COTTON COLLEGE STATE UNIVERSITY

DEPARTMENT OF CHEMISTRY

Postgraduate Chemistry Syllabus

DISTRIBUTION OF PAPERS/CREDITS (L+T+P format)

Semester – I

Paper Code	Paper Name	Credits
CHM 701C	Physical Chemistry – 1	3 + 1 + 0
CHM 702C	Organic Chemistry – 1	3 + 1 + 0
CHM 703C	Inorganic Chemistry – 1	3 + 1 + 0
CHM 704C	Laboratory Course (Organic Chemistry)	0 + 0 + 4
	Elective Paper (to be selected from list given here)	2 + 1 + 0

Semester – II

Paper Code	Paper Name	Credits
CHM 801C	Physical Chemistry – 2	3 + 1 + 0
CHM 802C	Organic Chemistry – 2	3 + 1 + 0
CHM 803C	Inorganic Chemistry – 2	3 + 1 + 0
CHM 804C	Laboratory Course (Inorganic Chemistry)	0 + 0 + 4
CHM 805C	Computer in Chemistry	2 + 1 + 0

Semester – III

Paper Code	Paper Name	Credits
CHM 901C	Environmental & Analytical Chemistry	3 + 1 + 0
CHM 902C	Molecular Spectroscopy- 1	3 + 1 + 0
CHM 903C	Molecular Spectroscopy- 2	3 + 1 + 0
CHM 904C	Laboratory Course (Physical Chemistry)	0 + 0 + 4
	Elective Paper (to be selected from the list given here)	2 + 1 + 0

Semester - IV

Physical Chemistry Special:

Paper Code	Paper Name	Credits
CHM 1001C	Advanced Quantum Chemistry	3 + 1 + 0
CHM 1002C	Chemical Kinetics & Electrochemistry	3 + 1 + 0
CHM 1003C	Heterogeneous Catalysis	3 + 1 + 0
CHM 1004C	Laboratory Course (Advanced Physical Chemistry Practical)/ Project Work/ Term paper	0 + 0 + 4
	Elective Paper (to be chosen from the list given here)	2 + 1 + 0

Organic Chemistry Special:

Paper Code	Paper Name	Credits
CHM 1031C	Natural Products Chemistry	3 + 1 + 0
CHM 1032C	Organic Synthesis	3 + 1 + 0
CHM 1033C	Bioorganic & Medicinal Chemistry	3 + 1 + 0
CHM 1034C	Laboratory Course (Advanced Organic Chemistry Practical)/ Project Work/ Term paper	0 + 0 + 4
	Elective Paper (to be chosen from the list given here)	2 + 1 + 0

Inorganic Chemistry Special:

Paper Code	Paper Name	Credits
CHM 1061C	Materials Chemistry	3 + 1 + 0
CHM 1062C	Bio-Inorganic Chemistry	3 + 1 + 0
CHM 1063C	Organometallic Chemistry & Catalysts	3 + 1 + 0
CHM 1064C	Laboratory Course (Advanced Inorganic Chemistry Practical)/ Project Work/ Term paper	0 + 0 + 4
	Elective Paper (to be chosen from the list given here)	2 + 1 + 0

SEMESTER-I

Paper : CHM 701C

PHYSICAL CHEMISTRY – 1

Credits: 4 (3+1+0)

Unit 1: Thermodynamics

(a) Non-ideal systems: Fugacity coefficients and activity coefficients– different scales of activity coefficients.
(b) Phase equilibrium: Gibbs phase rule and its application to three component systems – triangular plots – water-acetic acid chloroform and ammonium chloride-ammonium sulphate water system.
(c) Non-equilibrium thermodynamics: Review of basic concepts of force, flow and entropy production. Coupled forces and flows and phenomenological relations; Onsager reciprocal relations. Thermoelectric effects – Seebeck, Peltier and Thomson effects.
(d) Statistical thermodynamics: Calculation of partition functions, thermodynamic function, principles of equipartition, heat capacities (Einstein model and Debye modification), residual entropy, equilibrium constant.

Unit 2: Dynamic electro-chemistry

(a) Ion-solvent interactions: The Born model-thermodynamic parameters of ion-solvent interactions -structural treatment; the ion-dipole model – its modifications, ion-quadrupole and ion-induced dipole interactions.
(b) Primary solution – determination of hydration number, compressibility method and viscosity-mobility method.
(c) Debye-Húckel theory of ion-ion interactions – derivation, validity and limitations; extended Debye-Húckel-Onsager equation.
(d) The random walk model of ionic diffusion - Einstein-Smoluchowski relation.

