University of Kalyani

Department of Chemistry

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

COURSE STRUCTURE

	S E M E S T E R								
Duration	I July – Dec		II Jan – June		III July – Dec		IV Jan - June		Total Marks
Marks	300		300		300		300		1200
Course Type	Theo	Pract	Theo	Pract	Theo	Pract	Theo	Pract	
General (G)	180	120	180	120	60	---	---	---	660
Special(S)					120	120	180	120	540
Total Marks	180	120	180	120	180	120	180	120	1200
Examination month	January		June		January		June		

Special Courses in Four Branches of Chemistry are:

(i) Analytical Special (ANL)

(ii) Inorganic Special (ING)

(iii) Organic Special (ORG)

(iv) Physical Special (PHY)

SEMESTER – I

General (G) Course: Compulsory

Marks – 300

Course CH	Marks		Total Marks
	Theo	Pract	
CHEM – G11	60	40	100
CHEM – G12	60	40	100
CHEM – G13	60	40	100
Total	180	120	300

SEMESTER – II

General (G) Course: Compulsory

Marks – 300

Course CH	Marks		Total Marks
	Theo	Pract	
CHEM – G21	60	40	100
CHEM – G22	60	40	100
CHEM – G23	60	40	100
Total	180	120	300

*(Physical: 20, Computer Application: 10)

SEMESTER – III

General (G) Course – Compulsory

Special (S)* Courses: One special course to be opted

Course ID	Marks		Total Marks
	Theo	Pract	
CHEM-G31** (IOP-3)	60	40	100
CHEM- S 31/S 32/S 33/S 34	60	40	100
CHEM – S 35/S 36/S 37/S 38	60	40	100
Total: CHEM – G 31+CHEM-S 31/S 32/S 33/S 34+CHEM – S 35/S 36/S 37/S 38	180	120	300

*One Special Branch among the following four to be pursued:
CHEM-S 31/35 (ANL): CHEM-S 32/36 (ING): CHEM-S 33/37 (ORG)
CHEM-S 34/38 (PHY)

**(IOP-3): General combined paper of Inorganic, Organic and Physical Chemistry in 3rd Semester

SEMESTER – IV

Special Courses
Same special course corresponding to that opted in Semester III to be pursued
Marks – 300

Course ID*	Marks		Total Marks
	Theo	Pract	
CHEM-S 41/S 42/S 43/S 44	60	60	120
CHEM- S 45/S 46 /S 47 /S 48	60	-	60
CHEM – S 49 /S 50 / S 51 / S 52	60	60	120
Total	180	120	300

*CHEM – S 41/45/49 (ANL); CHEM – S42/46/50 (ING); CHEM – S43/47/51 (ORG); CHEM – S44/48/52 (PHY)

Course Structure of Theoretical Papers

Full Marks: 60

Unit – 1: 10 marks

Unit – 2: 10 marks

Unit – 3: 10 marks

Unit – 4: 10 marks

Unit – 5: 10 marks

Continuous Internal Assessment: 10 marks

Question format of theoretical papers:

Two questions per unit are to be set of which one question to be answered.

Continuous internal assessment will be based on performance in Midterm Examination.

Course Structure of Practical Papers

Semester – I

Course ID	Continuous assessment	Experiment	Viva-Voce	FM
CHEM-G11	20	10	10	40
CHEM-G12	20	10	10	40
CHEM-G13	20	10	10	40

Semester – II

Course ID	Continuous assessment	Experiment	Viva-Voce	FM
CHEM-G21	20	10	10	40
CHEM-G22	20	10	10	40
CHEM-G23	20	10	10	40

Semester – III

Course ID	Continuous assessment	Experiment	Viva-Voce	FM
CHEM-G31	20	10	10	40
CHEM-S/31/S32 /S33/S34	20	10	10	40
CHEM-S35/S-36/ S37/S-38	20	10	10	40

*One special Branch ANL / ING / ORG / PHY to be pursued.
CHEM- S 31/35 (ANI); CHEM-S 32/36 (ING)
CHEM- S 33/37 (ORG); CHEM-S 34/38 (PHY)

***Semester – IV**

Course ID	Expt. performance	Continuous assessment/ Project report writing and defence	Grand Viva/Seminar	FM
CHEM-S41/S 42/S 43/S44	30	10 + 10	10	60
CHEM-S 49/S 50/S 51/S 52	30	20	10	60

*CHEM-41/45/49 (ANL): CHEM-42/46/50 (ING)
CHEM-43/47/51 (ORG); CHEM-44/48/52 (PHY)
Viva- Voce Group Viva, FM: Full Marks

Plan of Conducting Different Semesters Together

Duration / Semester ⟶ ↓	**I**	**II**	**III**	**IV**
July – December	A (in)			
January – June '09	---	A		
July – December '09	B (in)	---	A	
January – June '09	---	B	---	A (out)

Odd Semesters: I & III to run simultaneously

Even Semesters: II & IV to run simultaneously

A = First batch of students (2008)

B = Second batch of students (2009)

Tentative Net Available Working Hours per Semester

Semester I, III (July – December)	Events	Semester II, IV (January – June)
180	Total no of days	180
26	Sundays	26
26	Saturdays	26
25	K.U. Holidays	13
-	Summer Preparatory leave	12
103	Available days	103
10	Preparatory leave	10
3 x 2	Theo. Exam.	3 x 2
3 x 3	Pract. Exam.	3 x 3
1 x 2	Lab Quiz.	1 x 2
3 x 2	Comprehensive viva	3 x 2
10	Mid-Semester exam	10
60	Net no. of teaching days	60
480	Net no. of lecture periods (L) @ 8L/day	480
40	Classes per week of 5 days	40
12	No. of teaching weeks	12
240	Available theoretical classes for 180 marks	240
240	Available practical classes for 120 marks	240
80	Classes available per theoretical Paper of 60 marks	80

Practical Schedule

First Semester:

The students enrolled will be divided into two groups of nearly equal numbers: A and B. The practical class of each semester will run approximately 60 days which will be divided into four approximately equal laps of 15 days (*1, 2, 3, 4*).

