reaction to determine the amount of a organic substance in unknown sample.

CORE COURSES: SEMESTER II

C05 – Inorganic Chemistry II   Credits: 3+1+0=4

Theory: 60Lectures

Learning Objectives:

LO1 To provide a general idea of electronic spectra of transition metal complexes of different geometries.
LO2 Reaction mechanism of metal complexes including electron transfer reactions and photo induced reactions of metal complexes.
LO3 To enhance knowledge about magnetic properties of inorganic compounds having different geometries.
LO4 To introduce synthesis, structure, bonding and catalytic properties of organometallic compounds.

Unit 1: **Electronic spectra of Transition metal complexes**

d-d transition, charge transfer transition, colour, intensity and origin of spectra, term symbols and splitting of terms in different geometries, selection rules for electronic transitions, correlation, Orgel and Tanabe-Sugano diagrams, calculation of Dq and Racah parameters, Nephelauxetic series.

(15 lectures)

Unit 2: Inorganic Reaction Mechanisms

Kinetic and thermodynamic stability, Lability and inertness, Stability Constants, Mechanisms of Substitution reactions in octahedral and square planer complexes, Trans effect and its application to the synthesis of metal complexes. Inner sphere and outer sphere mechanisms of Redox Reactions, MarcusTheory, Concept of Photochemical Reactions.

(15 lectures)

Unit 3: Magnetic Properties

Ferro and antiferro-magnetism, temperature independent paramagnetism, magnetic susceptibility - Van Vleck equation, experimental measurement, magnetic moment - orbital contribution, quenching of contribution, effect of spin orbit coupling, spin crossover. Temperature dependence of magnetic susceptibility, exchange coupling effects. Magnetic properties of second and third transition series.

(15 lectures)

Unit 4: Organometallic Chemistry

18-Electron rule, metal alkyl, metal carbonyl, metal-olefin and metal carbene complexes, synthesis, structure and bonding in metallocenes, Fluxionality in organometallic complexes, Types of organmetallic reactions, Homogeneous catalysis - Hydrogenation, hydroformylation, acetic acid synthesis, metathesis and olefin oxidation. Heterogeneous catalysis - Fischer-Tropsch reaction, Ziegler-Natta polymerization.

(15 lectures)

Course Outcomes:

After the completion of the course, the students are expected to acquire knowledge regarding:
CO1 Interpretation of the electronic spectra of transition metal complexes
CO2 The reaction mechanism including photochemical reactions of metal complexes.
CO3 Magnetic properties of inorganic compounds.
CO4 Basic knowledge of organometallic compounds and their role in catalysis.

C06 – Organic Chemistry II   Credits: 3+1+0=4

Theory: 60Lectures

Learning objectives:

LO1 Organic reaction intermediates, their stability and mechanisms related to these intermediates.
LO2 Biomolecules and their structures.
LO3 Role of biomolecules in different biochemical reactions.

Unit1: Reaction intermediates and related reactions: I

Carbanions: enolates and enamines, Kinetic and thermodynamic enolates, lithium and boron enolates and silyl enol ethers in aldol reactions (Zimmerman-Traxler model), conjugate addition, Michael reactions, Robinson annulation, alkylation and acylation of enolates; name reactions under carbanion chemistry - Claisen, Dieckmann, Knoevenegal, Stobbe, Darzen, Acyloin condensations, Shapiro reaction, Julia olefination, Brook rearrangement, Sakurai reaction, Henry reaction, Kulinkovich reaction, Nef reaction, Baylis-Hillman reaction.

Ylids: Chemistry of phosphorous and sulfur ylids - Wittig and related reactions, Peterson olefination

Carbocation: structure and stability of carbocations, classical and non-classical carbocations, neighbouring group participation and rearrangements including Wagner-Meerwein, pinacol-pinacolone, semi-pinacol rearrangement, Fries rearrangement, C-C bond formation involving carbocations, oxymercuration, halo-lactonisation,Tishchenko reaction, Ritter reaction, Prins reaction.

(20 Lectures)

Unit 2: Reaction intermediates and related reactions: II

Carbenes: Structure of carbenes, generation of carbenes, addition and insertion reactions, rearrangement reactions of carbenes such as Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition (existence of O and N based ylids),

Nitrenes: Structure of nitrene, generation and reactions of nitrene and related electron deficient nitrogen intermediates, Curtius, Lossen, Hoffmann, Schmidt, Beckmann rearrangement, Tebbe olefination reactions.

Radicals: Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter & intramolecular) for C-C bond formation and Baldwin‘s rules (b) fragmentation and rearrangements. Name reactions involving radical intermediates such as Barton deoxygenation and decarboxylation, McMurry coupling.

Benzyne: Generation and reactions involving benzyne.

(12 Lectures)

Unit 3: Bioorganic chemistry

Prokaryotic and eukaryotic cells; structure of plant and animal cells; intracellular organelles and their functions; metabolic processes- catabolism and anabolism; Constituents of cell nucleus, structure of chromosomes; composition and functions biological membranes- lipids and lipoproteins. **(3 Lectures)**

Nucleic acid chemistry- structure and functions of DNA and RNA, the double helical structure of DNA; unusual DNA structure- DNA hairpins, triple helix, G-quadruplex; stability of the double helix- thermal denaturation and renaturation of DNA double helix; chemical and enzymatic hydrolysis of nucleic acids; DNA replication, RNA transcription and translation of genetic information; chemical basis of heredity.

(6 Lectures)

Carbohydrate metabolism- glycolysis, gluconeogenesis and Kreb‘s cycle, oxidative phosphorylation. **(4 Lectures)**

Biochemistry of lipids- biosynthesis of fatty acids, triacylglycerols, phospholipids, cholesterol and related steroids; prostaglandins. **(4 Lectures)**

Protein biochemistry- amino acids, biosynthesis of amino acids, activation of amino acids, mechanism of translation, sequencing of amino acids in polypeptides; protein structure- primary, secondary, tertiary and quaternary structure of proteins, post-translational modifications and protein folding. **(6 Lectures)**

Enzymes- classification and catalytic behavior, enzyme kinetics, mechanism of action, factors affecting enzyme activity, enzyme regulators and inhibitors, enzyme models-host-guest chemistry, biotechnological applications of enzymes. **(5 Lectures)**

(28 Lectures)

Course outcome:

After completion of the course students will be able to-

CO1 find out the relative stability and reactivity of different reaction intermediates.
CO2 predict the outcome of an organic reaction based on the different intermediates that might be involved.
CO3 understand the structures and properties of biomolecules.
CO4 interpret the complexity of biochemical reactions for sustaining a living system.

C07 – Physical Chemistry II **Credits: 3 + 1 + 0 = 4**

Theory: 60 Lectures

Learning Objective:

LO1

1. To introduce different theories of reaction rates, factors affecting solution kinetics and fast reaction kinetics.
2. To give brief idea about the kinetics of heterogeneous catalysis and oscillating reactions.

LO2

1. To provide concepts about atom transfer and electron transfer processes.
2. To introduce students about different types of reactions in homogeneous catalysis including metal clusters and phase transfer catalysis.

LO3

1. To introduce the structural and non-structural models of ion-solvent interactions.
2. Learning different techniques to calculate the hydration number of ions.
3. Understanding the distribution of ions in solution via Debye-Hückel theory, its postulates and mathematical deductions.
4. To provide the idea of movement of ions in solution through Random walk model.

LO4

1. To get introduced about errors, accuracy and precision as measurements invariably involve errors and uncertainties.
2. To learn about significant figures and deviations, important in reporting measured data.
3. To understand determinate and indeterminate errors.
4. To learn various regression analyses like least-square fitting and also correlation analyses.
5. To introduce the concepts of confidence levels and reliability of results.

Unit 1: Kinetics

Theories of reaction rate: Collision theory, basic ideas of potential energy surfaces, Eyring equation, its thermodynamic and statistical thermodynamic formulation. Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment.

Solution kinetics: Factors effecting reaction rates in solutions, Effects of solvent and ionic strength (primary salt effect) on the rate constant, secondary salt effects.

Oscillating reactions: Belousov-Zhabotinski reaction, concept of chemical chaos.