Unit 3: Basic principles of quantum mechanics

(a) Wave functions of one-particle and many-particles system; Born interpretation. Well-behaved functions and normalized functions. Schwartz inequality (without derivation).
(b) Dynamic variables and quantum mechanical operators – Hermitian operators and their properties.
(c) Eigenvalues and eigenfunctions of quantum mechanical operators, their physical significance. Schródinger's wave equation. Orthogonal functions – Schmidt's orthogonalisation technique.
(d) Expectation values of observable properties. Compatible observables and compatibility theorem. Incompatible observables and the (generalized) uncertainty principle from Schwartz inequality.
(e) Basic ideas about the theory of angular momenta – spin and orbital angular momenta, conservation of angular momenta. General angular momentum operators J_x, J_y, J_z step-up and step-down operators, Eigenvalues of J^2 and J_z operators. Coupling of orbital and spin angular momenta – theoretical basis of the L-S and j-j coupling schemes.

Unit 4: Exactly solvable problems in quantum mechanics

Solutions of the energy eigenvalue equations for:
(a) Problem of two interacting particles – separation of center of mass and relative motion.
(b) Linear harmonic oscillator, vibrational energy levels of diatomic molecules.
(c) Particles in a ring. Free electron MO theory of benzene.
(d) Rectangular potential problems. Quantum mechanical tunneling.
(e) The two-particle rigid rotor problem, rotational energy levels of a diatomic molecule.

(f) The hydrogen atom. Radial solution-radial probability distribution function. Angular solutions, representation of orbitals.

SEMESTER-I

Paper : CHM 702C

ORGANIC CHEMISTRY - 1

Credits: 4 (3+1+0)

Unit 1: Aromaticity and stereoelectronic factors

Aromaticity and antiaromaticity – nonclassical concepts should be emphasized. HSAB concepts and their applications; symbiosis.

Stereoelectronic effects on reactivity – effect through bonds, through space; conformation and reactivity.

Unit 2: Stereochemistry

Brief overview of the following:

Designation of configuration; Fischer- Sawhorse-Newman interconversion. Molecular symmetry, asymmetry and dissymmetry; classification of organic molecules into different Point Groups; concept of stereogenic center – chirotopic and achirotopic center; homotopic and heterotopic ligands and faces (prostereoisomerism and prochirality etc); optical purity and enantiomeric excess; meaning of absolute and relative configuration; chirality in molecules devoid of chiral centers- allenes, spiranes andbiphenyls. Conformation of cyclohexane and decalins.

Unit 3: Reactivity and selectivity principles

Reactivity-selectivity principle – chemoselectivity, regioselectivity, stereoselectivity & stereospecificity in substitution, elimination and addition reactions; steric accelearation and steric retardation.

Unit 4: Reaction mechanism

Kinetic and non-kinetic methods; kinetic isotope effects and isotope labelling studies; significance of rate limiting step in multi-step reactions; from rate law to mechanism and from mechanism to rate law. Hammett & Taft equation; partial rate factor. Cross-over experiment.

SEMESTER-I

Paper : CHM 703C

INORGANIC CHEMISTRY - 1

Credits: 4 (3+1+0)

Unit 1: Chemical bonding

Chemical bonding of simple inorganic covalent compounds- molecular orbital treatments, hybridization; understanding molecular properties from bonding. Molecular orbital theory of homo and heteronuclear diatomics, molecular orbitals of polyatomic molecules, molecular shape in terms of molecular orbitals – Walsh diagrams.

Atomic and ionic radii- bond length and bond strength, van der Waals forces. Hydrogen bonding interactions. Effect of hydrogen bonding and other chemical forces on melting and boiling points and solubility.

Unit 2: Structure of simple solids

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

Unit 3: Acid base

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

Unit 4: Redox chemistry

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

SEMESTER – I

LABORATORY COURSE: CHM 704C

(ORGANIC CHEMISTRY)

Credits: 4 (0+0+4)

A student should do experiments from each unit. End-semester examination will be of 12 hours duration extending over 2 (two) days. There should be at least one experiment from each unit. Number of experiments to be conducted in the end-semester examination will be decided by the examiners. Internal evaluation will have a weightage of 40 per cent.