Name of the lap	A Group of students	B Group of students
1	Organic	Inorganic
2	Physical	Preparatory Library work
3	Preparatory library work	Organic
4	Inorganic	Physical

Second Semester:

Name of the lap	A Group of students	B Group of students
1	Organic	Preparatory Library work
2	Inorganic	Physical computer
3	Preparatory library work	Organic
4	Physical computer	Inorganic

Third Semester:

60 working days to be utilized to special Practical class being common for all the students of a particular semester.

Fourth Semester:

60 working days to be devoted to Project work.

SEMESTER – I

CHEM - G11

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. Applications in terms of structural information. 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 homonuclear 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, Walsh 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. Spectrophotometric and pH metric determination of binary formation constants.

Unit 4:

a. Bioinorganic Chemistry 1

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.

b. Poly acids: Iso and hetro poly acids: Synthesis, structure and bonding. Types and classifications of heteropolymetallates (Dawson, Keggin etc.). Polyoxometallates, heteropoly blue. Utilities and applications.

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 - G11 (Practical) : Quantitative estimations and inorganic preparations

CHEM – G12

Unit – 1: Structure – Activity Relationship

MO treatment of acyclic and cyclic conjugated systems, Huckel rule and concept of aromaticity; annulenes, heteroannulens, fullerenes (C60), alternate and non-alternate hydrocarbons, anti-aromaticity, pseudo-aromaticity, homo-aromaticity, Frost diagram, Huckel treatment – applications to ethylene, allyl, cyclopropenyl, butadiene, cyclobutadiene, Importance of antibonding orbitals in organic reactions.

Unit 2: Stereochemistry

Concept of chirality: Recognition of symmetry elements and chiral structures; configurational descriptors: R-S nomenclature; diastereoisomerism in acyclic and cyclic systems. Point groups; correlation of Axial dissymmetry and centrodissymmetry Winstein Holness equation, Curtin-Hammet Principle; Conformational Analysis of Cyclohexane, cyclohexene, decalin and their derivatives: Effects of conformation on reactivity in acyclic compounds and cyclohexanes.

Unit – 3: Pericyclic Reactions

Classification and stereochemical modes; Thermal and photopericyclic reactions, selection rules and stereochemistry of electrocyclic reactions, 2-component cycloadditions – antarafacial and suprafacial additions; Rationalization based on Frontier M.O. approach, correlation diagram, Dewer-Zimmermann approach, Mobius & Huckel systems; Claisen, Cope, Aza-Cope and Oxy-Cope rearrangements, Sommelet - Hauser, Ene reaction – Applications in Organic synthesis; Fluxional tautomerism.

Unit – 4: Organic Reaction Mechanisms

Reactive intermediates – Formation and stability of classical and non-classical carbonium ions, carbanions, carbenes, nitrenes, radicals and arynes; Nucleophilic, electrophilic and radical substitutions, addition and elimination reactions; Methods of determining reaction mechanisms, Kinetic isotope effect, Hard and soft acids and bases; Hammet equation.

Mechanisms of some familiar name reactions: Robinson annulation, Peterson elimination, Stork enamine reaction, Mannich reaction, Sharpless asymmetric epoxidation, Barton reaction, Hofmann-Loffler-Freytag reaction, Shapiro reaction, Baeyer-Villiger reaction, Chichibabin reaction.

Unit – 5: Natural Products – Terpenoids

Isoprene rule; Structure elucidation (by chemical and spectroscopical methods); synthesis, Biogenesis and Biosynthesis of representative examples of acyclic,

monocyclic and bicyclic monoterpenes. Structural types – general introduction to sesqui, di-and tri-terpenoids.

CHEM G-12 (Practical):

Identification of Single Organic Liquids and Solids containing one or more functional groups.

CHEM G – 13

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: Thermodynamics

Resume of thermodynamics; partial molar quantities, their significance and determination; non ideal systems – excess functions, fugacity, activity, activity coefficient, their determination; phase transitions (basic idea).

Unit 3: Symmetry & Group Theory

Symmetry elements & operations; group, subgroup etc., class, character; point groups, symbols, representations; great orthogonality theorem (no derivation) and its consequences; character table.

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, photochemical & oscillatory reactions (basic idea only).

Unit 5: Spectroscopy I

Basic idea of transition, transition probability & transition integral, selection rule, Fermi golden rule (no derivation), Einstein A, B, coefficients (no derivation); basic idea of uv-vis, vibration, rotation, nmr & esr spectra; idea of other types of spectra.

G -13 (Practical)

One day / two day instrument-based / analytical physicochemical experiments

SEMESTER – II

CHEM – G21

Unit 1: Coordination Chemistry I

(a) Metal – ligand bonding

CFT and VBT to rationalize the bonding in transition metal complexes. Limitations of CFT and VBT. MOT to rationalize σ and π interactions in octahedral , square planar and tetrahedral metal complexes. Symmetry designations of LGOs and MOs. Simplified MO diagrams.

(b) Magnetic properties and coordination compounds

Spin and orbital moments, spin – orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable temperature magnetic moments, antiferromagnetic interactions and spin crossover.