Fast reaction kinetics: Introduction to relaxation and flow methods, idea of relaxation kinetics and stopped flow technique.

Kinetics of heterogeneous catalysis – Langmuir-Hinselwood and Eley-Riedel models.

(20 Lectures)

Unit 2: Homogeneous catalysis

Atom transfer and electron transfer processes. Role of transition metal ions with special reference to Cu, Pd, Pt, Co, Ru and Rh, catalysis in non-aqueous media. Rates of homogeneously catalysed reactions, turnover number and frequency. Catalysis of isomerisation, hydrogenation, oxidation and polymerisation reactions. Metal clusters in catalysis, phase-transfer catalysis.

(10 Lectures)

Unit 3: Dynamic Electrochemistry

Ion-solvent interactions: The Born model – thermodynamic parameters of ion-solvent interactions. Structural treatment: the ion-dipole model – its modifications.

Primary solvation – determination of hydration number, compressibility method and viscosity method.

Debye-Húckel theory of ion-ion interactions – derivation, validity and limitations; extended Debye-Húckel-Onsager equation.

The random walk model of ionic diffusion - Einstein-Smoluchowski relation.

(15 Lectures)

Unit 4: Data Analysis

Errors and deviations in measurements of physical quantities: accuracy and precision. Absolute, relative and mean errors. Relative and mean deviation, standard deviation. Significant figures in reporting measurements and calculation results, its relation to precision. Types of errors: determinate and indeterminate errors, various types of determinate errors.

Propagation of errors in calculations. Uncertainty in measurement of physical quantities and in universal constants.

Regression analysis – linear least-square fitting of experimental data-points. Correlation analysis – positive, nil and negative correlations, calculation of Pearson's correlation coefficient.

Tests of significance: Concept of confidence level and confidence interval. Reliability of results – Dixon's Q Test. Comparison of results – Student's t test and the F test.

(15 Lectures)

Course Outcome:

After completion of the course, students will acquire knowledge on

CO1 the detailed concepts of different theories of reaction rates and kinetics of heterogeneous catalysis.

CO2 the basic principles various types of homogeneous catalysis reactions along with metal clusters and phase transfer catalysis.

CO3 (i) the structural and non-structural models of ion-solvent interactions, (ii) hydrations numbers (iii) the postulates and mathematical treatments of Debye-Hückel theory to visualise the distribution of ions in solution of strong electrolytes. Also, achievements and limitations of the theory. (iv) the movement of ions in solution.

CO4 (i) the significant figures, errors, accuracy, precision and deviations. (ii) know the determinate and indeterminate errors. (iii) various regression and correlation analyses. (iv) the concepts of confidence levels and reliability of results.

C08 – Quantum Chemistry and Molecular Spectroscopy

Credits: 3 + 1 + 0 = 4

Theory: 60 Lectures

(The answers to the two parts must be written in separate answer-scripts)

Learning Objectives:

On completion of this course, the students would learn the following:

LO1 Basic principles of quantum mechanics such as the postulates, the Schrödinger equation and its variations, well-behaved functions, physical observables, etc.
LO2 Quantum mechanical treatment of some important model systems such as one-dimensional and three-dimensional box problems, harmonic oscillator, rigid rotor, H atom etc.
LO3 To introduce the basic concepts of spin resonance spectroscopy
LO4 To impart knowledge about the advanced experimental techniques used for simplification and improvement of proton NMR, ^{13}C NMR and ESR spectra
LO5 To introduce basic principles and instrumentation used in mass spectrometry and to explain important features in mass spectra
LO6 To make students familiar with the basic principles and features of Mossbauer spectroscopy

Part A: Quantum Chemistry

Unit 1: Basic principles of quantum mechanics

Review of the postulates of quantum mechanics and of Schrödinger wave equation – both time dependent and time independent forms. Wave functions of one-particle and many-particle systems, their Born interpretation. Well-behaved functions and normalized functions. Orthogonal functions – Schmidt's orthogonalization technique.

Physical observables and corresponding quantum mechanical operators. Eigenvalues and eigenfunctions of quantum mechanical operators, the physical significance of the eigenvalues. Expectation values of observable properties. Hermitian operators and the theorems they obey. Concept of degeneracy. Compatible observables and compatibility theorem, incompatible observables and the (generalised) uncertainty principle (derivation not required).

Basic ideas about the theory of angular momenta – spin and orbital angular momenta, ways of their coupling. Conservation of angular momenta.

(15 lectures)

Unit 2: Some Model Systems with Exact Solutions

Solutions of the Schrödinger time-independent equations for:

(i) Particle in a one-dimensional box and in a three-dimensional box.

(ii) Linear harmonic oscillator, vibrational energy levels of diatomic molecules.

(iii) Rectangular potential barrier problems, quantum mechanical tunnelling.

(iv) Problem of two interacting particles: separating centre of mass and relative motion.

(v) The two-particle rigid rotor problem, rotational energy levels of a diatomic molecule.

(vi) The hydrogen atom: representation and solution of the Schrodinger equation for electronic motion in spherical polar coordinate system. Radial solution: radial wavefunction and radial probability distribution function. Angular solution: the angular wavefunction and the representation of the shapes of atomic orbitals.

(15 lectures)

Part B: Molecular Spectroscopy II

Unit 3: Spin Resonance Spectroscopy

Basic Concepts, Chemical Shift, splitting patterns of signals; coupling constant and its distinction from chemical shift – use of coupling constant in structural elucidation. Simplification of spectra by use of shift reagents and high magnetic fields, Integration and its use in proton count and molecular ratios- determination of enantiomeric excess. Deuterium exchange technique in the determination of labile hydrogen, spin-decoupling and NOE, 2D NMR (^{1}H- ^{1}H and ^{1}H – ^{13}C COSY), DEPT. Complexity of ^{13}C NMR spectra and use of spin decoupling in its simplification; CINDP and its applications., Simple worked out examples using application of NMR. A brief introduction to solid state NMR.

(12 lectures)

Unit 4: ESR and NMR Spectroscopy

Applications of NMR spectroscopy to diamagnetic and paramagnetic inorganic compounds; paramagnetic shifts, ^{11}B, ^{14}N, ^{19}F, and ^{31}P NMR in inorganic compounds.

Electron Spin Resonance (ESR spectroscopy): Basic principles, factors affecting g-tensors, hyperfine splitting in free radicals and metal complexes, zero field splitting, application of ESR for d^1 and d^9 complexes.

(8 lectures)

Unit 5: Mass Spectrometry

Basic Principle of mass spectrometry, Instrumentation: Ionization methods, Mass Analysers, Base peak, molecular ion peak and isotope peak. Nominal mass and exact mass, determination of molecular formula, McLafferty Rearrangement, Metastable peak, The Nitrogen Rule, General fragmentation modes, Important features of the mass spectra of aliphatic, aromatic and cyclic hydrocarbons, primary alcohols and carbonyl compounds, Analyzing Mass Spectrum and solving simple problems in Mass Spectra.

(6 lectures)

Unit 6: Mössbauer Spectroscopy

Basic principles, isomer shift, quadrupole splitting and effect of magnetic field. Mössbauer Spectra of high-spin and low-spin iron complexes.

(4 lectures)

Course Outcomes:

After completion of the course the students will be able to

CO1 gain an in-depth understanding of the fundamentals of quantum chemistry. They will gain knowledge of the basic postulates of quantum mechanics, the concept of quantum mechanical operators and their utility, the uncertainty principle and some exactly solvable quantum mechanical problems.

CO2 elucidate the structure of simple organic molecules from the chemical shift and coupling constant values

CO3 determine the enantiomeric excess from the peak integration area

CO4 interpret the structure of a molecule from 13C NMR spectra

CO5 understand the application of decoupling technique

CO6 determine the structure from the ESR spectra of organic and inorganic molecules

CO7 relate the molecular structure with the mass spectra

CO8 determine the oxidation and spin states of inorganic metal complexes from Mossbauer spectra

LAB COURSE: SEMESTER II

LAB 2 – Inorganic and Physical Chemistry Practical   Credits: 0+0+4 = 4

Practicals: 120 Hours

Learning objectives:

LO1 To introduce quantitative estimation of metal ions present in ores/alloys, cement, steel and water

LO2 To learn the synthetic methods of inorganic complexes and their characterization.

