Department of Chemistry
University of Kalyani
Kalyani 741235

S Y L L A B U S

TWO-YEAR FOUR-SEMESTER M.Sc. COURSE IN CHEMISTRY

(Effective from the Academic Session 2017-18)

UNIVERSITY OF KALYANI

Department of Chemistry

TWO-YEAR FOUR-SEMESTER M.Sc. COURSE IN CHEMISTRY

COURSE STRUCTURE

	SEMESTER								Total Marks
	I		II		III		IV		
Marks	400		400		400		400		1600
Course Type	Theo	Pract	Theo	Pract	Theo	Pract	Theo	Pract	
General (G+O)	300	100	200+100	100	---	---	---	---	800
Special (S)	---	---	---	---	300	100	300	100	800
Total Marks	300	100	300	100	300	100	300	100	1600

Special Courses in Four Branches of Chemistry are:

(i) Analytical Special (ANAL)
(ii) Inorganic Special (INORG)
(iii) Organic Special (ORG)
(iv) Physical Special (PHY)

Duration and expected schedule of End-Semester Examinations of each Semester would be according to the Academic Calendar of the University.

General (G) courses are Hard Core (compulsory) courses, General (O) course is **choice based** for students other than Chemistry (M.Sc.), while Special (S) courses are Soft Core (optional). Credit

for each course listed would be 4 units. Therefore, there are 4 x 4 or 16 credits in each semester, and 16 x 4 or 64 credits altogether in the Two-year, Four-semester M.Sc. course.

SEMESTER – I

General (G) Course: Hard Core / Compulsory

Marks – 400

OURSE	Marks		Total Marks
	Theory	Practical	
CHEM-G11	100	---	100
CHEM-G12	100	---	100
CHEM-G13	100	---	100
CHEM-G14	---	100	100
Total	300	100	400

SEMESTER – II

General (G) Course: Hard Core / Compulsory and Choice-based

Marks – 400

COURSE	Marks		Total Marks
	Theory	Practical	
CHEM-G21	100		100
CHEM-G22	100		100
CHEM-O23	100		100
CHEM-G24		100	100
Total	300*	100	400

*Chemistry students will take one choice-based course from other departments

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SEMESTER – III

Special (S) Course: Soft Core / Optional

Marks – 400

COURSE	Marks		Total Marks
	Theory	Practical	
CHEM-SA /SI /SO /SP-31	100		100
CHEM-SA /SI /SO /SP-32	100		100
CHEM-SA /SI /SO /SP-33	100		100
CHEM-SA /SI /SO /SP-34		100	100
Total	300	100	400

One set of special courses is to be selected by the student. SA stands for Analytical special (ANAL), SI for Inorganic special (INORG), SO for Organic special (ORG), SP for Physical special (PHY).

SEMESTER – IV

Special (S) Course: Soft Core / Optional

Marks – 400

COURSE	Marks		Total Marks
	Theory	Practical	
CHEM-SA /SI /SO /SP-41	100		100
CHEM-SA /SI /SO /SP-42	100		100
CHEM-SA /SI /SO /SP-43	100		100
CHEM-SA /SI /SO /SP-44		100	100
Total	300	100	400

Special courses would be as in Semester III

Course Structure of each Theoretical Paper

Full Marks: 100

Unit – 1: 16 marks

Unit – 2: 16 marks

Unit – 3: 16 marks
Unit – 4: 16 marks
Unit – 5: 16 marks

Continuous Internal Assessment: 20 marks

Question format of theoretical papers:

Each unit of any theoretical paper carries 20 marks, of which 20% or 4 marks are set for Internal Assessment and final or End-Semester Examination will be on the remaining 80% or 16 marks.

It is expected that, on the average, 12 one-hour classes or contact hours may suffice for one unit carrying 20 marks for any theoretical paper.

Continuous internal assessment will be based on performance in Midterm/ class test

Examination or Class Test or as decided by the concerned Board of Studies or the Departmental Committee.

Course Structure of Practical Papers

Semester I

Course ID	Continuous Assessment	Experiment	Viva-voce	Full Marks
Chem-G14	15 (5 x 3)	75 (25 x 3)	10	100

5 marks Continuous Assessment and 25 marks Experiment for each of Inorganic / Organic / Physical practical

Semester II

Course ID	Continuous Assessment	Experiment	Viva-voce	Full Marks
Chem-G24	15 (5 x 3)	75 (25 x 3)	10	100

5 marks Continuous Assessment and 25 marks Experiment for each of Inorganic / Organic / Physical practical

Semester III

Course ID	Continuous Assessment	Experiment	Viva-voce	Full Marks
Chem-SA /SI /SO /SP-34	20	70	10	100

Semester IV

Course ID	Internal Assessment	Project report submission / presentation	Project defense	Full Marks
Chem-SA /SI /SO /SP-44	20	70	10	100

In Semester I and II, students may be divided into 2 or more groups of nearly equal number. These groups would perform practical work in Inorganic, Organic and Physical sections by rotation, spanning approximately 60 days. In Semester III, practical sessions for each special experimental papers would last approximately 60 days also. In Semester IV, project work is expected to be carried out in 60 days. Marks in the experiment part (for Semesters I, II and III) would be based on performing given experiment(s) in the End-Semester Examinations.

For Semester IV, Project reports / presentation and Project defense would be evaluated during the End-Semester Examinations of Chem-SA /SI /SO /SP-44 paper.

SEMESTER – I

Paper: CHEM-G11 (Inorganic)

Unit 1: Coordination Chemistry I

Metal centered electronic spectra of transition metal complexes: Microstates, R-S terms, ground state terms of d^n metal ions. Splitting of ground state terms in crystal fields of octahedral and tetrahedral geometry. Orgel diagrams, Examples and assignments of d- d spectra. Hole formalism, crystal field parameters. Nephelauxetic series.

Unit 2: Theories of Bonding

Heitler – London theory of hydrogen molecule. Molecular Orbital theory. Salient features of valence bond theory (VBT) and molecular orbital theory (MOT). Bonding in homo-nuclear and heteronuclear diatomic molecules of 2^{nd} period. Bonding in triatomic (H_3^+, BeH_2, H_2O), tetraatomic (BH_3, NH_3) and CH_4. MO diagrams. Model of structure predictions: VSEPR and hybridization models, Bent's rule.

Unit 3: Metal – ligand Equilibria in Solution

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic effect.

Unit 4: Bioinorganic Chemistry I

Principles of coordination chemistry related to bioinorganic chemistry, Essential and trace metal ions in biological systems,

Porphyrin and related ligands, ATP as energy source, oxidative phosphorylation and phosphorylation of glucose. Transport and storage of dioxygen: Structure and function of hemoglobin, myoglobin, hemocyanin and hemerythrin. Synthetic oxygen carriers.

Unit 5: Electrochemical Analyses

Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, current – voltage relationship during electrolysis. Principles and applications of amperometry, coulometry and cyclic voltametry.