Unit 2: Ring, cage and clusters: Structure and bonding

Higher boranes and carboranes, Lipscomb's topological concept, styx rule, Wade's rule. Metal – metal bonding, metal – metal single and multiple bonds, Low nuclearity (M_3, M_4) and high nuclearity ($M_5 – M_{10}$) carbonyl clusters, skeletal electron counting, Wade – Mingos – Lauher rule. Bonding in metalloboranes and metallocarboranes.

Unit 3: Metal complexes of π acid ligands

Preparation , properties , structures and reactivities of metal carbonyls, nitrosyls, dinitrogen and dioxygen complexes. Tertiary phosphines as ligands. Application 18 and 16 electron rules to transition metal organometallic complexes. Isolobal relationships with examples.

Unit 4: Raman Spectroscopy

Raman spectroscopy. Scattering of electromagnetic radiation, Classical and quantum theories of Raman effect, Stokes and anti-Stokes lines; molecular polarizability, polarisability tensor, pure rotational, vibrational and vibrational – rotational Raman spectra,. Selection rules for vibration and rotation, mutual exclusion principle. Some applications of Raman spectroscopy in structure determination.

Unit 5: Instrumental techniques II

Errors in quantitative analysis, types of errors, handling of systematic error, random and non random error, distribution, standard deviation and confidence limit. Nature of radioactivity, isomeric transition, detection and measurement of radioactivity, ionization chamber. Flow scintillation and semiconducting counters. Types of radiometric analysis, radiometric titration, study of chemical reactions.

CHEM – G21 (Practical) : Qualitative analysis

CHEM-G 22

Unit-1: Photochemistry

Basic principles, Jablonski diagram, photochemistry of olifinic compounds, *Cis-trans* isomerization, Paterno-Buchi reaction, Norrish Type-I and II reactions, Photoreduction of ketons, di-π methane rearrangement, Photochemistry of arenas; Photoreactions in solid state, synthetic applications; cyclization of radicals.

Unit – 2: Synthetic Methodology-I

Organoboron chemistry: carboranes, hydroboration, reaction of organoboranes, unsaturated hydrocarbon synthesis, allyl borones, allyl enolates.

Organophosphorous chemistry: phosphorus ylides- Wittig reaction and its modifications; phosphine oxides and its applications.

Organosulfur chemistry: sulfur-stabilization of anions and cations, sulfur ylides, sulfoxides and sulfones.

Unit-3: NMR Spectroscopy

Principles, instrumentation and different techniques (CW and FT) of NMR spectroscopy, factors influencing chemical shift, spin-spin interactions, coupling constant (J), spin-decoupling, spin – tickling, classification of ABX, AMX, ABC, A_2B_2 in proton NMR. Introduction to ^{13}C-NMR spectroscopy, application of NMR and other spectroscopic techniques to solve structures and mechanistic problems.

Unit-4: Heterocyclic chemistry

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

Unit-5: Natural Products – Alkaloids

Familiarity with methods of structural elucidation (chemical and spectroscopical methods, biosynthesis, synthesis of alkaloids (nicotine, ephedrine, atropine, coniine and papaverine)

CHEM G-22 (Practical)

Organic preparations.

CHEM G – 23

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, ergodic hypothesis, ensembles & averaging; canonical, micro-canonical & grand canonical ensembles, corresponding distributions; partition functions, fluctuations; perfect gas, Gibbs' paradox, Sackur Tetrode eqn; MB, FD & BE statistics.

Unit 3: Spectroscopy II

Some details of rotation, vibration, rotation-vibration spectroscopy; application of symmetry principles to selection rules, vibration analysis, normal modes.

Unit 4: Electrochemistry I

Debye Huckel theory and its extension; Debye Huckel Onsager theory and its extension; ion solvent interaction; electrode surfaces, potentials & measurement; thermodynamics of such systems, Lippman equation, Gouy Chapman & Stern models.

Unit 5: Macromolecules

Polymer: definition, types of polymers – electrically conducting, fire resistant, liquid crystal polymers; polymerization – condensation, addition, radical chain, ionic, condensation polymerization, copolymerisation; kinetics of polymerization: chain transfer, retardation, inhibition; polymerization in homogeneous and hetero-geneous systems, polymerization conditions; mechanisms of polymerization; molecular mass of polymers: no. averaged and mass averaged molecular mass, their determination.

Course G -23 (Practical)

One day / two day instrument-based / analytical physicochemical experiments.

SEMESTER – III

CHEM – G31

Unit 1: EPR and Mossbauer Spectra

EPR Spectra: Principle and spin Hamiltonian (comparison to NMR spectra), spectro-Meter, external standard, linewidth, nuclear hyperfineinteractions, anisotropy in Lande g factor and hyperfine interaction, magnetically equivalent and nonequivalent sets of nuclei, intensity, structural information of organic radicals and inorganic molecules from EPR spectra.

Mossbauer Spectra: Principle, experiment, linewidth, centre shift, quadrupole interaction, magnetic interaction, information on spin and oxidation states, structure and bonding, spin transition from spectra of different Mossbauer active nuclei in various environments.

Unit 2: PES and Diffraction Methods

Photoelectron spectroscopy – photoexcitation and photoionization, XPS, UPS, experiments; chemical shift, detection of atoms and molecules, effect of environment; UPS of single molecules, AES, ZEKE spectroscopy; electron energy loss spectroscopy, EELS, HREELS.

Unit 3: Mass Spectroscopy

Principles, instrumentation and applications of mass spectrometry – methods of generation of ions in EI, CI, FD and FAB and other techniques. Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotope, ion-molecule interaction and analysis of fragmentation patterns.