LO3. Understanding, performing and interpreting physical chemistry experiments on advanced kinetics and basic electrochemical conduction problems involving titrimetry, polarimetry, catalyst concentration dependence, kinetic salt effect and ionic interactions.

Unit 1: Inorganic Chemistry Practical   90 Hours

(Each Student should perform one experiment from each unit during end semester examination)

A. Quantitative analysis

(a) Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe, etc. involving volumetric and gravimetric methods.

(b) Analysis of ores/alloys, cement and steel, etc.

Ores: Hematite, Limestone, Dolomite, Cement, Pyrolusite and other ores.

Alloys: Brass, Gunmetal, Cupronickel, Solder, Bronze, Phosphor Bronze, Steel, Copper-Nickel, other alloys.

(c) Determination of hardness of water

B. Preparation and Characterization of Inorganic Complexes

Preparation of selected inorganic complexes (Linkage isomers, Cis-Trans isomers etc.) and their physico-chemical characterization by elemental analysis, IR and electronic spectrophotometry, magnetic susceptibility measurements, magnetic resonance spectroscopy, and solution conductivity measurements wherever appropriate and possible.

Unit 2: Physical Chemistry Practical   30 Hours

(1) Study of the inversion of sucrose in presence of two acids polarimetrically using Guggenheim plots and hence determination of the relative strengths of the acids.

(2) Verification of the proportionality of the rate constant for acid-catalysed hydrolysis of methyl acetate to the concentration of the mineral acid catalyst (linear least square fitting method is to be used for calculation of the rate constants instead of the common graphical method).

(3) Study of the progress of the autocatalytic reaction between oxalic acid and $KMnO_4$ with time and identification of its autocatalytic nature.

(4) Study of the dependence of the rate constant of the ionic reaction $S_2O_8^{2-} + 2\,I^- = 2\,SO_4^{2-} + I_2$ on the ionic strength of the aqueous reaction medium in presence of varying concentrations of NaCl.

(5) Verification of the Debye-Huckel-Onsager equation for aqueous solutions of a strong electrolyte.

(Any new experiments may be added from time to time)

Course Outcomes:

After the completion of the course students will be able
CO1to gain skills on estimating metal ions and synthesizing inorganic complexes that is important in the present context of research.
CO2 to gain skills about conducting physical chemistry experiments on investigating various advanced kinetics problems and on electrochemical conduction.

CORE COURSES: SEMESTER III

C09 – Inorganic Chemistry III Credits: 3+1+0 =4

Theory: 60 Lectures

Learning Objectives:

LO1 To understand the structure and bonding of inorganic chain, ring, cage and cluster compounds.
LO2 To understand elaborately the role of metal ions in biological systems.
LO3 To learn about nuclear reactions and their applications
LO4 To study the properties and uses of superconducting and nanomaterials.

Unit 1: Inorganic Chains, rings, cages and clusters

Catenation, Heterocatenation, Zeolites, Intercalation , Structure and bonding in borazine, phosphazenes, polyhedral boranes, carboranes, metalloboranes and metallocarboranes, Styx notation, Wade's rules, Synthesis and electron count in polyhedral boranes. Inorganic clathrates.

Synthesis and bonding in metal clusters. Metal-metal quadruple bonding in $Re_2Cl_8^{2-}$.

(15 Lectures)

Unit 2: Bio Inorganic Chemistry

Active ion transport across cell membrane: Na^+/K^+ Pump, Oxygen: binding, transport and utilization, Photosynthesis, Nitrogen Fixation, Metalloenzymes: Haemoglobin, Myoglobin, Catalase, Peroxidase, Superoxide Dismutase, Cytochrome P-450. Nitrogenase, Chlorophyll, Carboxypeptidase, Carbonic anhydrase, Coenzyme Vitamin B_{12}, Xanthine Oxidase, Metal Complexes in Medicine.

(15 Lectures)

Unit 3: Nuclear and Radio Chemistry

Radioactive decay processes, half-lives, auger effect. Nuclear reactions – notations, comparison with chemical reactions, types of nuclear reactions, reaction cross section, mechanism of nuclear reactions. Radiation detection & measurements, Geiger-Muller and Scintillation counters, applications of radioisotopes as tracers (reaction mechanism, structure determination, activation analysis, isotope dilution technique, age determination)

(15 Lectures)

Unit 4: Inorganic materials

Superconducting materials: discovery, magnetic properties, theory, examples and uses of high temperature superconductors.

Nanomaterials: concept, novel optical and magnetic properties, synthesis, characterization techniques and applications.

(15 Lectures)

Course Outcomes:

After the completion of the course the students will acquire knowledge about
CO1 structure and bonding of inorganic chain, ring, cage and cluster compounds.
CO2 the role of metal ions in biological systems and metal complexes in medicine.
CO3 Nuclear reactions and their applications
CO4 Superconductivity and Nano chemistry.

C10 – Organic Chemistry III Credits: 3+1+0 =4

Theory: 60 Lectures

Learning objectives:

LO1 Introduction to various photophysical processes and application of these in different photochemical reactions.
LO2 Comprehensive idea of reducing and oxidising agents used in organic transformations.
LO3 Pericyclic reactions and their utilities.

Unit1: Organic Photochemistry

Introduction to organic photochemical-photophysical processes, chemiluminescence, photosensitization.

Photochemistry of carbonyl compounds: α-cleavage, β-cleavage, intramolecular H-abstraction, addition to π-systems, Paterno-Buchi reaction; Photochemistry of olefins - photostereomutation of cis-trans isomers, optical pumping, cycloaddition, photochemistry of conjugated polyenes, photochemistry of vision

Photochemistry of enones; Photo-rearrangement reactions, di-π-methane rearrangement, Photo-rearrangement of cyclohexadienones, Barton rearrangement; Singlet oxygen photochemistry.

(10 Lectures)

Unit 2: Oxidation Reactions

Metal based and non-metal based oxidations (Cr, Mn, Al, Ag, Os, Ru, Se, DMSO, hypervalent iodine and TEMPO based reagents). Reagents (Fremy's salt, silver carbonate, peroxides/per-acids, TPAP, Oxone).

Named reactions: Sharpless epoxidation and dihydroxylation, Baeyer-Villiger oxidation, Wacker oxidation, hydroboration-oxidation, Prevost reaction and Woodward modification, Oppenauer oxidation,.

(16 Lectures)

Unit 3: Reduction Reactions

Catalytic hydrogenation (Pd/Pt/Rh/Ni/Ir). Wilkinson catalyst

Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium, Zinc, Titanium and Samarium (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations);

Hydride transfer reagents from Group 13 and Group 14 in reductions (Borane, $NaBH_4$, $NaBH_3CN$, $LiBH_4$, Zn $(BH_4)_2$, triacetoxyborohydride, superhydride, selectrides, Luche reduction, $LiAlH_4$, DIBAL-H, and Red-Al, Diimide reduction, Trialkylsilanes and Trialkylstannane, Meerwein-Pondorff-Verley reduction)

(16 Lectures)

Unit 4: Pericyclic Reactions

MO symmetry, FMO of conjugated polyenes. Woodward-Hoffmann principle of conservation of orbital symmetry, allowed and forbidden reactions, stereochemistry of pericyclic reactions, orbital symmetry correlation method, PMO method.

Cycloaddition reactions: [2+2], [4+2], [6+2] cycloadditions, [3+2] and [4+3] dipolar cycloadditions; stereoselectivity of the reactions, regioselectivity of [4+2] cycloaddition reaction.

Sigmatropic rearrangement: (m+n) sigmatropic rearrangement of hydrogen and chiral alkyl groups; Divinyl cyclopropane rearrangement, fluxional molecules, stereoselectivity in Cope, and Claisen rearrangement. Sommelet-Hauser rearrangement. Aza-Cope rearrangement, Overman rearrangement.

Electrocyclic reactions and cyclo-reversions: Conrotatory and disrotatory process, Stereoselectivity of the reactions.

Linear and nonlinear cheletropic rearrangement, theories of cheletropic reactions, stereoselectivity of the reactions.