CHEM – G12 (Organic)

Unit 1: Stereochemistry

(a) Introduction: Chirality, stereoisomerism, configurational descriptors, topicity.

(b) Conformational analysis of six-membered carbo- and heterocyclic ring compounds; 6,6; 6,5-fused bicyclic compounds.

(c) Effects of conformation on reactivity in cyclic and acyclic systems.

Unit 2: Organic Reaction Mechanism

(a) Reactive intermediates: Formation, stability and reactivity of carbanions, carbocations (classical and non-classical), carbenes, nitrenes, free radicals and arynes with reference to basic types of organic reactions.

(b) Determination of reaction mechanism: Hammett equation, Taft equation.

(c) C-C and C-heteroatom bond forming reactions.

Unit 3: Fundamentals of Organic Synthesis

(a) Ring-closure reactions: Baldwin rules and exceptions.

(b) Ring-expansion and ring-contraction reactions: general utility in organic synthesis

(c) Protection and deprotection reactions.

(d) C=C bond forming reactions, rearrangement reactions involving electron rich and electron deficient centres.

Unit 4: Oxidising and reducing agents in organic synthesis

(a) Oxidation: metal-based oxidants (Cr, Mn, Os, Ag, Ru and Pb); non metal- based oxidation: Swern oxidation, Moffat oxidation, hypervalent iodine based oxidants, CAN as oxidant.

(b) Reduction: metal hydrides (B-H, Al-H, Zn-H, Sn-H, Si-H based reagents); hydrogenation; dissolving metal reductions; samarium iodide.

Unit – 5: Natural Products (Terpenoids and Alkaloids)

(a) Terpenoids: Introduction, isoprene rule, general methods of isolation, structure elucidation and synthesis of some representative members of mono and sesquiterpenes. Biogenesis and biosynthesis of mono-, sesqui- and di-terpenoids.

(b) Alkaloids: Definition and classification, general methods of isolation and structure elucidation, structure and synthesis of ephedrine, piperine, nicotine and papaverine. Biosynthesis of ephedrine and nicotine.

CHEM G – 13 (Physical)

Unit 1: Quantum Chemistry I

Stern-Gerlach expt., ket, bra, operator algebra, representations & transformations, uncertainty relation, translation & momentum, position & momentum wave function; simple potential systems – free particle, wells, barriers; simple harmonic oscillator

Unit 2: Introduction to Biophysical Chemistry

Introduction to the structural hierarchy in proteins, nucleic acids and lipids, basic features of primary, secondary, tertiary and quaternary structures of proteins, nucleic acid and lipids, explanation of various interactions determining the structures of biomolecules features and importance of hydrogen bonding in biomolecules and hydrophobic effect in biological structures.

Unit 3: Symmetry & Group Theory

Symmetry elements & operations; group, subgroup, class, point groups, group multiplication tables for cyclic and non-cyclic groups; matrix representations of symmetry operations and their characters, reducible representations, irreducible representations and great orthogonality theorem (no derivation), construction of character tables; application of group theory.

Unit 4: Kinetics I

Brief review of collision theory & activated complex theory; ionic reaction, kinetic salt effect; steady state kinetics, kinetic & thermodynamic control of reactions; unimolecular reactions; chain reactions, fast reactions.

Unit 5: Spectroscopy I

Rotation, vibration and vibration-rotation spectra of diatomic molecules; electronic spectra of diatomic molecules – progressions, band structure.

CHEM G – 14 (Practical)

Unit 1: Quantitative estimations and inorganic preparations

Unit 2: Preparation of selected organic compounds involving electrophilic substitution, addition, elimination and condensation reactions.

Unit 3: One day / two day instrument-based / analytical physicochemical experiments.

SEMESTER – II

CHEM G – 21

Unit 1: Coordination Chemistry II

Symmetry designation of LGOs and metal orbital's. Simplified MO energy level diagrams of octahedral and square planar complexes. Symmetries of the metal-ligand σ and π MOs. Magnetic properties of metal complexes when multiplet width is large, comparable and small compared to kT, anti-ferromagnetic interactions.

Unit 2: Ring, Cage and Cluster Compounds

Higher boranes and carboranes, Lipscomb`s topological concept, styx rule, Wade`s rule, skeletal electron counting, Wade – Mingos – Lauher rule. Bonding in metalloboranes and metallocarboranes. Low nuclearity (M_2, M_3) carbonyl clusters.

Unit 3: Metal Complexes of π acid Ligands

Characteristic Features of π-acid ligands. Preparation, properties, structures and reactivities of metal carbonyls, nitrosyls, dinitrogen and dioxygen complexes. Tertiary phosphines as ligands.

Unit – 4: Synthetic reagents and reactions

Organosilicon: Generalisations in silicon chemistry, Use of arylsilanes, vinylsilanes, epoxysilanes, allylsilanes.

Organoboron chemistry: Hydroboration, region-, chemo- and stereoselectivity. Conversion of C-B bond to C-hetero and C-C bonds. Use of allylboration and crotylboration.

Organophosphorous chemistry: phosphorus ylides, Wittig reaction and its modifications. Phosphines and phosphites. Arbutsov reaction.

Organosulfur chemistry: application of sulphoxides, sulfones and sulphur ylides in organic synthesis.

Unit-5: Heterocyclic chemistry and Steroids

Systematic nomenclature for monocyclic, fused– and bridged heterocycles, modern approaches of synthesis of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; their reactivities.

Steroids: Introduction, classification, nomenclature and general properties. Chemistry of Vitamine-D.

CHEM G – 22

Unit 1: **Quantum Chemistry II**

Rotation & angular momentum, spherical harmonics; H atom solution; many electron systems, variation, perturbation theory; Born-Oppenheimer separation; basic ideas of bonding.

Unit 2: Statistical Mechanics I

Phase space, introduction to ensembles and distributions, partition functions, fluctuations; introduction to Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein statistics.

Unit 3: Macromolecules

Polymer: definition, types of polymers – electrically conducting, fire resistant, liquid crystal polymers; condensation polymerization, copolymerisation; kinetics of polymerization; molecular mass of polymers: no. averaged and mass averaged molecular mass, their determination.

Unit-4: Pericyclic Reactions

Pericyclic Reaction: Introduction, classification and stereochemical modes, selection rules of electrocyclic reactions, 2-component cycloadditions and sigmatropic rearrangements. Rationalization based on PMO and FMO approach. Fluxional tautomerism.

Unit-5: Atomic absorption and atomic emission spectroscopy

Principles, instrumentation, and comparison of these techniques. Interferences such as background, spectral, vaporization, ionization, etc. Atomization techniques, relations and comparison, advantages and disadvantages. Applications for trace, speciation and multiple analysis. Specificity, sensitivity and detection limits in analysis.

CHEM O-23 Chemistry: Concept and Applications

Unit 1: Thermodynamics and Chemical Kinetics

Basic chemical thermodynamics: system and environment, intensive and extensive variables, state of a system, state functions, internal energy, entropy, free energy, reversible, irreversible, adiabatic, isothermal processes, three laws of thermodynamics.