Unit 4: Problem-solving methods in spectroscopy

Applications of Mass, UV-VIS, IR and NMR spectroscopy to structural and mechanistic problems

Unit 5: Laser and Laser Spectroscopy

General principles of laser action – population inversion, features of lasers, mode locking, Q-switching; some practical lasers – solid-state lasers, gas lasers, dye lasers, excimer lasers, diode lasers; laser spectroscopy – flash photolysis, time-resolved fluorescence, femtosecond transient absorption and up-conversion, multi-photon absorption, jet spectroscopy, use of lasers in Raman spectroscopy, single molecule spectroscopy.

CHEM – G31 (Practical): Preparation and characterization of inorganic compounds.

CHEM – G31 (Practical): Multistep organic synthesis and chromatographic separation techniques.

CHEM – G31 (Practical): One day / two day instrument based / analytical physicochemical experiments

CHEM-S31

Unit-1: Basic steps of chemical analysis

Sampling - plan and protocol, single and multiple stage sampling, sampling of solid/liquid/ gaseous materials, sampling uncertainties, safety in chemical laboratory, problem and measures of occupational health, health standard.

Unit-2: Electronics and instrumentation

Active and passive networks, tuned and crystal oscillators, power supply, bipolar and field effect transistor, transducer, amplifier circuit, operational amplifiers and their uses in chemical devices, optical devices

Unit 3: Molecular absorption and x-ray spectroscopy

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

Unit-4: NMR spectrometry

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

Unit-5: Automation in analytical laboratory

Principles in automation, autoanalyser, microprocessor controlled instruments, chemical sensors, automatic chemical and elemental analyzer, oxygen analyzer, flow injection analysis.

Chem S31 (Practical): Analysis of ore/mineral/alloys/cement/municipal/industrial wastes

CHEM – S32

Unit 1: **Group theory and Quantum mechanics**

Point groups; Representation; Atomic and molecular orbitals as bases of representation; Reducible and irreducible representations; Character table. Great Orthogonal theorem, GOT and its importance; Bridging group theory and quantum mechanics: symmetry aspects of molecular orbitals, Wigner's theorem: symmetry rules of chemical reactions (introduction only). Molecular vibrations: symmetry normal modes of vibrations, determination of the symmetry types normal modes, contribution of particular internal coordinates to normal modes, selection rules for fundamental vibrational transitions.

Unit 2: Quantum mechanics

Schrödinger equation, problem of solving many electron Schrödinger equation: Introduction Self Consistent Field (SCF) theory, orbital approximation, Hartree's method, electron spin, identical particles and symmetry and antisymmetry law of nature, Slater determinant, Fock's extension of Hartree's work – Hartree-Fock SCF theory, exchange and coulomb integrals, Koopmann's theorem. Slater type orbitals (STO) and its importance in quantum chemistry.

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. Specific defects in magnetite, $\gamma - Fe_2O_3$, silver iodide and in fluorite lattice. 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: Application of spectroscopy in inorganic chemistry

Vibrational spectroscopy: Infrared and Raman spectroscopy, selection rules for IR and Raman activity. Symmetry and shapes of AB_2, AB_3, AB_4, AB_5, AB_6 . Mode of bonding ambidentate ligands, ethylene diamine and diketonato complexes, application of resonance Raman spectroscopy, particularly for study of active sites of metallo proteins. Application of IR and Raman spectroscopy for the determination of structural features of Inorganic compounds.

Electron spin resonance spectroscopy: Theory. 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 a $[PH_4]^-$, F_2^-, and $[BH]^-$.

Unit 5: Reaction mechanism of transition metal complexes

Energy profile of reactions, discussion on general reactivity of metal complexes, inert and labile complexes, Techniques for experimental measurements of reaction rates, techniques for fast reaction.

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 – S32 (Practical)

Physicochemical experiments.

CHEM-S33

Unit 1: Stereochemistry-II

Conformation and reactivity of monocyclic systems-3 to 10 membered rings, 6-6, 6-5, 6-4, 5-5 bicyclic systems, 6-6-6, 6-5-6, 5-6-5 and 5-5-5 tricyclic systems, enantioselective and diastereoselective synthesis, Addition to carbonyl compounds.

Unit 2: Synthetic strategy

Disconnection approach: basic principles, one-group, two-group disconnections, selectivity aspects: Chemoselectivity, regioselectivity, stereoselectivity, Retron, Umpolung concepts; uses of aliphatic nitro, amines; radical reactions in synthesis-FGA and its reverse, Protection and deprotection of common functional groups (hydroxy, carbonyl, carboxylic and amino groups).

Unit 3: NMR Spectroscopy II

Theory and Applications of DEPT, ^1H-^1H COSY, HMBC, HMQC, NOESY in structure elucidation of organic compounds, reaction monitoring.

Unit 4: Heterocyclic Chemistry II

Synthesis and reactions of azidirines, azetidines, oxazoles, thiazoles, isoxazoles, pyrazoles; Nomenclature of bicyclic and tricyclic fused systems; Introduction to the chemistry of arzepins, oxepins.

Unit 5: Medicinal Chemistry I

Chemical basis of disease states, definition and classification of drugs, drug metabolism and drug excretion, development of new drugs, concepts of prodrugs and soft drugs, pharmacophores, lead compounds and molecular modification, qualitative and quantitative structure activity relationship.

Concept of pharmacokinetics and pharmacodynamics, enzyme inhibitors, receptors, chemical messengers, agonists and antagonists. 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 and synthesis of some antipyretics and non-steroidal anti-inflammatory drugs (NSAID).