Ene reactions of 1,7-dienes, carbonyl enophiles, simple problems, metallo-ene, Conia-ene reaction.

(18 Lectures)

Course outcomes:

After completion of the course students will be able to-

CO1 interpret the photophysical processes that might take place in a given organic molecule.

CO2 predict outcomes of photochemical reactions.

CO3 select a reducing/oxidising agent for a chemoselective organic synthesis.

CO4 predict the substrates for a pericyclic reaction and the selectivity in such reactions.

C11 – Advanced Quantum Chemistry　　　　Credits: 3 + 1 + 0 = 4

Theory: 60 Lectures

Learning Objectives:

This course aims to impart to the students' knowledge of the following:
LO-1. Concept of approximate methods of quantum mechanics with perturbation and variation methods in some details.
LO-2. Electronic structure of many-electron atoms in terms of their complete, spin-included wavefunctions including independent particle central field model, atomic orbital theory, electron repulsion parameters and concepts of spectroscopic atomic terms as well as levels.
LO-3. Quantum chemical expression of chemical bonding in molecules in terms of simple LCAO-MO theory, simple VB theory, improvements of both these theories, extension to diatomic and some simple polyatomic molecules and also the pi-electron Hückel MO theory of unsaturated organic compounds.
LO-4. General concepts in molecular quantum chemistry namely Born-Oppenheimer approximation, Hellmann-Feynman theorem, electrostatic theorem, force concept in molecules and molecular electronic virial theorem.
LO-5. Introductory concepts in quantum chemical SCF method in particular Hartree-Fock theory in some details, as well as in density functional theories.

Unit 1: Approximate Methods of Quantum Mechanics

(a) Time-independent first order perturbation theory for – (i) non-degenerate, and (ii) degenerate systems applications to the ground and first-excited states of the helium atom. Calculation of energy up to the second-order corrections.

(b) The variation theorem, linear variation function – secular equation.

(10 Lectures)

Unit 2: Electronic Structure of Many-Electron Atoms

(a) Product wave functions- complete many-electron wave functions including electron spin. Pauli's anti-symmetry and exclusion principles. Spin states of a two-electron system- singlet and triplet states.

(b) Independent particle central field model of many-electron atoms- the helium atom. Atomic orbital theory – Slater type orbitals (STO); electron repulsion parameters (Racah and Condon-Shortly types).

(c) Spectroscopic term symbols for the s^1p^1, p^2 and d^2 configurations – splitting of term energies due to inter-electronic repulsion and spin orbit coupling, magnetic effects and Zeeman splitting.

(15 Lectures)

Unit 3: Chemical Bonding

(a) The hydrogen molecule ion: linear combination of atomic orbital (LCAO)-molecular orbital (MO) theory- ground and excited electronic states.

(b) The hydrogen molecule: LCAO-MO and valence bond (VB) treatments.

Equivalence of the MO and VB methods.

(c) Extension of the LCAO-MO method to homo- and heteronuclear diatomics-inclusion of hybridization.

(d) Term symbols for molecular electronic states, their symmetry classification. Correlation diagrams and the non-crossing rule.

(e) LCAO-MO theory of simple polyatomic molecules (e.g., the H_2O molecule).

(f) π-electron theory: Hückel molecular orbital (HMO) method for unsaturated carbon compounds showing chain and ring structures; introduction to extended Hückel theory.

(15 Lectures)

Unit 4: General Theorems in Molecular Quantum Mechanics

(a) Born-Oppenheimer approximation, separation of electronic and nuclear motion.

(b) Hellmann-Feynman theorem and its chemical applications. The electrostatic theorem (derivation not required) and the force concept in chemistry, binding and anti-binding regions.

(c) Molecular electronic virial theorem, its simplified expression for diatomic molecules, resulting ideas about contribution of kinetic and potential energies to molecular bonding.

(10 Lectures)

Unit 5: Introduction to Quantum Chemical SCF and Density-Functional Theories

(a) Review of the principles of quantum mechanics, Born-Oppenheimer approximation, separation of electronic and nuclear motion

(b) The self consistent field method, Hartree-Fock theory of closed shell electronic configurations of atoms and molecules, Coulomb and exchange integrals, Hartree-Fock equations, Koopman's theorem without derivation. Gaussian basis sets.

(c) Linear SCF LCAO-MO theory of molecules – the Roothan equations.

(d) Density-functional theories: basic ideas, Hohenberg-Kohn theorem and its derivation, Kohn-Sham formulation.

(10 Lectures)

Course Outcome:

On completion of this course, students will gain an advanced-level understanding of approximation methods namely perturbation theory and variation principles as applied to many-electron systems, their complete wavefunction forms in terms of orbitals and spin functions, MO and VB theories for molecules along with their improvements, Hartree-Fock Self Consistent Field method, density functional theory, the Hellmann-Feynman and electrostatic etc. theorems in quantum chemistry along with their chemical applications.

CORE COURSES: SEMESTER IV

C12 – Analytical Methods in Chemistry Credits: 3+1+0 =4

Theory: 60 Lectures

Learning Objectives:

LO1 To impart advanced knowledge on instrumental techniques for structural elucidation of molecular solids and thermal and electrochemical properties.

LO2 To impart knowledge on various microscopic techniques for understanding phenomenon occurring at atomic and molecular levels.

LO2 To comprehend the knowledge on chromatographic techniques.

LO4 Structural determination of organic/inorganic compounds using various spectroscopic techniques

Unit 1: Electrochemical, Thermal and X-ray Diffraction Methods

(a) Electrochemical methods: Principles, instrumentation and applications of cyclic voltammetry. Anodic stripping voltammetry.

(b) Thermal methods: Principles, instrumentation and applications of TG, DTG, DTA and DSC in analysis of chemical compounds.

(c) X-ray diffraction: Principles, instrumentation and application of Powder XRD and Single crystal XRD. Indexing reflection patterns, Scherrer equation.

(16 lectures)

Unit 2: Electron Microscopy and Scanning Probe Microscopy

(a) Scanning electron microscopy/Energy Dispersive X-ray (SEM/ EDX) and Transmission electron microscopy/ Selected Area Electron Diffraction (TEM/SAED): principle, instrumentation, applications.

(b) Surface Tunnelling Microscopy (STM) and Atomic Force Microscopy (AFM): principle, Instrumentation and Applications.

(8 lectures)

Unit 3: Chromatographic Techniques

Gas Chromatography (GC), Gas Chromatography- Mass Spectrometry (GCMS), Liquid Chromatography- Mass Spectrometry (LCMS), High Performance Liquid Chromatography (HPLC), Gel permeation chromatography (GPC): Techniques, Instrumentation and Applications.

(12 lectures)

Unit4: Electron Spectroscopy

Photoelectron Spectroscopy: Basic principles and applications of XPES (O_2, N_2 and N_3), Koopman's Theorem, Chemical information from ESCA.

Chiroptical properties: Introduction to CD (Circular Dichroism), ORD (Optical Rotatory Dispersion) and Magnetic Circular Dichroism (MCD) - Octant rule.

(14 lectures)

Unit 5: Structure Elucidation using various Spectroscopy

Determination of chemical structure of organic/inorganic compounds by analysing UV-Vis, IR, NMR and Mass Spectrometry data.

(10 lectures)

Course Outcome: After the completion of the course students will acquire knowledge in structural elucidating techniques, chromatographic techniques and gain insight towards characterizing materials by electron microscopy.

Special Papers (SPL): Department of Chemistry

SPL 1 :: Semester III

SPL – Organometallics and Photo-Inorganic Chemistry

Credits: 4 + 1 + 0 = 5

Theory: 75 Lectures

Learning Objectives:

LO1 To impart elaborate knowledge on Alkyls and Aryls, Metal-Carbon Multiple Bonds and π-complexes of transition metals.
LO2 To understand the role of various inorganic catalysts in different reactions.
LO3 To impart knowledge on the photochemical reactions of metal complexes.

Unit 1: Alkyls and Aryls of Transition Metals

Types, routes of synthesis, characteristics, stability, decomposition pathways, structure and bonding. Organocopper in organic synthesis.