A. Qualitative organic analysis

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

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

B. Organic estimation

i. Glycine by sodium hydroxide in the presence of formaldehyde
ii. Number of hydroxy groups in a disaccharide by acetylation
iii. Percentage purity of carbonyl compounds by 2, 4-dinitrophenylhydrazine
iv. Carboxylic acid by Ag-salt method
v. Glucose & sucrose in a mixture

C. Chromatographic application

i. Separation and identification of aromatic nitro compounds present in a binary mixture by TLC
ii. Separation and identification of aminoacids present in a ternary mixture by paper chromatography

D. Organic preparation: Two-step preparation

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

ELECTIVE PAPER
Credits: 3 (2+1+0)

One topic to be chosen from the list of Elective Papers given at the end of Semester- IV syllabus.

SEMESTER-II
Paper : CHM 801C

PHYSICAL CHEMISTRY - 2
Credits: 4 (3+1+0)

Unit 1: Chemical kinetics

Steady-state approximation and its applications. Oscillating reactions, chemical chaos. Belousov-Zhabotinski reaction. Chain reaction – alkane pyrolysis. Branching-chain reactions – the hydrogen-oxygen reaction, explosion limits. The transition state theory (TST) of bimolecular gaseous reactions, statistical thermodynamic formulations. Comparison between TST and hard-sphere collision theory.

Unit 2: Homogeneous catalysis

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

Unit 3: Adsorption on solid surfaces

Adsorption of gases on solid surfaces – Langmuir's theory and its limitations. Derivation of BET equation – determination of surface area of an adsorbent, thermodynamics of adsorption processes. Capillary condensation – adsorption in micro pores, hysteresis loop. Kinetics of heterogeneous catalysis – Langmuir-Hinselwood model and Riedel-Eley model, electrokinetic phenomena at the interface – electrical double layer.

Unit 4: Polymer science

Polymer and polymerization – natural and synthetic polymers- molecular weights, control of molecular mass. Technological applications of polymers. Frictional properties of macromolecules (polymers) in solution, the concept of free draining, equivalent sphere model. Chain configuration of macromolecules- root mean square end to end distance and radius of gyration; random flight model and chain stiffness, average dimension of polymer chains.
Kinetics of step polymerization and copolymerization – ring-scission polymerization.

SEMESTER-II

Paper : CHM 802C

ORGANIC CHEMISTRY - 2

Credits: 4 (3+1+0)

Unit 1: Stereodifferenting reactions

General aspects of stereoselective synthesis, enantiodifferenting reactions, diastereodifferenting reactions. Applications of Cram's, Ahn-Felkin and prelogs rule in strereodifferenting reactions. Use of chiral reagents, chiral catalyst and chiral auxilliaries in organic synthesis. Double stereodifferentation.

Unit 2: Oxidation reactions

Allylic oxidation of alkenes- use of chromium trioxide-pyridine complex (Collin's reagent) and selenium dioxide.

Oxidation of alcohols- use of PCC, PDC, DCC oxidation, Swern oxidation, tetrapropylammonium perruthenate (VII). Mn (IV) oxide, silver carbonate.

Oxidation of carbon-carbon double bonds- Sharpless dihydroxylation & epoxidation, oxidation with iodine; introduction to electrooxidation – oxidation of tertiary amines and carboxylates. Oxidation by potassium permanganate, osmium tetroxide and per acids.

Unit 3: Reduction reactions

Use of H_2/Pd-C, LAH, $NaBH_4$, $NaCNBH_3$, 9-BBN, Lindlar catalyst, DIBAL, diimide, super hydride and selectrides; introduction to electroreduction- reduction of carbonyl compounds, alkyl halides and nitro compounds.

Unit 4: Pericyclic reactions and photochemistry

Cycloaddition reactions - |2+2|, |4+2|, |6+2| cycloadditions, stereoselectivity of the reactions, Sigmatropic rearrangement – fluxional molecules, stereoselectivity in Cope and Claisen rearrangement.

Photochemistry of alkenes, dienes and Aromatic compounds; Cis-transisomerization, photodimerization, Paterno Buchi reactions.

SEMESTER-II

Paper : CHM 803C

INORGANIC CHEMISTRY - 2

Credits: 4 (3+1+0)

Unit 1: Coordination Chemistry

Crystal field theory of bonding in octahedral, tetrahedral and square planar transition metal complexes. Factors affecting crystal field splitting, crystal field stabilization energy, spectrochemical series. Ligand field theory of metal complexes-electronic spectra – *d-d,* spectra interpretation of spectral behaviour of octahedral and tetrahedral complexes. Charge transfer spectra.