Classification and mechanism of action of antibiotics. Synthesis of penicillin-G, penicillin-V, ampicillin, amoxycillin, chloramphenicol, norfloxacins, cephalosphorins an other new generation antibiotics.

CHEM S33 (Practical)

Multistep organic synthesis, chromatographic separation techniques.

Course S 34

Unit 1: Advanced Quantum Chemistry I

Addition of angular momenta; coupling schemes, electronic configurations, term symbols; time evolution, pictures & representation, Heisenberg eqn of motion,

Ehrenfest relations; 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

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

Unit 3: Biophysical Chemistry I

Structural hierarchy in proteins (titration curves), nucleic acids and lipids in living systems; forces involved in biopolymer interactions; structure & function of cells.

Unit 4: Advanced Spectroscopy I

Interaction of radiation with matter, transition probability, Fermi golden rule, Einstein A, B coefficients; selection rules, exceptions to selection rules.

Unit 5: Solid State Chemistry I

Theory of crystalline solids, free electron model, its limitation, Kronig Penny model, tight binding model, band structure, Brillouin zones, insulators, conductors, semiconductors; Bragg condition, Laue method.

Course S 34 (Practical)

One day instrument-based / analytical physicochemical experiments

CHEM-S35

Unit-1: Data treatment

Evaluation and presentation of analytical data, propagation of uncertainty, probability and distribution, test of significance, ANOVA and chi square test, least square method, regression and correlation analysis.

Unit-2: Numerical analysis

Iterative solution of f(x)=0, finite differences and approximate representation of functions, polynomial building, interpolation, numerical integration and differentiation, numerical solution of ordinary differential equations, solving of simultaneous and linear algebric equations.

Unit-3: Radiochemical analysis

Nuclear reactions and radiation, tracer techniques, role of carrier, isotope exchange reactions, preparation of carrier free tracer, kinetic isotope effect, activation analysis, isotope dilution analysis.

Unit-4: Kinetic methods of analysis

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

Unit-5: Thermal methods of analysis

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

CHEM S35 (Practical)

Physicochemical experiments: Potentiometry/conductometry/spectrophotometry

CHEM – S36

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.* $\Gamma_d = T_{2g} + E_g$. Correlation upon descending and ascending symmetries. Transition metal ions (d^n) 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: 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 3: Bioinorganic Chemistry II

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.

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 I

Organotransition metal chemistry: History, Nature of metal – carbon bonding and definition and classification of organometallic compounds, classification 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. Role in organic synthesis.

Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, technoiques of study.

Unit 5: Organometallics II

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 hydrido species, terminal metal- hydrogen, bridged metal hydrogen bonds, coordination dihydrogen, clusters and encapsulated hydrides.

CHEM – S36 (Practical)

Analysis of ores/minerals.

CHEM- S37

Unit 1: Applications of M.O. Theory

M.O. theory and its applications to organic molecules, construction of M.O.s - linear and cyclic conjugated systems, Walsh orbitals of cyclopropane and cyclobutane, stability of carbocations, strained organic molecules, calculation of strain energies.

Unit 2: Organometallic Chemistry of Transitional Elements-I

Synthesis, structure, bonding, oxidative addition, migratory insertion, reductive elimination, ligand migration from metal to carbon. Organometallic reagents in organic synthesis and in homogeneous catalytic reactions (hydrogenation, hydroformylation, isomerization and polymerization), π-acid metal complexes, complexation and decomplexation.

Unit 3: Synthetic Methodology-II

Organosilicon chemistry, synthetic uses of silyl ethers, silylenol ethers, TMSCl, TMSI, TMSCN, alkene synthesis, alkenyl, vinyl, aryl, allyl and acyl silanes, Brook rearrangement, silicon Baeyer Villiger rearrangement.

Unit 4: Natural Products I

Steroids – General methods of study and structural types, chemistry of cholesterol, hormones, bile acids, Vitamins of D-group, diosgenin. Terpenoids: Chemistry of some

representative members of diterpenoid and triterpenoids (synthesis of steroids and terpenoids excluded).

Unit 5: Asymmetric Synthesis I

Addition to C=C double bonds (electrophile induced cyclization, iodolactonization), Hydroboration, conjugate additions, Diels-Alder cycloaddition, π-facial selectivity and Cieplak model.

CHEM S37 (Practical)

Preparation of organic reagents and their applications.

CHEM- S 38

Unit 1: Advanced Spectroscopy II

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

Unit 2: Solid State Chemistry II

Debye Scherrer method, unit cells & diffraction patterns, reciprocal lattice, simple lattices & x-ray intensities, relation to electron density; x-ray analysis; crystal defects & non-stoichiometry: perfect, imperfect crystals, intrinsic, extrinsic defects, point defects – vacancies, Schottky, Frenkel defects, defect concentration, colour centre.

Unit 3: Advanced Polymers I

Characterisation, polydispersity & molecular weight distribution, measurement of molecular weight; osmometry, viscometry, diffusion & light scattering methods; sedimentation; chain configuration of macromolecules, calculation of average dimensions of various chain structures; analysis & testing of polymers – chemical, spectroscopic, XRD, microscopy; mechanical testing – thermal, physical, fatigue, tear,

hardness, etc.; Flory Huggins theory, chemical potential & virial coefficients, excluded volume, polymer solvent interaction, its parameter.

Unit 4: Statistical Mechanics II

Chemical potential & chemical equilibrium; liquid state, its thermodynamics, eqns of state, critical constants, types of intermolecular forces, potential functions, pair potential approximation; classical partition function for liquid, correspondence principle, configuration integral & properties; cell model; entropy, Lennard Jones Devonshire, significant structure model.

Unit 5: 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.