Basic chemical kinetics: concept of rates and rate constants of chemical reactions, zeroth order, 1^{st} order and 2^{nd} order chemical reactions, determination of rate constant (elementary idea only).

Unit 2: Essential of Inorganic chemistry

Werner`s theory, Coordination compounds, geometries, VB, CFT and MO to understanding simple metal-ligand bond; Isomerism, Spin-only magnetic moment of d and f block elements, Colors and d-d transitions; Classification of metal ions and their roles in various basic chemical reactions in biological systems. Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs (examples only), metal dependent diseases.; Theories of catalysis, general principles, physical, dynamic and thermodynamic principles and applications of homogeneous and heterogeneous catalysis, various actions of promoters/poisons and inhibitors, catalysis by metal ions in industrial and biological processes.

Unit 3: Bioorganic chemistry

Structure and utility of natural and unnatural compounds, carbohydrates, biopolymers, nucleic acids, amino acids, peptides, drug molecules.

Unit 4: Exploring Chemical Analysis

Sampling, general protocols, classification and overview on some selected analytical techniques. Principle and instrumental features of spectrophotometry, thermogravimetry and voltammetry. Applications of various analytical techniques in different fields such as biology, pharamaceuticals, agriculture and environment.

Unit 5: Characterization and analytical tools in chemistry

Concept of surface tension, viscosity, conductivity in chemical systems, Infrared, UV-vis, Atomic absorption and emission, Electrochemistry.

CHEM G – 24 Practical

Unit 1: Inorganic qualitative analysis

Unit 2: Two-step synthesis of some selected organic compounds involving electrophilic substitution, addition, elimination and condensation reactions.

Unit 3: One day / two day instrument-based / analytical physicochemical experiments.

SEMESTER – III

CHEM SA-31

Unit 1: Basic steps of chemical analysis

Sampling - plan and protocol, single and multiple stage sampling, Importance of sampling to analytical processes, sampling of solid/liquid/ gaseous materials, sampling uncertainties, occupational health and hazards.

Unit 2: Molecular absorption and x-ray spectroscopy

Instrumentation and applications of IR, UV-VIS and X-ray spectroscopy, direct x-ray methods, x-ray absorption and emission, Auger emission spectroscopy.

Unit 3: Nuclear magnetic resonance spectroscopy

Theory, instrumentation and applications of proton NMR, C-13 NMR, application ofNMR to other nuclei, elucidation of NMR spectra, magnetic resonance imaging.

Unit 4: Mass spectrometric analysis

Theory and instrumentation. Different ionization techniques such as EI, CI and FAB techniques. Interpretation of mass spectra. Molecular ion or parent ion peak and their important features. General rules for predicting the prominent peaks in a mass spectra. Metastable peaks. Fragmentation patterns and modes. Mass spectra of some organic compounds and other applications.

Unit 5: Photoluminescence & laser spectroscopy

Principles, instrumentation and applications of fluorescence and phosphorescence. General principles of laser action, features of lasers and population inversion. Examples of some common lasers – solid state, gas and dye lasers.

CHEM-SA-32

Unit 1: Statistical & numerical analysis

Evaluation and presentation of analytical data, test of significance, ANOVA, correlation and regression analysis. Finite differences and approximate representation of functions, polynomial building, numerical integration and differentiation.

Unit 2: Liquid chromatography

Theory of chromatographic migration, plate theory, retention parameters, factors influencing band broadening and resolution, selection of phases and instruments for liquid chromatography, partition, adsorption, reverse phase chromatography, efficiency of LC separation, scope of HPLC, instrumentation and applications.

Unit 3: Hydrosphere Chemistry

Importance of hydrosphere, major water resources, hydrological cycle, origin of waste water from point and non-point sources and their classification, eutrophication, organic and inorganic pollutants and their public health significance, wholesome water, water borne pathogens and contaminants.

Unit 4: Kinetics & catalysis

Comparison of kinetic and non kinetic methods, rate analysis for slow and fast reactions, differential reaction rate methods and applications, catalyzed and non catalyzed reactions, enzyme catalyzed reactions.

Unit 5: Thermal methods of analysis

Thermogravimetry (TG), derivative of thermogravimetry (DTG), differential thermal analysis (DTA), differential scanning calorimetry (DSC), combination of thermal analysis techniques, instrumentation and application of thermal methods.

CHEM-SA-33

Unit 1: Solvent extraction

Solvent extraction and other separation techniques, distribution behavior, single, multiple and counter current extraction, salting out agent, kinetics of solvent extraction, metal ion extraction.

Unit 2: Nanochemistry & nanotechnology

Fundamental concepts of nanochemistry synthesis & characterization of nanometerials & nanocomposites, examples of some important nanomaterials. Applications of nanomaterials in spectrometry, electrochemistry, separation science, water treatment, food and agriculture. Future aspects of nanochemistry.

Unit 3: Bioanalytical chemistry

Trace elements in biological systems, classification and importance. Determination of serum electrolytes, blood glucose, cholesterol, uric acid, urea, billirubin, albumin, globulin etc.

Unit 4: Concept of radioactivity

Nature of radioactivity and radioactive disintegration, application of radioisotopes as tracers and in nuclear reactions, detection and measurement of radioactivity using ionization chamber, GM counter, flow scintillation and semiconducting devices. Analytical application of radiometric methods and radiometric titrations.

Unit 5: Automation in analytical techniques

Principles of automation, examples of automated and automatic instruments, chemical sensors, on-line analyzers, flow injection analysis.

CHEM-SA-34 (Practical)

Analysis of ores / minerals / alloys / cement / municipal and industrial wastes / drugs / physicochemical experiments: potentiometry / conductometry / spectrophotometry.

CHEM-SI-31

Unit 1: Principles of EPR Spectroscopy

Principle, comparison to NMR spectra, spectrometer, external standard, linewidth, nuclear hyperfine interactions, anisotropy in Lande g factor, magnetically equivalent and nonequivalent sets of nuclei, intensity, structural information of organic radicals and inorganic molecules from EPR spectra.

Unit 2: Electrochemistry and Coordination Compounds

Basic principles, metal and ligand centred redox chemistry,, innocent and non-innocent ligands, effect of ligands on metal redox chemistry, hard and soft ligands in tuning metal redox potential, electronic communication in dimetal and mixed metal assembly, Hammett constant and Hammett plot.

Unit 3: Application of IR and Raman Spectroscopy in Inorganic Chemistry

Vibrational spectroscopy: Infrared and Raman spectroscopy: S election rules for IR and Raman activity. Symmetry and shapes of AB2, AB3, AB4, AB5, AB6 . Application of IR and Raman spectroscopy for the determination of structural features of Inorganic compounds.

Unit 4: Application of NMR Spectroscopy

Application of NMR spectroscopy towards elucidation of structure of metal complexes and compounds containing various NMR active

nuclei – B, F, P, Si, Na, K, Al, V, Cr, Mn, Ni, Cu, Mo, Ru, Pd, I, Ir, Au, Pt etc. NMR of paramagnetic substances, contact shift.