Unit 2: Complexes of *Л* – acceptor ligands

Metal carbonyl hydrides and metal carbonyl clusters. Metal-metal bonding in $Re_2Cl_8^{2-}$. Complexes

containing alkenes and alkynes as ligands. Ferrocene-synthesis, structure, bonding and reactivity.

Unit 3: Reactivity of complexes.

Stability constants, the chelate effect, labile and inert complexes, mechanism of substitution reactions in octohedral complexes and associated stereochemical changes, isomerisation and racemisation of tris-chelate complexes. The trans effect. Electron transfer reactions- outer and inner sphere mechanism.

Unit 4: Chemistry of lanthanides and actinides

Important aspects of the chemistry of the lanthanides- oxidation states, lanthanide contraction, separation of lanthanide elements, lanthanide shift reagents. Chemistry of actinides- electronic configurations, oxidation states, sources of the actinide elements, their extraction and application. Radioactivity of actinides.

SEMESTER – II

LABORATORY COURSE: CHM 804C

(INORGANIC CHEMISTRY)

Credits: 4 (0+0+4)

A student should do experiments from each unit. End-semester examination will be of 12 hours duration extending over 2 (two) days. There should be at least one experiment from each unit. Number of experiments to be conducted in the end-semester examination will be decided by the examiners. Internal assessment will have a weightage of 40 per cent.

A. Qualitative and quantitative analysis

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

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

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

Alloys: Brass, Gunmetal, Cupronickel, Solder, Bronze, Phosphor Bronze, Steel, Copper concentrate, other alloys

(c) Determination of hardness of water

B. Preparation and characterization

Preparation of selected inorganic compounds and their physico-chemical characterization by elemental analysis, IR and electronic spectrophotometry, magnetic susceptibility measurements, magnetic resonance spectroscopy, solution conductivity measurements, wherever appropriate and possible.

SEMESTER-II

Paper : CHM 805C

COMPUTERS IN CHEMISTRY

Credits: 3 (2+1+0)

Unit 1: Introduction to computers

The components of a computer, Central Processing Unit, Secondary Storage Devices (magnetic disks, FD, HD, CD), Input and Output Devices, Hardware and Software Types of Computers, The Personal Computer.

Programming languages- Algorithms, flow charts and Computer Programs. An example: Program to reverse a four-digit number 1234 to 4321. Windows Operating System, Software Packages in Windows and their use.

Unit 2: Principles of FORTRAN and BASIC programming

Elements of FORTRAN and BASIC languages, constants and variables, expressions, operations and symbols, common mathematical functions, arithmetic expressions and assignment statements, input and output statements, Format statement, Termination statement, GO TO, Arithmetic IF and Logical IF statements, Complex and Logical Variables, Subscripted Variables and DIMENSION and DO statements, Subprograms, Functions and Subroutines, Arraying and Dimensioning, EQUIVALENCE, COMMON and DATA statements.

Unit 3: Computer applications in chemistry

(a) **Applications in Chemistry- I**

Solution of simultaneous equations with examples from chemistry, solution of quadratic equations with examples from chemistry, Least squares method of fitting data to a straight line, applications of programming for Huckel Molecular Orbital calculations, calculation of delocalization energy of an aromatic system.

(b) **Applications in Chemistry- II**

Computer program for calculation of rate constants of reactions from concentration vs. time data. Calculation of concentration of a [Fe(II)- phenantroline] complex from absorbance data for calculation of wavelength maxima of conjugated dienes. Plotting of data of an experiment (eg., first order kinetics, spectra at different concentrations), data-fitting and evaluation of the parameters (eg., rate constants, extinction coefficient). Learning to use MOPAC and CHEMDRAW for chemical applications. Drawing of molecular and crystal structure- practical work. Practical work- using the internet for chemical information retrieval.

SEMESTER – III

Paper code: CHM 901C

ENVIRONMENTAL AND ANALYTICAL CHEMISTRY

Credits: 4 (3+1+0)

Unit 1: Environmental chemistry: Global perspective

Introduction to environmental chemistry, chemical processes in the environment, water cycle and its implications, water resource flux, case histories of environmental disasters and accidents; Green chemistry concepts.

Unit 2: Atmospheric chemistry

Temperature and pressure variations in the atmosphere, chemical composition of the atmosphere and the influence of solar radiations; thermodynamic, kinetic and photochemical considerations; role of free radicals in atmospheric chemistry.