CHEM S 38 (Practical)

Two day instrument-based / analytical physicochemical experiments

SEMESTER – IV

CHEM-S41

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: 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-3: 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, ion and size exclusion chromatography, efficiency of LC separation, scope of HPLC, instrumentation and applications of HPLC.

Unit-4: Gas and other chromatographic techniques

Types and operation in gas chromatography, instrumentation, first and second family detector, temperature programming, applications, relative advantages of GLC and GSC, supercritical fluid chromatography, size exclusion chromatography.

Unit-5: Fuel analysis

Ultimate and proximate analysis, heating values, grading of coal, determination of calorific value by BOMB calorimeter, determination of flash point and aniline point of an oil, octane number and carbon residue, producer gas and water gas.

Chem S41 (Practical): Project work

CHEM – S42

Unit 1: Density Functional Theory (DFT)

Definition of electron dencity and functionals, Hohenburg – Kohn theorem (without proof) and importance of theorem.

Chemical application of DFT, density functional definition of chemical potential, global hardness and global softness of Parr and Pearson, Principle of maximum hardness (PMH)- its significance and importance in structural chemistry. The density functional definition of electronegativity, justification of chemical potential, and electronegativityequalisation principle. Application of PMH to the physical process of molecular inversion, internal rotation, isomerisation process and the formation of transition state for chemical reaction.

Unit 2: Solid state II

Diffusion in solids: Atomic approach, bulk diffusion, surface diffusion, grain boundary diffusion. Mechanism of diffusion, equations, temperature dependence of diffusivity, experimental studies.

Ionic drift – ionic conductivity and diffusivity, diffusion controlled reactions.

Metallic solids: Alloy, solid solutions, substitutional alloys, order- disorder phenomenon – super lattice structures, Hume – Rothery rules. Interstitial alloys – general preparative techniques, properties, structure and utilities of refractory carbides, borides and nitrides.

Unit 3: Materials chemistry

Superconductivity and HTSC materials: The superconducting state, effect of magnetic field- Meissner efeect, type –I and type – II superconductors. High temperature superconductivity (HSTC) 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 nano materials. Electronic properties of low dimentional materials. Nano/molecular magnets.

Unit 4: Crystallography II

Geometric data collection with simple examples, structure factor, systematic absence and space groups.

Structure solution: Fourier synthesis, Patterson and direct method.

Unit 5: Magnetochemistry

First order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes in cubic and

axially symmetric crystal fields, low spin – high spin crossover, magnetic behaviour of lanthanides and actinides, magnetic exchange interactions, magnetic materials.

CHEM – S42(Practical)

Analysis of alloys.

CHEM-S43

Unit 1: Stereochemistry-III

Chirooptical properties of organic molecules: Origin, Theory of CD, ORD, their applications, haloketone rules, sector rules, helicity rules, excitation chrality. Chiral analysis by polarimeter, NMR, GC, HPLC and Capillary Electrophoresis (CE) methods, Baldwin's rules.

Unit 2: Asymmetric Synthesis II

Reduction of C=C bonds, carbonyl and imine groups, oxidation: epoxidation, dihydroxylation and amino hydroxylation; Rearrangement: [3, 3]-sigmatropic, (2, 3)-Wittig, alkene isomerization; Hydrolysis and esterification.

Unit 3: Heterocyclic Chemistry-III

Indoles, pyrimidines, pyridazines, pyrazines, purines, pteridines. Role of heterocyclic compounds in biological systems. Application of heterocycles in pharmaceutical and electronic industry.

Unit 4: Organometallic Chemistry of Transitional Elements-II

Applications of organotransition metals in organic synthesis-preparative, structural and mechanistic aspects, Davies rule, catalytic nucleophilic addition and substitution reaction, coupling reaction-Heck, Stille, Suzuki coupling, Zieglar Natta reaction, Olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, functional organometallic compounds, use of indium and zinc.

Unit 5: Supramolecular Chemistry- Basics and Theory:

Basic concepts of supramolecular chemistry, different non-covalent forces (hydrogen bonding, cation-π, CH-π, π-stacking, hydrophobic, hydrophilic interactions etc.) leading to strong bonding of guest molecules to the host, thermodynamics of host-guest complexation, solvent effects and salt effects in complexation, design principle of host or receptor molecules, different experimental techniques to characterize the host – guest complexation, example of molecular receptors: crown ethers, ionophores, cyclophanes, cyclodextrins.

CHEM-S43 (Practical)

Project, Grand Viva

CHEM - S 44

Unit 1: Advanced Quantum Chemistry III

DFT, Hohenberg Kohn theory, Kohn Sham eqns, some theorems, examples of functionals, applications; path integral formalism, formulation & 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 III

Nature of excited state, Jablonski diagram, various processes, fluorescence, quenching, Stern-Volmer plots; single molecule spectroscopy; photoacoustic spectroscopy, applications.

Unit 3: Biophysical Chemistry II

Bioenergetics, ion transport through cell membrane, nerve conduction, muscle contraction & energy generation in mechanochemical systems; thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibria.

Unit 4: Solid State Chemistry III

Property of crystalline materials – electrical properties, conduction, resistance, band gap; magnetic properties, classification, magnetic domains, theory of paramagnetism, ferromagnetism, anti-ferromagnetism, ferrimagnetism, hysteresis; optical properties, reflectance, photoelectrons, photoconduction; superconductors, their properties, BCS theory.

Unit 5: Advanced Polymers II

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

CHEM S 44 (Practical)

One day / two day instrument based / analytical physicochemical experiments / seminar on current topics

CHEM-S45

Unit-1: Forensic analysis

Chemistry of fire, analysis of flammable residues, explosives and their analysis, narcotics and drugs identification, screening and testing.