Unit 5: Mossbauer Spectroscopy

Theory, presentation, isomer shifts, electric quadrupole interaction, magnetic interaction. Structural elucidation of compounds containing ^{119}Sn, ^{57}Fe, ^{129}I, ^{197}Au etc.

CHEM-SI-32

Unit 1: Application of EPR spectroscopy in Inorganic Chemistry

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including bilological systems and to inorganic free radicals such as $[PH_4]^{\cdot}$, $F_2^{\cdot}$, and $[BH]^{\cdot}$.

Unit 2: Polyacids, Clusters and Metal-metal Bonded Complexes

Iso and Hetero poly acids: Synthesis, Structure and Bonding. Types and classification of Heteropolymetallates (Dawson, Keggin etc.). Polyoxometallates, heteropoly blue. Utilities and application. High nuclearity (M_4-M_{10}) carbonyl clusters. Metal-metal single and multiple bonds, metal-metal bonding in Mo, Re, W, Cr, V etc. Bridging ligands and metal-metal bonded paddle wheel complexes. Synthesis and properties of metal-metal bonded complexes.

Unit 3: Solid State I

Crystal defects and non-stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects, point defects, Schotky and Frenkel defects, concentration of defects. Line and plane defects. Non stoichiometric defect, thermodynamics of non stoichiometric phases, color centres. Electronic properties and band theory: Free electron model and its limitations: Periodic potential field, Zone or

band models, Brillouin zones, band structure of insulators, conductors and semiconductors. Intrinsic and extrinsic semiconductors. Semiconductivity in nonstoichiometric compounds.

Unit 4: Organometallics I

Organotransition metal chemistry: History, Nature of metal – carbon bonding and definition and classification of organometallic compounds, classification of ligands, kinetic and thermodynamic stability of organometallic compounds. Compounds with metal carbon σ bond: alkyls and aryl complexes, Synthesis, stability and decomposition pathway. Compounds with metal carbon multiple bond: Alkylidenes and alkylidynes, Fischer and Schrock type of complexes. Low valent carbenes and carbines, Synthesis, bonding and reactivity.

Unit 5: Reaction Mechanism of Transition Metal Complexes

Energy profile of reactions, discussion on general reactivity of metal complexes, inert and labile complexes, Substitution reactions: Application of CFT, mechanism of ligand substitution in octahedral complexes, mechanism of isomerisation and racemisation, substitution reactions in square planar complexes. Cis- and trans effects.

CHEM-SI-33

Unit 1: Application of Group Theory in Inorganic Chemistry

Determination of the pattern of splitting of orbitals and R-S terms in a particular geometry. Assign ment symmetry designations, *e.g.* Γd = T2g + Eg. Correlation upon descending and ascending symmetries. Transition metal ions (dn) in weak and strong crystal fields. Correlation diagram. Tanabe – Sugano diagram. Revisit to d-d and

charge transfer spectra of transition metal complexes. Racah parameters.

Unit 2: Bioinorganic Chemistry II: Ion Transport Across the Membrane

Passive transport of alkali and alkaline earth metal ions through cell walls – ionophores, active transport - Na^+/ K^+ pump. Calcium in living cells, transport and regulation aspects of intramolecular process, extra cellular binding proteins.

Unit 3: Bioinorganic Chemistry III: Electron Transport Metalloproteins

Electron transport proteins: Cytochromes and Fe-S proteins-ferridoxins. Respiratory electron transfer chain, cytochrome c oxidase, photosynthetic electron transport chain– PS –I and PS- II

Unit 4: Organometallics II

Fluxional organometallic compounds: Classification of fluxional organometallic compounds. Fluxionality and dynamic equilibria in compounds such as η2 olefins, η3 ally and dienyl complexes, techniques of study.

Unit 5: Organometallics III

Transition metal π complexes with unsaturated organic ligands: alkenes, alkynes, allyl, diene, dienyl, arenes and trienyl complexes. Preparation, properties, reactivities, structure and bonding. Transition metal compounds with bonds to hydrogen: General features, preparative methods, types of hydrido species, terminal metal-hydrogen, bridged metal-hydrogen bonds, coordination dihydrogen,

CHEM-SI-34 (Practical)

1. Physicochemical experiments
2. Analysis of ores/minerals.

CHEM-SO-31

Unit 1: Alkaloids

Structural types, general introduction to phenylethylamine, pyrrolidine, pyridine, indole, isoquinoline type alkaloids. Quinine, morphine, yohimbine, reserpine, strychnine, lysergic acid and their uses.

Unit 2: Steroids

Chemistry of cholesterol, bile acids and some important steroidal hormones. Structure and biosynthesis of cholesterol and other related steroids.

Unit 3: Terpenoids

Chemistry of some representative members of diterpenoids, sesquiterpenoids, triterpenoids and tetraterpenoids (carotenoids) and their biogenetic routes.

Unit 4: Carbohydrate Chemistry

Conformational analysis of monosaccharides (pentoses and hexoses). Structure of maltose and gentiobiose. Protection and deprotection. *O*-glycosylation, *C*-glycosylation, Deoxysugars, amino sugars, glycal sugars and their synthetic aspects. Carbohydrates as chiral pools in organic synthesis.

Unit 5: Bioorganic Chemistry of Amino Acids

Introduction – importance of amino acids and peptides in chemical biology; Amino acids and their asymmetric synthesis; Amino acids

as building blocks; Chemistry of peptide bonds; synthesis of peptides, N-protection, Carboxy protection, activating agents, determination of N-terminus and C-terminus, Edman degradation; Peptide secondary structures and tools for stabilization; Synthetic peptides of importance, solid phase synthesis of peptides.

CHEM-SO-32

Unit 1: NMR Spectroscopy

NMR phenomenon (CW and FT-NMR), ^{1}H NMR: Chemical shift δ, inductive and anisotropic effects on δ, chemical and magnetic equivalent / non-equivalent protons, spin-spin coupling (hydrogen-hydrogen and hydrogen with other spin active nuclei such as ^{13}C, ^{19}F), structural correlation to coupling constant J, First order patterns, Second order effects, Nomenclature of spin system, Examples of A_2, AB, AX, AMX, ABX, ABC systems etc, Techniques for simplification of ^{1}H NMR spectra (Chemical techniques: deuteration, trifluoroacetylation, lanthanide shift reagents, chiral resolving agents; Instrumental techniques: use of higher magnetic field, spin decoupling, NOE); ^{13}C NMR spectroscopy, Application of NMR and other spectroscopic techniques to solve structures and mechanistic problems.

Unit 2: Synthetic Methodology I

A review of various synthetic methods in organic chemistry: Formation of C—C, C=C, C≡C triple bonds and selected syntheses of natural and unnatural products using these chemistry.

Rearrangement reactions.

Unit 3: Stereochemistry of ring systems

Stereochemistry of ring compounds: Conformations of monocyclic systems (small, common and medium ring compounds), fused and bridged cyclic systems, small tricyclic ring compounds.