(8 Lectures)

Unit 2: Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural, characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

(12 Lectures)

Unit 3: Transition Metal π - Complexes

Transition metal π-complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. lmportant reactions relating to nucleophillc and electrophilic attack on ligands and to organic synthesis.

(15 Lectures)

Unit 4: Organometallic Reactions and Catalysis

Organometallic reactions for catalysis, Examples of catalysis: hydrogenation by Wilkinson's catalyst, Zeigler-Natta polymerization of olefins, hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions (Wacker process), Monsanto acetic acid synthesis, activation of C-H bond.

(20 Lectures)

Unit 5: Photo Inorganic Chemistry

Ligand field and charge transfer state (Thexi & DOSENCO states), Photo physical processes in electronically excited molecules, Types of excited states (radiative and non-radiative processes), Jablonski diagram. Photo substitution and photo redox reactions of chromium, cobalt and ruthenium compounds, Photo rearrangement reactions: Cis-trans isomerization, Linkage Isomerism. Photo catalysis and solar energy conservation by ruthenium complexes.

(20 Lectures)

Course Outcomes:

This course helps to acquire knowledge of

CO1 various aspects of transition metal based organometallic compound as well as the reactions catalyzed by them.

CO2 acquire knowledge on the photochemical reactions of transition metal complexes.

SPL – Advanced Organic Synthesis Credits: 4 + 1 + 0 = 5

Theory: 75 Lectures

Learning objectives:

LO1 Introduction to recent and advanced organic reactions for C-C, C-N, C-O, C-X and C-S bond formation.

LO2 Use of heterogeneous catalysis for organic transformations.
LO3 Asymmetric synthesis and different methods for induction of asymmetry.
LO4 Strategies for synthesizing cyclic compounds.
LO5 Protection-deprotection strategies in organic synthesis.
LO6 Introduction to retro synthetic analysis.
LO7 Introduction to total synthesis of targeted organic molecule.

Unit 1: C-C bond forming reactions

C-C bond formation reactions using organometallic compounds (orgnao Li, Mg, Zn, B, Sn, Si, Cu reagents). Pd catalyzed coupling reactions (Heck, Suzuki, Sonogashira, Stille and Negeshi coupling). Formation of C-C multiple bonds involving Csp2 and Csp carbon centers (with emphasis on important name reactions, e. g. Corey–Fuchs reaction, Horner–Wadsworth–Emmons reaction, Simmons−Smith Reaction), pyrolytic syn elimination reactions (Chugaev reaction and Cope reaction). Alkene from hydrazones, sulfones.

(15 Lectures)

Unit 2: C-heteroatom bond forming reactions

Formation of carbon-heteroatom bonds: New methods for the construction of C-N, C-O, C-S and C-X bonds (including aspects related to the activation of C-H bonds), Ullmann reaction, Buchwald-Hartwig reaction, Ugi reaction, Stork-enamine reaction, hetero Diels-Alder reactions.

(10 Lectures)

Unit 3: Asymmetric synthesis

Enantioselective synthesis (alkylation, allylation and crotylation reactions), use of chiral reagent; Chiral catalyst and chiral auxiliary; Use of chiral auxiliaries (Evans oxazolidones, Oppolzer sultams, Myers amides, Schöllkopf Chiral Auxiliaries), use of chiral pool.

Kinetic resolution (including enzymatic resolution), desymmetrization reactions.

Asymmetric reactions: Epoxidation (Sharpless, Jacobsen, Shi, Julia-Colonna), Dihydroxylation (Sharpless); Stereo/enantioselective reductions (Pfaltz catalyst, Chiral Boranes, Corey-Bakshi-Shibata catalyst, use of BINOL, BINAP, chiral phosphine ligands).

(16 Lectures)

Unit 4: Construction of Ring Systems

Different approaches towards the synthesis of three, four, five and six-membered rings; photochemical approaches for the synthesis of four membered rings, oxetanes and cyclobutanes. Diels-Alder reaction (inter- and intra-molecular), ketene cycloaddition (inter- and intramolecular), Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization, radical-olefin cyclization, Hofmann- Loeffler-Freytag reactions, cyclization reactions of nitrenes,

Heterocyclic rings (with two or more heteroatoms): Pyrazoles, isoxazoles, thiazoles, triazoles and pyrimidines (Claisen synthesis, Fischer synthesis)

Inter-conversion of ring systems (contraction and expansion); construction of macrocyclic rings, ring closing metathesis.

(12 Lectures)

Unit 5: Protecting Groups

Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection. Illustration of protection and deprotection in peptide and carbohydrate synthesis.

(6 Lectures)

Unit 6: Retrosynthetic Analysis

Basic principles and terminology of retrosynthesis, synthons and synthetic equivalents, synthesis of aromatic compounds, one group and two group C -X disconnections,

One group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions, Umpolung of reactivity.

(8 Lectures)

Unit 7: Synthesis of Complex Molecules

Total synthesis of Terpene (caryophylene), alkaloid (morphine), and drug (efavirenz)

(8 Lectures)

Course outcome:

After completion of the course students will be able to-

CO1 select an advanced catalyst for C-C, C-heteroatom bond formation.

CO2 choose a catalytic/a non-catalytic synthetic pathway for a given reaction.

CO3 understand the concept in different asymmetric synthesis strategies.

CO4 interpret product ratios in different asymmetric syntheses.

CO5 select a protecting group for a particular functional group in a multifunctional molecule.

CO6 work out the synthetic pathway for a given ring system.

CO7 predict reactants for an organic synthesis using disconnection approach.

CO8 design a synthesis involving 3-5 steps.

SPL - Chemical Kinetics and Electrochemistry Credits: 4 + 1 + 0 = 5

Theory: 75 Lectures

Learning Objective:

LO1:

1. Introduction to advanced theories of chemical reaction dynamics such as Lindemann, RRK etc. along with their limitations
2. Factors affecting reaction rates in solutions including electron transfer reactions.
3. Theories and mathematical equations about reactions in solutions.
4. Mechanisms and kinetics of photochemical reactions.

LO2:

1. To give knowledge of fast reactions along with various techniques.
2. To make students familiar with elucidating reaction mechanism from chemical kinetic studies by giving examples.

LO3:

1. To have a quantitative understanding of electrified interfaces (metal-solution) through the mathematical models like Helmholtz-Perrin model, Gouy-Chapman model and Stern model.
2. Understanding electrocapillary phenomena to deduce the Lippmann equation.
3. Knowing charge leakage behaviour on polarizable and non-polarizable interfaces.
4. To have a brief idea of electrode kinetics and a detailed knowledge of Butler-Volmer equation.

LO4:

1. To have sound knowledge of important electrochemical methods like, polarography, cyclic voltammetry, chronopotentiometry and rotating disk electrodes.
2. To have a brief idea about convective diffusion processes.
3. Learning application of electrochemistry like electrodeposition.

Unit 1: Chemical Kinetics - I

Drawbacks of Lindemann theory- Hinselwood modification, RRK theory, Slater's treatment, RRKM theory.

Effect of dielectric constant on reaction rate in solution, effect of pressure on rate, cage reactions, electron transfer reactions in solution, linear free energy relationship, Hammett equation, Taft equation, their applications.

Photochemical reactions: photophysical kinetics, state energy diagrams. Delayed fluorescence: the mechanism and kinetics of fluorescence quenching – Stern-Volmer equation.

(25 Lectures)

Unit 2: Chemical Kinetics - II

Review of stopped flow technique, temperature and pressure jump methods. NMR studies in fast reactions, shock tube kinetics, relaxation kinetics. Linearised rate equation, relaxation time in single step fast reactions, determination of relaxation time.

Chemical kinetics in the elucidation of reaction mechanism: hydrolysis of lactones and aldol condensation, thermal decomposition of dinitrogen pentoxide and ligand replacement reactions of octahedral complexes.

(20 Lectures)

Unit 3: Electrochemistry - I

Theories of electrical interface – Helmholtz-Perrin model, Gouy-Chapman model, Stern model. Electrocapillary phenomena – Lippmann equation. Electron transfer at interfaces – polarisable and non-polarisable interfaces, Butler-Volmer equation, Tafel Plots.