Unit-2: Bioanalytical chemistry

Trace elements in biological systems, determination of serum electrolytes, blood glucose, cholesterol, uric acid and urea, albumin, globulin, billirubin, analysis of blood for alcohol, mercury, lead and arsenic in urine.

Unit-3: Atmospheric chemistry and ambient air pollution

Composition of atmosphere, heat budget, chemistry of upper atmosphere, source and classification of air pollutants and their effects on human, livestock, vegetation and inanimate objects. Vehicular emission and their control, atmospheric stability and meteorology inversions, transport of air pollutants, air pollution monitoring, abatement and control of air pollution.

Unit-4: Optical methods of analysis

Principles, instrumentation and application of atomic absorption, atomic emission spectroscopy, phosphorescence and fluorescence.

Unit-5: Geochemistry and surface analysis

Redox chemistry and release mechanism of toxic metals in natural system, importance of geochemical environment, surface analysis by spectroscopic methods using electron spectroscopy/ ion spectroscopy/ surface photon spectroscopy/ electron simulated microanalysis/ scanning probe microanalysis.

CHEM – S46

Unit 1: Bioinorganic Chemistry III

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, transferring, siderophores. Role of phosphate in glucose storage.

Unit 2: Bioinorganic Chemistry with chemotherapeutic drug

Copper containing enzymes: Blue and non-blue copper enzymes, ascorbate oxidase, cerulopasmin laccase, tyrosynase, galactose oxidase, super oxide dismutase. Cobalt

containing coenzymes: Vitamin B_{12} and Vitamin B_{12} 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. Photochemical processes: photosubstituional and electron transfer reactions of transition metals. Applications in photochromism and other.

Unit 4: Supramolecular chemistry

Concepts and terminologies, Synthesis and structures of different types of molecular receptors and recognition of cations and anions. Application in analytical techniques.

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-S47

Unit 1: Oxidations in Organic Chemistry

Different oxidative processes based on one-electron and two-electron oxidants, oxidations with Cr(VI) oxidants; Collin oxidation, PCC, PDC and PFC, DMSO-based oxidations: Swern, Moffat, DMSO-SO_3 complex, DMSO-Ac_2O, Hypervalent iodine oxidations: Dess-Martin periodinane, IBX, iodobenzene diacetate, Oxidations with MnO_2, $Tl(NO_3)_3$, Ag_2O, RuO_4 and OsO_4.

Unit 2: **Reductions in Organic Chemistry:**

Different reductive processes, reduction with metal hydrides of B, Al, Sn and Si, catalytic and transfer hydrogenations, dissolving metal reductions, synthetically useful hydrogenolysis reactions, samarium and indium-based reducing agents, enzymatic and microbial reductions.

Unit 3: Medicinal Chemistry-II

Cardiovascular drugs: Introduction, cardiovascular diseases, lipoproteins (LDL, HDL etc.) and their role in atherosclerosis, synthesis and mechanism of action of some cardiovascular and antianginal drugs (Dalvastatin, Fulvustatin, Simvastatin etc. and other nitrate drugs).

Psychoactive drugs-the chemotherapy of mind:

Introduction, CNS depressants, general anesthetics, mode of action of hypnotics, sedatives, anticonvulsants, antianxiety and other psychotic drugs. Synthesis of diazepam, oxazepam, chlorpromazine, Librium, alprazolam, barbiturates etc.

Antineoplastic agents:

Introduction, cancer chemotherapy, special problems, role of alkylating agents, antimetabolites and antibiotics in treatment of cancer and their mechanism of action.

Antihistamines anti-ulcer agents:

Introduction and general mode of action. Synthesis and uses of cimetidine, ranitidine, famotidine, omeprazole, lansoprazole and other new generation drugs.

Local anti-infective drugs: Introduction, general mode of action and synthesis of sulphonamides, chloroquine, pamaquine, mefloquine, albendazole.

Unit 4: Natural Products I

Alkaloids: Structure, transformation and biosynthesis of alkaloids from terrestrial and marine sources; chemistry of quinoline alkaloids with special reference to cinchona group alkaloids; peptide alkaloids.

Unit 5: Carbohydrate Chemistry

Basic structure and type of sugars. Protection and deprotection. Deoxysugars, amino sugars, glycal sugars and their synthetic aspects. Carbohydrates as chiral pools in organic synthesis.

CHEM S 48

Unit 1: Statistical Mechanics III

Structure factor & radial distribution function, eqn of state, relation between potential function & radial distribution function; cluster expansion, PY eqn, HNC & BGY eqns;

Cohen-Turnbull free volume model, configurational entropy model, Macedo Litovitz hybrid model, glass transitions in supercooled liquids

Unit 2: Multiphase materials, Glasses, Ceramics & Composites

Ferrous alloys, Fe-C phase transformations in such alloys, stainless steels; non-ferrous 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, fibre-reinforced and macroscopic composites.

Unit 3: Advanced Polymers III

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: Electrochemistry II

Overpotential, exchange current density, Butler-Volmer and Tafel equations, electrolysis, polarography; photoelectrochemistry – band structure at semiconductor / solution interface, photocathode, photoanode, Schottky barrier, surface states & potential distribution at semiconductor / solution interface, photoelectrocatalysis, photoelectrochemical splitting of water, CO_2 reduction, waste reduction;

Unit 5: 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 – wt loss, electrochemical & Stern Geary method; fuel cells.

CHEM-S49

Unit-1: Hydrosphere chemistry and water pollution

Water resources, point and non point source of pollution, public health significance of heavy metals and pesticides, water pollution monitoring, water pollution laws and standards.