Unit 4: Template-mediated Organic Synthesis

Definition of molecular template, Role of templates (thermodynamic and kinetic templates, covalent and non-covalent template-substrate interaction, Topology of reactions, Cyclization templates, Linear templates, Interweaving templates, Scavenger templates, Negative templates), Templated synthesis of polymers – Molecularly imprinted materials for recognition and catalysis, Biomimetic reactions directed by templates and removable tethers, use of temporary connection in organic synthesis.

Unit 5: Synthesis in solid phase

Introduction, geneal techniques and analytical tools for solid phase organic synthesis, supports for solid-phase synthesis, linkers for solid phase synthesis, preparation of organic compounds: preparation of alkanes, alkenes, alcohols, ethers, sulphur, nitrogen, carboxylic acids, carbonic acid and heterocyclic compounds.

CHEM-SO-33

Unit 1: Molecular Orbital Theory

M.O. Theory: M.O. theory and its applications to simple organic molecules, Walsh model for cyclopropane, HMO treatment to cyclic and acyclic conjugated systems, Huckel rule and concept of aromaticity, antiaromaticity, homoaromaticity.

Unit 2: Pericyclic Reactions

Stereochemistry of pericyclic reactions, reactivity, regioselectivity and periselectivity. Rationalization based on FMO method and aromatic transition state concept. Catalysis in pericyclic reactions.

Cheletropic reactions, dipolar cycloadditions, Claisen, Cope, oxy-Cope, aza-Cope and Ene reactions etc. Retropericyclic reactions.

Unit 3: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olefinic compounds, *cis-trans* isomerization, Paterno-Buchi reaction, Norrish Type-I and Type-II reactions, photoreduction of ketons, di-π methane rearrangement, photochemistry of arenes, photoreactions in solid state, photochemistry of nitro, azo and diazo compounds, photo-fragmentation reactions (Barton, Hofmann-Loffler-Freytag).

Unit 4: Green Chemistry

Green Chemistry: Introduction, principles, green synthetic methods, catalytic methods, organic synthesis in aqueous media, ionic liquid, supercritical fluids, MCR reactions, microwave-induced organic reactions, real-world cases of green chemistry.

Unit 5: Supramolecular Chemistry

Basic concepts of supramolecular chemistry, different non-covalent forces (e.g. H-bonding, cation-π, anion-π, π-stacking, hydrophobic, hydrophilic interactions etc.) leading to strong bonding of guest molecules to the hosts, thermodynamics of host-guest complexation, solvent effects and salt effects in complexation, design principle of host molecules, experimental techniques for characterization of host–guest complexation, examples of different design-based receptor molecules for cation, anion and neutral molecules binding, chiral recognition with examples, supramolecular devices (optical and electrochemical) and molecular switches, self-organization process-template association and supramolecular synthesis, self-replication and autocatalysis, supramolecular reactivity and catalysis, transport processes and carrier design, supramolecular gel, cyclodextrins, catenanes and rotaxanes.

CHEM-SO-34 (Practical)

1. Preparation of some selected reagents and their use in organic synthesis
2. Purification of organic compounds by column chromatography
3. Review and presentation of a current topic of interest

CHEM – SP-31

Unit 1: Advanced Spectroscopy I

Spectroscopy of polyatomic molecules -- rotation, vibration (normal modes, vibration analysis of H_2O), rotation-vibration spectra; special effects in vibration-rotation spectra of polyatomic molecules.

Unit 2: Biophysical Chemistry I

Detailed study of interactions in structure of biomolecules like protein, nucleic acid and lipid (charge-charge interaction, ion-dipole interaction, Lennard Jones type interaction, dipolar interaction, induction interaction), secondary structure of proteins and nucleic acids, interactions in tertiary and quaternary structures of proteins and nucleic acids, introduction to amphiphile aggregates

Unit 3: Advanced Spectroscopy II

Magnetic resonance spectroscopy, Bloch eqn, resonance, saturation, shielding of magnetic nuclei; chemical shift & measurements, factors affecting it, relaxation, factors affecting coupling constants, decoupling; FT nmr; ^{1}H, ^{13}C, ^{19}F, ^{31}P nmr; instrumentation, applications.

Unit 4: Multiphase materials, Glasses, Ceramics & Composites

Ferrous alloys, Fe-C phase transformations in such alloys, stainless steels; nonferrous alloys, their properties & applications; glassy state, glass formers & modifiers, applications; ceramic structures, mechanical properties, clay products; refractories, characterizations, properties & applications; microscopic composites, dispersion strengthened, particle-reinforced, fiber-reinforced and macroscopic composites.

Unit 5: Advanced Polymer I

chain transfer, retardation, inhibition; polymerization in homogeneous and heterogeneous systems, polymerization conditions; mechanisms of polymerization; polymerization – condensation, addition, radical chain, ionic, copolymerisation; Details kinetics of polymerization

CHEM – SP-32

Unit 1: Advanced Quantum Chemistry I

Addition of angular momenta; coupling schemes, electronic configurations, term symbols; WKB method; Hartree & Hartree-Fock theories; self-consistent fields; post-Hartree-Fock theories – CI, MCSCF, GVB and other methods, applications.

Unit 2: Non-equilibrium thermodynamics

Reversible and irreversible processes, Clausius inequality, thermodynamic criteria for non-equilibrium states; balance equations for irreversible processes; phenomenological equations, microscopic reversibility and Onsager reciprocity relations; examples and illustrations.

Unit 3: Advanced Spectroscopy III

Interaction of radiation with matter, transition probability, Einstein A, B coefficients; Fermi golden rule; basic selection rules and exceptions to selection rules: derivation of selection rules for rotational and vibrational transitions.

Unit 4: Solid State Chemistry I

X-Ray diffraction: Bragg's treatment, Von Laue's treatment, X-Ray diffraction methods, Reciprocal lattice, Brillouin zone, atomic scattering factor, geometrical structure factor.

Unit 5: Electrochemistry

Ion solvent interaction; electrode surfaces, potentials & measurement; thermodynamics of such systems, Lippman equation, Gouy Chapman & Stern models. Overpotential, exchange current density, electrolysis, polarography; photoelectrochemistry – band structure at semiconductor / solution interface, photocathode, photoanode, surface states & potential distribution at semiconductor / solution interface, photoelectrocatalysis, photo-electrochemical splitting of water, CO_2 reduction, waste reduction.

CHEM – SP-33

Unit 1: Solid State Chemistry II

Theory of solids: Free electron theory of metals and its applications, Band theory of solids and its applications; Semiconductors: Intrinsic semiconductors, extrinsic semiconductors, carrier concentration, Fermi level, conductivity

Unit 2: Advanced Polymers II

Characterisation, polydispersity & molecular weight distribution, measurement of molecular weight; osmometry, viscometry, diffusion

& light scattering methods; sedimentation; Flory Huggins theory, chemical potential & virial coefficients, excluded volume, polymer solvent interaction, its parameter.