(15 Lectures)

Unit 4: Electrochemistry - II

Electrochemical methods used in electrode kinetics: polarography, chrono potentiometric method, cyclic voltammetry. Convective diffusion, rotating disc electrode (RDE). Applications in electrode processes, electrodeposition on metals.

(15 Lectures)

Course Outcomes:

After completion of the course, students will understand:

CO1 (i) the basic principles and models of advanced theories of chemical reaction dynamics such as Lindemann, RRK etc. along with their limitations, (ii) to solve problems relating to reaction rates in solutions, (iii) to interpret the theories and mathematical equations about reactions in solutions and also mechanisms and kinetics of photochemical reactions.

CO2 the basic idea about the kinetics of fast reactions and elucidate the reaction mechanism with suitable examples from chemical kinetic studies.

CO3 (i) the basic principles and models to describe electrified interfaces and electrocapillary behaviour. (ii) insights of electrode kinetics and Butler-Volmer equation.

CO4 the important principles and methods of applied electrochemistry and applications.

SPL 2 Semester IV

SPL – Advanced Bioinorganic Chemistry Credits: 4 + 1 + 0 = 5

Theory: 75 Lectures

Learning Objectives:

LO1 To introduce the basics of Supramolecular Chemistry involving supramolecules like cryptands, Valinomycin, DNA etc. to explain their role in various biochemical processes.
LO2 To enhance the knowledge of structure and functions of oxygen carrying proteins, dioxygen toxicity and the role of detoxifying enzymes.
LO3 To understand the mechanism of electron transfer process involving metalloenzymes.
LO4 To introduce the role of various metalloenzymes in biological systems.
LO5 To introduce the role of metals in treatment of various diseases.

Unit 1: Supramolecular Chemistry and Ion Transport

Definition and examples of Supramolecules, Self assembly and membranes, Molecular receptors: Cryptands, Valinomycine, Spherands, Molecular recognition, interaction of metal ions and metal complexes with DNA.

Supramolecular Transport: Active transport of ions across cell membranes, selectivity of Na and K with crown ethers, cryptands and ionophores, Na/K pump, transport of Ca^{2+}, Biominerals containing Ca and Fe, Storage and Transport of Fe: Ferritin, Transferrins, Siderophores.

(20 Lectures)

Unit 2: Carrier, Transport, Storage and Activation of Dioxygen

Structure of active site and functions of oxygen carrying proteins: Haemoglobin, Myoglobin, Haemerythrin and Haemocyanin, Model O_2 carriers. Mechanism of cooperativity in Haemoglobin, Dioxygen toxicity. Detoxification enzymes – Catalases, Peroxidases, Superoxide dismutases.

(15 Lectures)

Unit 3: Electron Transfer Proteins

Mechanism of electron transfer reactions in: Blue Copper Proteins, Iron Sulphur Proteins: Rubredoxin, Ferridoxin and HiPIP, Cytochromes (a, b and c types).

(10 Lectures)

Unit 4: Metalloenzymes

Structure of active sites and functions of Zn containing enzymes: carboxypeptidase, carbonic anhydrase, Effect of Co (II) substitution in Zn enzymes, Cytochrome P-450, Coenzyme B_{12}, Nitrogen fixation: Nitrogenase – structure, N_2 activation and fixation. Role of Ni, Cr and Vanadium in enzymes.

(15 Lectures)

Unit 5: Metals in Medicine

Metal deficiency and disease, toxic effects of metals: Fe and Cu overload, Thalassemia, toxicity due to Hg, As, Cd, and Pd. Chelation Therapy: EDTA, BAL and Penicillamine. Gold compounds in Rheumetic Arthritis, Cisplatin and related anticancer drugs.

(15 Lectures)

Course Outcomes:

After the completion of the course the students will acquire knowledge on

CO1 the fundamentals of supramolecular chemistry and its importance in Biology.

CO2 role of metalloenzymes in Biology.

CO3 mechanism of electron transfer by various metal containing enzymes.

CO4 importance of metals in medicine.

SPL – Natural products and Medicinal Chemistry

Credits: 4 + 1 + 0 = 5

Theory: 75 Lectures

Learning objectives:

LO1 Natural products, their occurrence, properties.
LO2 Biological role and industrial use of natural products.
LO3 Introduction to basics of medicinal chemistry and drug discovery.
LO4 Study of drugs on basis of pharmaceutical effect.
LO5 Structure activity relationship and mode of action of drugs.

Unit 1: Introduction to natural products

Natural products chemistry: a general treatment. Classification: Primary and secondary metabolites.

(2 Lectures)

Unit 2: Carbohydrates

Open chain and ring structure of monosaccharides, reactions of the anomeric centre, reactions of hydroxyl groups, Cyclic acetals, Glycosyl activation.

Disaccharides- Ring structure of sucrose, maltose, lactose and their hydrolysis. Introduction to deoxysugars, glycosides, glycals, glycosamines and glycosans.

Polysaccharides- Representative structure of starch, glycogen and cellulose. Chemical disaccharide formation, Enzymatic dissacharide formation, Introduction to chemical glycobiology.

(14 Lectures)

Unit 3: Terpenoids, Steroids and Alkaloids

Terpenoids: Chemistry of - caryophyllene, α-santonin (with structure determination), biogenetic pathway of mono- and sesquiterpenes.

Introduction to carotenoids, Discussion on β-carotene and lycopene, vitamin-A. Singlet oxygen quenching and food coloring properties of carotenes.

Steroids: Introduction to steroids: cholesterol, sex hormones, cardiac glycosides and corticosteroids.

Alkaloids: Chemistry of reserpine, and morphine including structural determinations. Industrial and medicinal uses of Terpenoids, Steroids and Alkaloids.

(16 Lectures)

Unit 4: Chemistry of vitamins

Classification and functional role in biological systems; chemistry of thiamine, riboflavin, retinol, tocopherols, vitamin C and pyridoxine.

(8 Lectures)

Unit 5: Drug action and drug development

Definition and classification of drugs, prodrugs, need of new drugs, history of drug development: Aspirin, paracetamol, sulpha drugs.

Receptors, drug-receptor interaction and Clark's Occupancy Theory, physiological response, drug agonist, antagonist, inverse agonist.

Need of quantification of drug action, definition of chemotherapeutic index & therapeutic index, factors affecting bioactivity of drugs, pharmacokinetics, pharmacodynamics,

Quantitative structure activity relationships (QSAR).

Lead compound, importance of SAR & molecular modification, combinatorial library and molecular modeling in drug discovery, introduction to gene therapy.

Phases in drug development.

(14 Lectures)

Unit 6: Antibiotics

Definition of antibiotics, their sources, classification (based on structure and biological activity) and basic structures, causes & concerns of bacterial resistance to antibiotics, Definition and need of broad spectrum antibiotics.

β-lactam antibiotics: Classification, History leading to the discovery of penicillins (β-lactam antibiotics) – natural & semi-synthetic penicillins, structure activity relationship & chemical modification, bacterial resistance to penicillins - causes and inhibitors, mode of action of β-lactam antibiotics, origin of high reactivity of penicillins and related consequences.

Teracyclines: uses and structure activity relationship, mode of action.
Macrolide antibiotics: structure activity relationship, mode of action.

(12 Lectures)

Unit 7: Antimalarials

Discovery of quinine and its SAR, importance of quinine as a lead to discovery of other low cost antimalarials, artemisinin and its derivatives, their SAR and importance in dealing with CQ resistant malaria, mode of action.

(4 Lectures)

Unit 8. **Antiviral and Anticancer drugs**

Difficulty in developing clinical solution to viral diseases, introduction to antiviral agents.

Cancer and its causes, difficulty in developing clinical solution, chemotherapy of cancer – uses of vinca alkaloids, taxol and its derivatives.

(5 lectures)

Course outcomes:

After completion of the course students will be able to-

CO1 understand the classification of drugs, structure activity relationship.

CO2 apply QSAR to interprete bioactivity of drugs.

CO3 classify and compare activity of drugs with knowledge of mechanism of action

CO4 classify natural products.

CO5 interpret the biological role of the natural products.

CO6 understand utility of natural products in pharmaceuticals and cosmetics.