Chemistry of the stratosphere; role of UV-radiations in production and destruction of ozone; catalytic decomposition processes with special reference to the role of NO, OH and ClO radicals; anthropogenic sources of Cl; formation of Antarctic and Arctic ozone holes.

Smog formation, chemical species in smog; VOCs and their oxidation; emissions from 2-stroke and 4-stroke gasoline engines, emission from diesel engines, CNG and other alternative fuels; production of ozone in the lower atmosphere and its impact.

Nitrogen and Sulphur species present in the atmosphere and their sources; production of nitric and sulphuric acids in the atmosphere; acidifying agents in rain, fog and snow; control of anthropogenic nitrogen and sulphur emissions- fluidized bed combustion, desulphurisation, SONOX process; conversion of coal to liquid and gaseous fuels.

Aerosol chemistry; polyaromatic hydrocarbons (PAHs) and heavy metal in aerosols; condensation aerosols; the Arctic haze; lifetime and transport of aerosol particles.

Pollutants in the urban atmosphere; indoor air pollution; radioactivity and radon pollution.

Energy balance of the earth in terms of black body radiation; greenhouse gases and their generation from various sources; the global warming potential.

Unit 3: Hydrosphere chemistry

Distribution of chemical species in water; the Phosphorous and Sulphur systems; gases in water; alkalinity; organic matter in water, humic matter in water- origin, formation and environmental role.

Environmental classification of metals in water; behaviour of Calcium, Copper and Mercury in the hydrosphere; formation of complexes between metals and anthropogenic pollutants in water. Partitioning of small organic molecules between water and soil or sediment; sorption organic species by soil; octanol-water partition coefficient; role of clay minerals in the environment.

Wastewater treatment processes; use of chemical coagulants; treatment of water containing excessive iron, phosphate, nitrate and flouride.

Unit 4: Soil chemistry

Composition of soil; chemical weathering; physical properties of soil- particle size, texture, bulk density, permeability. Chemical properties- Cation exchange capacity, pH, macro and micro nutrients, Leachate formation.

Wastes from mining and metal production; Acid mine drainage; sewage sludge, biogas synthesis, hazardous wastes and their disposal, incineration.

Pesticides and their role in the environment, DDT and its fate in the environment.

Unit 5: Analytical techniques

Analysis of common ions – ultraviolet and visible spectrometry, emission spectrometry, ion chromatography.

Preparation of sample for trace metal analysis in water, air, soil and plants; extraction and dissolution technique, microwave digestion; chemical separation technique.

Analysis of metal ions- atomic absorption spectrometry, anodic stripping voltammetry, inductively coupled plasma mass emission spectrometry, neutron activation analysis.

Analysis of trace organics with particular reference to phenolic compounds; PCBs and PAHs- extraction techniques for chromatographic analysis; gas chromatography, HPLC, GC-MS; immunoassay technique.

Sampling and analysis of PM10 and gases in air.

SEMESTER – III

Paper code: CHM 902C

MOLECULAR SPECTROSCOPY – I

Credits: 4 (3+1+0)

Unit 1: Introduction

Electromagnetic spectrum, interaction of electromagnetic radiation with molecular systems; Spectroscopic transition- absorption, emission, reflection, polarization and scattering processes; Natural line width and broadening- intensity of spectral transitions, selection rules; sampling techniques in different branches of spectroscopy.

Unit 2: Electronic spectroscopy

Electronic transitions, the Frank-Condon principle, ground and first excites states of diatomic molecules, selection rules on the basis of the symmetry properties of the electronic states; Vibronic transitions; flourescence and phosphorescence, laser action; electronic spectra of conjugated, aromatic and coordination compounds- *d-d* and charge-transfer spectra; change of molecular shape upon electronic excitation.

Unit 3: Rotational (microwave) spectroscopy

(a) Classification of molecules according to their moments of inertia; rotational energy levels of HCl. Determination of molecular geometry by isotopic substitution effects on pure rotational spectrum; Stark effect, estimation of molecular dipole moments; spectra of symmetric top and asymmetric top type molecules.

(b) Rotational Raman spectra- anisotropic polarisability. Specific selection rule in Raman spectroscopy; Stokes and anti-Stokes lines.

Unit 4: Vibrational rotational spectroscopy

(a) Diatomic molecules- force constants; fundamental vibration frequencies; the unharmonicity of molecular vibrations and its effect on vibrational frequencies, second and harmonics.