Unit 3: Statistical Mechanics II

Introduction to liquid state, dominant intermolecular interactions in various liquids, brief summary of potential functions, probability density, configuration integral and classical partition function for liquid, distribution function, correspondence principle.

Unit 4: Interfacial Chemistry

Nature of surfaces & their properties, experiments on surfaces; adsorption & theories of adsorption, various eqns; thin films & clusters; catalysis; micelles, micellisation, reverse micelles, properties, related factors, thermodynamics of micellar systems.

Unit 5: Advanced quantum chemistry II

Pictures and representations: Schrodinger, Heisenberg, interaction pictures; Ehrenfest relations and other applications; Density Functional Theory: introduction, Hohenberg-Kohn theorems, N and V representability, Kohn-Sham equations, functionals, some examples.

CHEM – SP-34 (Practical)

Two day instrument-based / analytical physicochemical experiments

SEMESTER – IV

CHEM-SA-41

Unit 1: Electrochemistry

Types of electroanalytical methods, electrode systems, electrode kinetics, general feature of diffusion.Polarography, amperometric and coulometric titration.Voltammetry - linear sweep voltammetry, cyclic voltammetry, pulse voltammetry, stripping methods.

Unit 2: Atmospheric chemistry

Atmosphere and its composition, Chemistry occurring in atmosphere and important chain chemical reactions, Photochemical smog, Classification of air pollutant sources, Air pollution in urban centers and megacities, Effects of air pollutants on vegetation, livestock and inanimate objects, including human health, Analysis of common air pollutants like dust fall, PMs, SO_x, CO, NO_x, oxidants, chlorine, benzene.

Unit 3: Green chemistry & green technology

Principle of green chemistry, development of green materials, prospects of green solvents. Alternative techniques and renewable sources.Supercritical carbon-dioxide and supercritical water.Role of green technology in chemical synthesis, separation science & purification, pharmaceutical, sustainable development.

Unit 4: Analysis of pharmaceuticals

Basic concept of pharmaceuticals; definition and classifications. Phamacokinetics and pharmacogenomics, dose-response relationship. Metabolism, identification and analysis of various pharmaceuticals in various matrices.

Unit 5: Chemical processes and measurement of water environment

Chemistry of water molecule, important chemical processes and mechanism in water environment, measurement of critical water quality parameters, role of inorganics, organics and biotic contaminants and their recycling and equilibrium studies.

CHEM-SA-42

Unit 1: Basic instrumentation for analytical tools

Fundamentals of analytical instruments, sensor, transducer, signal conditioning, read out system, performance requirement, calibration techniques and validation. Basic concepts of some typical analytical instruments such as spectrophotometer/ fluorimeter/ potentiostat/ electrochemical & automated chemical analysis system.Electronic devices & circuits.

Unit 2: Forensic analysis

Chemistry of fire, analysis of flammable residues, study of explosives, Classification, properties and their analysis. Narcotics and drugs: Metabolism in human, identification, screening and testing.

Unit 3: Lithosphere chemistry and soil pollution

Soil composition, role of micro and macro nutrients, determination of critical soil properties including exchange capacity, C, N, K and P. Cations and anions adsorption in soils. Sources of soil pollution, importance of bio-fertilizers.

Unit 4: Gas and other chromatographic techniques

Types and operation in gas chromatography, instrumentation, first and second family detectors, temperature programming.

Performances & advantages of GLC and GSC. Supercritical fluid chromatography, size exclusion chromatography.

Unit 5: Fuel analysis

Ultimate and proximate analysis, coal ranking, determination of flash point and aniline point, octane number and carbon residue, producer and water gas.

CHEM-SA-43

Unit 1: Radiochemical analysis

Nuclear reactions, radioisotopes as tracers for application, isotope exchange reactions, preparation of carrier free tracer, isotope dilution analysis, activation analysis.

Unit 2: Electron spin resonance spectroscopy

Theory and instrumentation. Comparison to NMR spectroscopy. ESR lines and intensity. g-values and factors affecting the ESR lines. Hyperfine interactions. Zero field splitting and Kramer's degeneracy. Applications of ESR for the characterization free radicals and metal compounds. Applications in chemical and biological fields.

Unit 3: Modern & hyphenated techniques in analytical chemistry

Hyphenated techniques: GC-IR, GC-MS, GC-MS/MS, LC-MS, LC-MS/MS, LC-NMR and ICP-MS, acceleration mass spectrometry. Instrumentation, advantages and applications.

Unit 4: Toxicology

Fundamentals of toxicology, molecular-cellular aspects of toxicity. Toxico-kinetics, dose effect and dose-response relationship, toxicity and chemical nature, factors determining the toxicity of various toxic substances.

Unit 5: Waste management

Industrial operation (continuous and batch); selection of methods for industrialwaste treatment such as distillery, sugar, paper and steel plants.

CHEM-SA-44 (Practical)

Project work / Seminar / Grand viva

CHEM-SI-41

Unit 1: Metal-organic Framework

Ligand design: pillar and layer principles, synthesis of metal-organic framework (MOF), hydrothermal and solvothermal techniques. Applications: hydrogen storage, gas purification, gas separation, heterogeneous catalysis and drug carriers.

Unit 2: Solid State II

Diffusion in solids: General principles of diffusion, atomic approach, self diffusion, bulk diffusion, surface diffusion, grain boundary diffusion. Mechanism of diffusion, temperature and pressure dependence of diffusivity, tracer diffusion method. Fick's law and Nernst-Einstein equation, ionic conductivity and diffusivity, diffusion controlled reactions, application of diffusion in solids. Metallic solids: Alloy, solid solutions, substitutional and interstitial solids, application of alloys, super lattice structures, Hume – Rothery rules. Refractory carbides, borides and nitrides -- general preparative techniques, properties, structure and utilities

Unit 3: Crystallography I

Crystal symmetry: Forms, lattice, primitive cells, crystal systems and symmetry, nonprimitive lattice, crystal classes, space groups. X-ray diffraction, lattice planes, indices, Brag's law, reciprocal lattice.

Unit 4: Crystallography II

Crystal lattice and Miller indices, structure factor, systematic absence and space groups, screw axis and glide plane, fractional coordinates. Geometric data collection with simple examples. Structure solution: Fourier synthesis, Patterson and direct method.

Unit 5: Magnetic Properties and Complex Ions

Theory of magnetic susceptibility: Van Vleck equation, application of Van Vleck equation for different energy levels with respect to thermal energy kT. First order and second order Zeeman effects, quenching of orbital angular momentum by ligand fields (octahedral and tetrahedral only). Magnetic properties of A, E and T terms; splitting by spin-orbit coupling. The effect of t2g electron delocalization on effective magnetic moment. Temperature independent paramagnetism (TIP).

CHEM-SI-42

Unit 1: Bioinorganic Chemistry IV

Zinc containing enzymes: Carboxy peptidase A, carbonic anhydrase, alcohol dehydrogenase, DNA polymerase. Molybdenum containing enzymes: Nitrogenases: biological nitrogen fixation, oxo transferase, nitrate reductase, xanthine oxidase, aldehyde oxidase and sulphite oxidase. Metal storage and transport: Ferritin, transferrin, siderophores.