SPL – Heterogeneous Catalysis **Credits: 4 + 1 + 0 = 5**

Theory: 75 Lectures

Learning Objective:

LO1

1. To give the fundamentals of determination of surface area and porosity with different techniques.
2. Factors affecting the reaction rates in heterogeneous catalysis.
3. To give idea about how to design a good catalyst for its industrial applications.

LO2

Introduction of zeolites and clays along with their applications in different domains.

LO3

To give basic idea about the applicability of catalysis in various processes in petroleum industry.

LO4

1. To know about the catalysis involved in environmental protection such as catalytic converters.
2. To give basic idea about the role of catalysis in controlling automobiles exhausts and industrial plants.

Unit 1: Introduction to Heterogeneous Catalysis

Surface area determination from adsorption isotherms and point-B methods, porosity determination by volumetric and gravimetric methods. Chemisorption on metals, semi-conducting oxides and insulator oxides.

Effect of temperature on rates of catalysed reactions, mass transport limitation of catalysed reactions. Surface dependence of reaction rates, volcano principles.

Characteristics of a good catalyst. Catalyst design methods, catalyst support and preparation of industrial catalyst, supported and unsupported metal catalysts, bimetallic catalysts.

(25 Lectures)

Unit 2: Zeolites and Clays

Zeolites (natural and synthetic), shape selectivity properties, solid acids, acidity of zeolites and clays. Mesoporous materials, poorly crystalline silicates and aluminosilicates.

Applications of zeolites and clays as heterogeneous catalysts in cracking, reforming and olefin reactions. Zeolites as catalyst supports.

(20 Lectures)

Unit 3: Catalysis in Petroleum Industry

Synthesis gas and production of chemicals from it. Hydrodesulphurization process and catalysts involved. Lewis acid catalysts, hydrogenation catalysts and bi-functional catalysts. Selective oxidation of hydrocarbon compounds – production of various petrochemicals. Manufacture and transformation of hydrocarbons – hydrogenation and isomerisation. Catalytic deactivation and reactivation.

(20 Lectures)

Unit 4: Catalysis in Environmental Roles

Control of pollution from automobile exhaust, catalytic converters – use of non-selective oxidation. Abatement of nitrogen oxides and industrial odours, cleaning of industrial effluents.

(10 Lectures)

Course Outcomes:

After completion of the course, students will acquire knowledge of

CO1 The fundamentals of determination of surface area and porosity with various techniques and application of heterogeneous catalysts in different areas.

CO2 The properties of zeolites and clays with applications in different industrial fields.

CO3 The basic principles of heterogeneous catalysts to be applied in different processes in petroleum industries.

CO4 To raise concern about environmental protection of the catalysts used in automobiles exhausts and industrial plants.

M.Sc. Skill Enhancement Courses (SEC): Department of Chemistry

SEC 1 :: Semester I

SEC – Chemistry of Environmental Pollution Credits: 2+0+0 = 2

Theory: 30 Lectures

Course Objective: The objective of this course is to make the students aware of environmental pollution and understand the role of chemistry in mitigating it.

Unit 1: Chemistry of air pollution

Parameters of air quality and their permissible limits. Contaminants and Pollutants. Primary air pollutants and formation of secondary air pollutants, smog formation. Automobile vehicles as a source of air pollution and its control using catalytic converters. Increasing level of CO_2 in air and green house effect, measures (such as shifting to greener energy sources, afforestation, preventing deforestation, etc.) to control CO_2 pollution. CFCs as pollutants, ozone layer depletion and measures for its mitigation.

(15 Lectures)

Unit 2: Chemistry of Soil and Water Pollution

Parameters of water and soil, their permissible limits. Soil and water pollution due to anthropogenic sources: changes in pH in both cases, reclamation of problem soil, adverse effects of petroleum exploration and processing on soil and water, increase of BOD in water, decrease of dissolved oxygen in water, effect of industrial effluents and thermal pollution on aquatic life, pesticides in soil and water, its trophic level biomagnification. Groundwater pollution by pesticides and heavy metals. Fertilizers, detergents and sewage as water pollutants, eutrophication of water bodies.

(15 Lectures)

Course Outcome: Students will acquire adequate knowledge about the chemicals and chemical phenomena related to environmental pollution. This will enable them to move towards greener aspects of chemistry.

SEC 2: Semester II

SEC – Computational Representations of MoleculesCredits: 2+0+0 = 2

Theory: 30 Lectures

Course Objective: The objective is to provide knowledge about usage of various software for actual visual representation of molecules in 3-D space.

Unit 1: Computer Models of Molecules and Macromolecules

Two-dimensional molecular drawings and three-dimensional molecular models. Sketching two-dimensional drawings using ChemSketch, ISIS Draw or ChemDraw. Building three-dimensional molecular models using ArgusLab, Avogadro or GaussView – constructing the raw backbone, selecting and changing an atom, adding and hiding the hydrogen atoms, cleaning (refining) molecular geometry, saving in various formats. Computer storage of the molecular model in the XYZ (*.xyz*) file format – the content pattern of the XYZ files, use of Angstrom unit of length, absence of bond connectivity data therein. The z-matrix specification of the molecular geometry, illustration with a suitable file format such as MOPAC input format, use of degree unit for angles. Downloading, storing and opening macromolecular structural data as PDB files, interpreting PDB files in terms of chains, ligands, water molecules, etc. using ArgusLab, etc. [Hands-on practice strongly advised.]

(14 Lectures)

Unit 2: Computational Approaches about Molecules and Intermolecular Interactions

Introduction to Molecular Mechanics (MM) approach – all-atom and united-atom approaches, potential energy as sum of various covalent and non-covalent interactions, idea of force fields, examples of common force fields in MM. Introduction to Molecular Dynamics (MD). Introduction to semi-empirical methods – commonly used methods. Use of MM and semi-empirical methods for molecular geometry optimisation in ArgusLab or Avogadro etc. Concept of docking of a drug molecule with a protein macromolecule, using an example in ArgusLab etc. Quantum Mechanics (QM) approach, commonly used level of theory and basis sets for QM calculations, use of charge and spin multiplicity parameters – example of a QM calculation about a simple molecule using Gaussian or Firefly (i.e., PC-GAMESS) etc. Approach for the QM calculation of interaction energy for two interacting molecules such as two water molecules.
[Hands-on practice strongly advised.]

(16 Lectures)

Course Outcome: Students will learn the usage of software and programs for better representation of molecules in 3-dimensions for scientifically relevant visualization and representation of molecules.

SEC – Computer Programming for Science Students Credits: 2+0+0 = 2

Theory: 30 Lectures

Course Objective: To provide students with knowledge of computer algorithms to tackle scientific problems.

Unit 1: Introduction to Computer Programming

Computer programming and programming languages: computational problems, algorithms, flow charts, computer programs, programming languages and their evolution. Structured programming, the compilation process – source code, object code and executable code. Fundamentals of C language: character set, identifiers, key words, data types, constants and variables, statements, expressions, operators, precedence of operators, input-output and assignments. Fundamentals of FORTRAN: constants and variables – real, double precision, integer, complex, character and logical constants and variables. Arithmetic operations and operator symbols, common mathematical functions, arithmetic expressions and assignment statements, input and output statements. Typing and running FORTRAN programs: common downloadable freeware compilers, text editors – Edit, Notepad and gedit, working with the command prompt and the terminal in Windows and Ubuntu Linux, common text commands therein, hard disk drives, folders and subfolders.

(12 Lectures)

Unit 2: Computer Programming Using FORTRAN

Program for calculating the number of gas molecules in a very small speed range. Comment lines, statement labels, declaration statements, termination statements, conditional IF-ELSE-ENDIF and IF-ENDIF structures and their syntaxes with the example of real solutions of quadratic equation. GO TO statements, DO-loop structure and syntax. Arrays and subscripted variables. Algorithm for summing a series, its implementation using array, DO loop and GO TO statement for calculation of average and sample standard deviation of a series of values. Formatted input-output including *Fw.d* and *Ew.d* formats, FORMAT statement and syntax. Reading program input from text files and writing output to text files: the OPEN statement. Subprograms in FORTRAN: functions and subroutines.

(18 Lectures)

Course Outcome: Students will learn different operating systems and computer programs such as FORTRAN and C languages.