Unit-2: Lithosphere chemistry and soil pollution

Soil composition, role of micro and macro nutrients, determination of soil properties such as pH, conductivity, exchange capacity, moisture, C, N, K and P, cations and anions adsorption in soils, organic pollutants and their soil chemistry, analysis of fertilizers, bio-fertilizers and identification.

Unit-3: Modern techniques in analytical chemistry

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

Unit-4: Toxicology

Fundamentals of toxicology, molecular-cellular aspects of toxicity, toxicokinetics, dose effect and dose response relationship, toxicity and chemical nature, factors determining toxicity of substances.

Unit-5: Industrial operation and green chemistry

Industrial operation and process analyzer, green technology chemistry for industrial waste treatment such as distillery, fertilizers, paper and steel plants.

CHEM S49 (Practical)

Analysis of oil/drugs; Separation techniques: solvent extraction/ion exchange and adsorption chromatography

CHEM – S50

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. hydrocyanation, hydroboration and hydrosilation reactions. Catalytic oxo transfer and oxygenation reactions – Model metal porphyrin complexes as catalyst, Sharpless, Jacobsen and Katsuki catalysts for achiral and chiral catalysis.

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: Application of NMR, Mössbaur and photoelectron spectroscopy

NMR: Theory, chemical shift and spin-spin interations, exchange phenomenon. Contact and pseudo contact shifts, relaxation and types of relaxation. Applications including biological systems. An overview of NMR of metal nuclides.

Mössbaur: Basic principles, spectral parameters and display of spectra. Application of techniques in the studies of

i. Bonding and structure of Fe(II) and Fe(III) compounds including those of intermediate spin.
ii. Sn(II) and Sn(IV) compounds – nature of M-L bonds, coordination number, structure and detection of oxidation states

Photoelectron spectroscopy and its application determining core binding energy.

Unit 4: Electron transfer reactions and twist 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.

Twist mechanism of racemisation, inversion of configuration and associated process, ORD and CD.

Unit 5: Density Functional Theory (DFT)

Difficulties with the traditional methods in electronic structure theory, in particular the Hartree-Fock theory and its descendants. The main objective of DFT to replace the many-body electronic wave functions with the electronic density as the basic quantity.

Electron density: Computation of molecular electron density: Functional.

Hohenberg-Kohn theorems: first theorem and second theorem; their statements, significance and mathematical proof.

Kohn-Sham theory: Statement of Kohn Sham theory. Mathematical formulation and interpretation of terms and recipe for obtaining density and other DFT parameters. The major problem with DFT – the exact functionals for exchange and correlation – the local – density approximation, LDA.

CHEM – S50 (Practical)

Project.

CHEM S51

Unit 1:Supramolecular Chemistry

Applications- Chiral recognition; Self-organization processes – Template association and supramolecular synthesis, Self-replication and autocatalysis; Supramolecular catalysis; Analytical applications- optical devices, electrochemical devices; Molecular switches, Gel, Membrane transport.

Unit 2: Total synthesis of some Naturally Occurring Molecules

Total synthesis of Longifolene, Reserpine, Juvabione, Aphidicolin and Fredericamycin A and prostaglandins (PGE_2, $PGF_{2\alpha}$), Taxol.

Unit 3:Green Chemistry

Green Chemistry-Introduction, Principles, Green synthetic methods, catalytic methods, Organic synthesis in aqueous media, Ionic liquid, super critical fluids, Microwave-induced organic reactions, Real-World cases of Green Chemistry.

Unit 4: Material Chemistry (including nanomaterials)

The nano-world -general definition, philosophy, physico-chemical considerations (band structures, nano effects), nano structure material catalysis reaction, applications of nano-gold, nano-palladium in organic synthesis, fullerenes, carbon nanotubes (synthesis, forms, properties, applications); Introduction to liquid crystals and linear optical properties of organic materials.

Development of problem solving skills - mechanistic, synthetic, stereochemical issues involved in units of organic (specialization) syllabus.

Unit 5: Natural Products-II

Alkaloids: Chemistry of Isoquinoline alkaloids – morphine group, berberine group; alkaloids derived from pyrrolidines and piperidine ring systems. Structure, transformations of yohimbine and reserpine.

CHEM S51 (Practical)

Isolation of naturally occurring compounds and their spectral analysis; Seminar on current topics in Organic Chemistry.

CHEM S 52

Unit 1: Advanced Spectroscopy V

Surface spectroscopy – STM, AFM, SEM, TEM, photoemission from adsorbed species; ion channeling & blocking; RAIRS; instrumentation and applications.

Unit 2: Advanced Materials

Nanomaterials – preparation methods, characterization, theoretical understanding, properties & applications; quantum dots; high Tc superconductors – preparation, properties, theory, applications; organic semi / superconductors, fullerenes, doped fullerenes, nano- & bio-composites; designing new materials with desired properties, models & methods involved, some examples.

Unit 3: 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 4: Surfaces, Thin Films & Clusters

Nature of surfaces, physisorption, chemisorption, catalysis, surface reactions, reconstructions & surface defects; thin films, methods of preparation e.g. evaporation, sputtering, CVD, sol-gel etc.; Langmuir & LB films, photolithography, examples, applications; clusters – preparation methods, beam experiments, magic number & stability, properties, examples, applications.

Unit 5: Biophysical Chemistry III

Ligand binding and multiple equilibria, protein folding; molecular recognition; physical chemistry of drugs & drug action, models of drug action, introduction to pharmacokinetics and pharmacodynamics.

CHEM - 52 (Practical)

Project work / computer practicals