Unit 2: Bioinorganic Chemistry with Chemotherapeutic Drug

Cobalt containing coenzymes: Vitamin B12 and Vitamin B12 coenzymes. Iron containing enzymes: Catalase, peroxidase and

cytochrome P-450. Metals in medicine: Metal deficiency and diseases, toxic effects of metals, detoxifications by chelate therapy. Chemotherapy and anticancer drugs - cis platin and carbo platin.

Unit 3: Inorganic Photochemistry

Excited states of transition metal complexes, photoexcited states – photophysics and photochemistry. Energy level diagram and characteristics of excited states. Photo-chemical processes: photosubstituional and electron transfer reactions of transition metals. Applications in photochromism and other.

Unit 4: Supramolecular Chemistry I

Introduction: Complimentarity in biology, lock (host) and key (guest) principle. Non-covalent interaction in supramolecular systems. Design principle: chelate and macrocyclic effects.

Cation binding: Introduction, synthesis of macrocyclic receptors for cations, techniques used for synthesis of macrocyclic-crown ethers, cryptands, spherands and siderophores.

Unit 5: Reactions and Catalysis Involving Organometallic Compounds

Insertion, oxidative addition and reductive elimination reactions. Hydride transfer processes. Stoichiometric reactions. Homogenous catalytic hydrogenation, Ziegler-Natta polymerization of olefins, catalytic reactions involving CO (hydroformylation, oxo insetion etc.), Wacker oxidation.

CHEM-SI-43

Unit 1: Catalytic Reactions Involving Coordination Compounds

Activation of C-H bond and O–H bond, activation of CO, CO_2 (water gas shift reaction, Reppe reduction and Monsanto acetic acid

synthesis), coupling reactions and their synthetic applications – Heck, Suzuki etc.

Unit 2: Metal Ligand Bonding: Group Theoretical and Semi-quantitative Approach

Application of group theory to determine the symmetry and combinations of ligand group Orbitals (LGO) and metal orbitals in octahedral, square planar, tetrahedral and other ligand environments using of projection operator. Construction of qualitative MO energy level and interaction diagram on the basis of symmetry considerations only. Drawing of LGO and MO diagrams. Appropriate symmetry designations of MOs. Semi quantitative treatment of CFT. Types of splitting, Crystal field potential and relative energies of d- orbitals in crystal fields.

Unit 3: Materials Chemistry

Superconductivity and HTSC materials: The superconducting state, theory of superconductivity, effect of magnetic field – Meissner efeect, type–I and type–II superconductors. High temperature superconductivity (HTSC) in cuprates – preparation and characterization of 1-2-3 compounds of YBCO type. Organic superconductors. Theoretical aspects, preparation, characterization and applications of nanomaterials. Optical properties of semiconducting nanomaterials. Electronic properties of low dimentional materials. Nano/molecular magnets.

Unit 4: Electron Transfer Reactions and Mechanisms

Mechanism of redox reactions with reference to metal complexes. Electron transfer reactions – outer sphere and inner sphere, atom transfer, induced electron transfer reactions, two electron transfer reactions, non complementary reactions, synthetic implications of electron transfer reactions, solid state electron transfer reactions.

Electroprotic reactions. Mechanism of racemisation, inversion of configuration and associated process.

Unit 5: Supramolecular Chemistry II

Anion binding: Receptor design principles; recognition using electrostatic interaction; hydrogen bonds. Lewis acid hosts, importance of anion binding.

Present and future applications of supramolecular systems: Phase transfer agents; separation of mixtures; molecular sensors (electrochemical and optical); molecular switches; pharmaceuticals (MRI contrast and anti-cancer agents, drug design).

CHEM-SI-44 (Practical)

Seminar / grand viva / Project work

CHEM-SO-41

Unit 1: Total synthesis of natural products

Total synthesis of longifolene, reserpine, juvabione, aphidicolin and Fredericamycin A and Prostaglandins (PGE_2, $PGF_{2\alpha}$), taxol etc.

Unit 2: Biogenesis and Biosynthesis of Natural Products

Biogenesis: Precursors, primary and secondary metabolites. Acetate hypothesis. Mevalonate and Shikimic acid pathways.

General principles involved in the biosynthesis of amino acids, alkaloids, steroids and terpenoids.

Biosynthesis of selected natural products: L-tryptophan, quinine, estrone, taxol

Unit 3: Natural Oxygen Heterocycles

Naturally occurring oxygen heterocyclic compounds: Natural pigments, polyphenolics and other anti-oxidants

Unit 4: Medicinal Chemistry

Chemical basis of disease states, definition and classification of drugs and theoretical aspects of drug action. Drug metabolism and drug excretion. Qualitative and quantitative structure activity relationship. Concepts of drug dosing and drug half-life, drug tolerance and physical dependence, drug potency and therapeutic index (LD-50 & CD-50)

Mechanism of action of NSAIDs as pain killers and statin group of drugs to prevent atherosclerosis

Concept of prodrugs, pharmacophores and lead compounds. Molecular modification of drugs.

Definition, classification and mechanism of action of antibiotics.

Unit 5: Advanced Heterocyclic Chemistry

Synthesis and reactions of aziridines, azitidines, imidazoles, oxazoles, thiazoles, isoxazoles, pyrazoles and their benzo derivatives.

Pyrimidines, pyridazines, pyrazines, purines, pteridines.

Nomenclature of bicyclic and tricyclic fused system heterocycles. Role of heterocyclic compounds in biological systems. Application of heterocycles in pharmaceutical and electronic industry.

CHEM-SO-42

Unit I: Catalysis in Organic Synthesis

General introduction, homogeneous catalysis, heterogeneous catalysis, acid catalysis, asymmetric catalysis, phase transfer

catalysis in organic synthesis, polymeric materials as catalyst in organic synthesis, transition metal catalysed organic reactions.

Unit 2: Synthetic Methodology II

A review of various symmetric methods in organic chemistry for the formation of various rings (viz. 3, 4, 5, 6, 7 and 8 membered rings) and selected syntheses of natural and unnatural products having these ring systems.

Introduction to domino and tandem reaction concepts with a detailed discussion on selected examples.

Selected examples of multi-component reactions.

Unit 3: Dynamic Stereochemistry

Stereoselective reactions, enantioselective and diastereoselective reactions. Addition to carbon-carbon and carbon-hetero double bonds, epoxidation, dihyroxylation, amino-hydroxylation, hydrolysis, esterification etc.

Unit 4: Organometallics in Organic Synthesis

Classification, synthesis, reactions, structure and bonding and applications with typical examples. Application of 18-electron and 16-electron rules to transition metal organometallics, structure, bonding (pictorial MO approach) and reactions of η^2-ethylinic, η^3-allylic and η^5-cyclopentadienyl compounds: $K[Pt(\eta^2\text{-}C_2H_4)Cl_3]$, $[(\eta^3\text{-}C_3H_5)PdCl]_2$, $[(\eta^5\text{-}C_5H_5)_2Fe]$; carbine and carbine complexes

Various transition metal catalysed coupling reactions: Heck, Suzuki, Stille, Kumada, Hiyama etc.