Open Elective Courses (OPE) :: Department of Chemistry

OPE 1 :: Semester III

OPE – Nanostructures and Nanomaterials Credits: 3+1+0 = 4

Theory: 60 Lectures

Course Objective: To provide students with the knowledge of nano-dimensional aspects of materials.

Unit 1: Introduction

Concept of nanosize, novel properties of nanomaterials, history of nanomaterials , nanomaterials in nature, scope and perspectives of nanoscience.

(10 Lectures)

Unit 2: Synthesis and Stabilisation of Nanomaterials

Top Down and Bottom Up approaches of fabricating nanomaterials, Challenges in nano fabrication, Different physical and chemical methods of synthesizing nanoparticles, Ostwald ripening, electrostatic and steric stabilization, synthesis of metal, semiconducting and oxide nanoparticles. A brief introduction to dimensional control of nanoparticles.

(20 Lectures)

Unit 3: Structural and Chemical Characterization

Electron Microscopy: Transmission Electron Microscopy/Selected Area Electron Diffraction Scanning Electron Microscopy/ Energy Dispersive X-Ray Analysis, Scanning Probe Microscopy: Surface Tunneling Microscopy and Atomic Force Microscopy, X-ray Diffraction. Miscellaneous Techniques.

(20 Lectures)

Unit 4: Applications and Ethical Issues

Applications of Nanomaterials in enviromental, industrial and medical fields. Toxicity, Biosafety and Ethical issues in application of nanoparticles.

(10 Lectures)

Course Outcome: Students will learn to synthesize and characterize nanomaterials and learn about their potential applications.

OPE 2: Semester IV

OPE – Chemistry in Human Life Credits: 3+1+0 = 4

Theory: 60 Lectures

Course Objective: This course is meant for all branches of students and hence the objective is to provide wider perspective of chemistry on human life.

Unit 1: Chemistry of Drugs and Medicines

Definition of Drugs, narcotic and non narcotic drugs, stages involved in drug development, determination of LD_{50} and ED_{50}, therapeutic index, over the counter and prescription drugs, drug regulatory agencies, side effects of drugs, drugs for metabolic and infectious diseases, Probiotics and antibiotics, antacids, anti inflammatory drugs, antidepressants, anti-viral and anti-fertility drugs. Drug tolerance and drug resistance. Harmful effects of nicotine consumption.

(15 Lectures)

Unit 2: Chemistry of Food and Nutrition

Macro and micro nutrients in food, basics of nutrition, calorie values of food, fats and oils, Unsaturated versus saturated fat, PUFA, MUFA, trans fat. Cholesterol, uric acid, and blood sugar. Role of minerals in metabolism. Dietary fibres.

Food colours and preservatives, MSG, Artificial sweeteners.

(12 Lectures)

Unit 3: Cosmetics and Personal Hygiene

A general study of the following: Hair oils, shampoo, sunscreen lotions, face powder, lipsticks, talcum powder, nail enamel, creams and moisturizers, toothpaste, antiperspirants and perfumes. Detergents and hair dye, hair curlers and straighteners.

(10 Lectures)

Unit 4: Petroleum and Non-Petroleum Fuels

Composition of crude petroleum, Refining and different types of petroleum products and their applications.

Fractional distillation (principle and process), Cracking (thermal and catalytic cracking), Reforming. Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals.

Biomass energy and biodiesel.

(15 Lectures)

Unit 5: Polymers and Industrial Chemicals

Biopolymers and man-made polymers, biodegradable and non-biodegradable plastics. Fibres and fabrics. Cellulose and pulp. Pesticides and fertilizers.

(8 Lectures)

Course Outcome: The outcome of this course will provide adequate knowledge of chemistry in the context of health, hygiene, nutrition, environment and other daily life activities.

Suggested Books in Chemistry for M.Sc. Course:

1. Basic Inorganic Chemistry by F.A. Cotton, G. Wilkinson, P.L. Gauss (John Wiley and Sons Ltd., Indian Edition)

2. Concise Inorganic Chemistry by J.D. Lee (John Wiley and Sons Ltd., Indian Edition)

3. Inorganic Chemistry by G.L. Meissler and D.A. Tarr (Pearson)

4. Shriver and Atkins's Inorganic Chemistry by P. Atkins, T. Overtone, J. Rourke, M. Weller and F. Armstrong (Oxford University Press, Indian Edition)

5. Inorganic Chemistry Principles of Structure and Reactivity by J. E. Huheey, E.A. Keiter, R.L. Keiter and O.K. Medhi (Pearson Education)

06. Oxford Chemistry Primer: Magnetochemistry by A.F. Orchard (Oxford University Press)

7. Oxford Chemistry Primer: Supramolecular Chemistry by P.D. Beer, P.A. Gale and D.K. Smith (Oxford University Press)

8. Fundamental Concepts of Inorganic Chemistry (Part I, II & III) by Ashim K. Das (CBS Publishers and Distributors)

9. Advanced Inorganic Chemistry (Volume I & II) by Satya Prakash, G.D. Tuli, S.K. Basu and R.D. Madan (S. Chand)

10. Principles of Inorganic Chemistry by B. R. Puri, L. K. Sharma and K. C. Kalia (Milestone)

11. Organic Chemistry by J. Clayden, N. Greevs and S. Warren (Oxford University Press)

12. Organic Chemistry by S.H. Pine (McGraw Hill)

13. Organic Chemistry (Volume I & II) by I.L. Finar (Pearson)

14. Advanced General Organic Chemistry by S.K. Ghosh (NCBA)

15. Organic Chemistry by S.M. Mukherji, S.P. Singh and R.P. Kapoor (Wiley)

16. Reaction Mechanism in Organic Chemistry by S.M.Mukherjee and S.P. Singh (Macmillan)

17. Basic Organic Stereochemistry by E.L. Eliel (Wiley)

18. Stereochemistry of Organic Compounds by D. Nasipuri (New Age International)

19. Polymer Science by V.R. Gowariker, N.V. Viswanathan and J. Sreedhar (New Age International)

20. Atkins's Physical Chemistry by P. Atkins and J.D. Paula (Oxford University Press)

21. A Textbook of Physical Chemistry (Volume 1, 2, 3, 4 & 5) by K.L. Kapoor (MacMillan)

22. Physical Chemistry by G.W. Castellan (Addison-Wesley)

23. A Textbook of Physical Chemistry by A.S. Negi and S.C. Anand (New Age International)

24. Quantum Chemistry by I.N. Levine (Prentice Hall)

25. Quantum Chemistry and Spectroscopy by B.K. Sen (Kalyani Publishers)

26. Fundamentals of Molecular Spectroscopy by C.N. Banwell and E.M. McCash (Tata McGraw Hill)

27. Organic Spectroscopy by W. Kemp (McMillan)

28. Introductory Organic Spectroscopy by B.K. Sen and Mousumi Ganguly (Kalyani)

29. An Advanced Course in Practical Chemistry by A.K Nad, Ghosal and Mahapatra (New Central Book Agency)

30. Chemical Kinetics by K. J. Laidler (Pearson)

31. Principles of Polymerisation by G. Odian (Wiley)

32. Textbook of Polymer Science by F. W. Billmeyer (Wiley)

33. Analytical Chemistry by G. D. Christian (Wiley)

34. Practical Organic Chemistry by A. I. Vogel (Longman)

35. Quantitative Chemical Analysis by A. I. Vogel (Longman)

36. Vogel's Textbook of Qualitative Inorganic Analysis by G. Svehla (Longman)

37. Modern Chemical Analysis by D. Harvey (Mc Graw Hill)

38. Catalytic Chemistry by B. C. Gates (Wiley)

39. Heterogeneous Catalysis by G. C. Bond (Oxford)

40. Principles and Practice of Heterogeneous Catalysis by J. M. Thomas and W. J. Thomas (VCH)

41. Modern Electrochemistry Vol. 1 by J. O. Bockris and A. K. N. Reddy (Kluwer)

42. Modern Electrochemistry Vol. 2A by J. O. Bockris and A. K. N. Reddy (Kluwer)

43. Professional Programmer's Guide to Fortran-77 by C.G. Page (University of Leicester)

44. Computers in Chemistry by K. V. Raman (Tata McGraw Hill)