Carbonylation reactions, Pauson-Khand reaction

Olefin metathesis, Tebbe reagent

Metal hydride catalysts: Isomerization reactions, olefin hydrogenation

C-H activation

Unit 5: Synthesis of Advanced Materials

Synthesis of novel advanced materials by new generation catalysts via ROMP (ring opening metathesis polymerization) reactions, nano structure material catalysis reaction, applications of nano-gold, nano-palladium, nano-copper in organic synthesis, carbon nanotubes (synthesis, forms, properties, applications).

CHEM-SO-43

Unit 1: Advanced Analytical Techniques in Organic Chemistry

Chiroptical properties of organic compounds: Origin, theory of ORD and CD, their applications, Cotton effects, axial haloketone rules, sector rules, helicity rules. Chiral analysis by polarimeter, NMR, GC, HPLC etc.

Unit 2: Mass Spectrometry

Theory and instrumentation. Importance of recognition of the parent peak. General rules of fragmentation and basic fragmentation types of simple organic molecules having different functional groups. Brief discussion on HR-, CI-, FAB- and MALDI-TOF MS techniques.

Unit 3: Two-dimensional NMR Spectroscopy

Application of proton (^{1}H), ^{13}C with advanced techniques (DEPT, COSY, NOESY, HETCOR) in structure elucidation of organic compounds.

Unit 4: Enzyme Chemistry

Introduction to enzymes: Molecular asymmetry and prochirality, factors responsible for enzyme specificity, Fischer's lock and key hypothesis, Koshland's induced fit hypothesis, kinetics of enzyme action, enzyme inhibitors, mechanism of enzyme action, different kinds of enzyme catalysed reactions, enzymes in synthetic organic

chemistry, brief introduction of coenzymes and some of their applications in organic synthesis, immobilization of enzymes, some examples of artificial enzyme models.

Unit 5: Advance spectroscopic techniques in structure elucidation

Different spectroscopic tools (FTIR, UV-vis, NMR, Mass etc.) and their role in structure elucidation.

CHEM-SO-44 (Practical)

Project work, presentation and defence. Grand viva

CHEM – SP-41

Unit 1: Advanced Quantum Chemistry III

Time dependence; path integral formalism, formulation and applications. Many body perturbation theory, interaction picture, GellMann & Low's theorem, normal & time ordering, Wick's theorem, level shift; diagrams, linked cluster theorem, applications.

Unit 2: Advanced Spectroscopy IV

Jablonski diagram, various processes occurring subsequent to excitation – radiative and non-radiative transitions, fluorescence spectroscopy, fluorescence quenching, Stern-Volmer plots, determination of fluorescence lifetime, single molecule spectroscopy, femtosecond spectroscopy.

Unit 3: Advanced Biophysical Chemistry II

Protein conformational transition, helix coil transition, protein folding, common folds in proteins, Ramachandran plot, supercoiled

structure of nucleic acid, organized structure of amphiphile aggregates

Unit 4: Solid State Chemistry III

Electrical properties: conduction, resistance, band gap; Magnetic properties: Diamagnetism, paramagnetism, ferromagnetism, anti-ferromagnetism, ferrimagnetism, hysteresis; Dielectric properties: Polarization, susceptibility, dielectric constant, ferroelectricity, piezoelectricity; Superconductivity: Theory and applications, high Tc superconductors – preparation, properties, theory and applications

Unit 5: Computational chemistry I

Introduction to computational chemistry and molecular modeling, potential energy surface, energy minimization, introduction to computational quantum mechanics and classical force field models, basic computations with reference to simple chemical and biological molecules

CHEM – SP-42

Unit 1: Advanced Polymers III

Structure & properties of polymers – morphology & order in crystalline polymers, polymer chains, effect of strain, crystallization & melting; structure & physical properties, melting point, effect of chain flexibility & other steric factors, entropy & heat of fusion; glass transition temperature; relation between Tm & Tg, effect of molecular weight, chemical structure, chain topology, branching & crosslinking, property requirements & polymer utilization.

Unit 2: Laser Spectroscopy

General principles of laser action – population inversion, features of lasers, some practical lasers – solid-state lasers, gas lasers, dye lasers, excimer lasers, diode lasers; laser spectroscopy – flash photolysis,

time-resolved fluorescence, Raman spectroscopy and use of lasers in Raman spectroscopy.

Unit 3: Corrosion

Corrosion – local cell theory, Pourbaix diagrams & corrosion of Fe & Zn, corrosion current & potential, Evans diagram, corrosion control – cathodic, anodic, mixed; inhibition, H_2 embrittlement, stress corrosion cracking, fatigue, corrosion measurement – weight loss, electrochemical & Stern Geary method; fuel cells.

Unit 4: Advanced Materials

Nanomaterials – preparation, characterization, theoretical understanding, properties & applications; quantum dots; nano-composites; organic semiconductors, fullerenes, carbon nanotubes, graphene.

Unit 5: Applications of Group Theory

Applications of group theory and molecular symmetry in molecular orbital theory, vibrational spectroscopy, chemical bonding, ligand field theory and electron spectroscopy, chemical reactions.

CHEM – SP-43

Unit 1: Advanced Spectroscopy V

Modern spectroscopic and microscopic techniques and applications: surface analysis (STM, AFM, SEM, TEM), fluorescence microscopy.

Unit 2: Numerical Analysis

Solution of algebraic equations; interpolation, extrapolation; linear & nonlinear fitting of data; finding eigenvalues & eigenvectors of matrices, determinants; numerical differentiation & integration; solution of ordinary differential equations of 1^{st} & 2^{nd} order;

modeling & testing of models; programming in Fortran / C for these methods.

Unit 3: Advanced Polymers IV

Processing of polymers – plastics, elastomers, fibres, compounding, techniques e.g. calendaring, die, rotational & film casting, injection, blow & extrusion moulding, thermoforming, foaming, reinforcing & fibre spinning; commercial polymers e.g. PE, PVC, polyamides, polyesters, phenolic & epoxy resins, silicones; functional polymers e.g. fire retarding, conducting polymers; bio-medical polymers e.g. contact lens, dental, artificial tissues & organs.

Unit 4: Computational Chemistry II

Dynamics of chemical and biological molecules, time dependent correlation function and relation with dynamical properties, introduction to computer simulation methods, molecular dynamics simulation, examples with reference to simple molecules

Unit 5: Surfaces, Thin Films

Nature of surfaces, physisorption, Chemisorption, catalysis, surface reactions, Surface defects; thin films, method of preparation e.g. evaporation, sputtering, CVD, sol-gel etc. Langmuir and LB films, photolithography, examples, applications;

CHEM – SP-44 (Practical)

Project work / Seminar