(b) Vibration-rotation spectrum of HCl – P, Q and R branches; vibrational Raman spectra of diatomic molecules.

(c) Polyatomic molecules (e.g. CO_2, NH_3)- normal modes vibrations, symmetry of vibrations- group theoretical treatment; elements of normal coordinate analysis for CO_2 molecule.

Unit 5: Mass spectroscopy

Mass spectroscopy: Ion fragmentation mechanism; base peak and molecular ion peak; nominal mass and exact mass; isotopic distribution-problems.

Unit 6: NMR spectroscopy

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

Unit 7: UV-visible and IR spectroscopy

λ_{max} and molar absorptivity, factors affecting them; calculation of λ_{max} – Woodward Fieser's rules.

IR spectroscopy: Characteristics bands for different functional groups; change in band frequency due to FGI; effects of hydrogen bonding on band frequency-problems.

SEMESTER – III

Paper code: CHM 903C

MOLECULAR SPECTROSCOPY – II

Credits: 4 (3+1+0)

Unit 1: Vibrational and electronic spectroscopy in Inorganic chemistry

(a) Symmetry criteria for intensity of spectroscopic transitions (qualitative treatment); symmetry and spectral changes upon coordination.

Infrared and Raman spectroscopy: Symmetry and IR/Raman activity of normal modes of vibrations; mutual exclusion principle; interpretation of IR and Raman spectra of simple inorganic and coordination compounds.

(b) Study of metal- ligand equilibria and Job's method, CD, ORD and MCD of inorganic compounds.

(c) Photoelectron spectroscopy: Basic principles and applications of PES (O_2, N_2 and N_3) only; chemical information from ESCA.

Unit 2: ESR, NMR and Mossbauer spectroscopy

(a) ESR spectroscopy: Basic principles, factors effecting g-tensors, hyperfine splitting in inorganic free radicals and metal complexes, zero field splitting; application of ESR to d^1 and d^9 complexes of various symmetry.

(b) NMR spectroscopy: Simple application to diamagnetic inorganic compounds; NMR paramagnetic shifts, simple application to paramagnetic compounds; NMR of ^{31}P and ^{19}F in inorganic compounds.

(c) Mossbauer: Basic principles, isomer shift, quadrupole splitting, and effect of magnetic field. Application to the study of high-spin and low-spin iron compounds,

and of Sn compounds in various oxidation states and coordination geometries.

Unit 3: Electrochemical, Thermal and X-ray diffraction methods

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

(b) Thermal methods: Principles and applications of thermogravimetry, DTA, TGA and DSC of inorganic compounds.

(c) X-ray diffraction: Crystal symmetry, Space groups, Bragg condition, Miller indices, Luae and Bragg methods, Debye and Scherrer method of X-ray structural analysis of crystals; reflection indexing, identification of unit cells from systematic absence in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem; description of the procedure for X-ray structure analysis of small molecules.

Unit 4: Chiroptical properties

Introduction to CD (Circular Dichroism), ORD (Optical Rotatory Dispersion) and CPE; applications of CD and ORD- octant rule.

SEMESTER – III

Paper code: CHM 904C

LABORATORY COURSE

(PHYSICAL CHEMISTRY)

Credits: 4 (0+0+4)

The students should complete 14 experiments, 7 instrumental and 7 non-instrumental. In the end-semester examination, students are to perform 2 experiments. The examination will be of 12 hours duration, extending 2 days. New experiments may be added from time to time.

Unit 1: Chemical kinetics

(a) Determine the temperature coefficient and energy of activation of acid hydrolysis of methyl acetate, using least-square calculation.
(b) Study the kinetics of the reaction between iodine and acetone in acidic medium by half-life period method and determine the order with respect to iodine and acetone.
(c) Determine the inversion of sucrose in presence of two acids polarimetrically using Guggenheim plots and hence determine the relative strengths of the acids.
(d) Study the saponification of ethyl acetate by sodium hydroxide and determine the order of the reaction and energy of activation.
(e) Study the autocatalytic reaction between oxalic acid and $KMnO_4$ and determine the order of the reaction.
(f) Study the mutarotation of glucose in presence of acid and base by polarimetric method. Investigate the influence of acid and base strength on the rate of reaction.
(g) Study the decomposition kinetics of the formation of complex between sodium sulphide and sodium nitroprusside spectrophotometrically. Determine the rate constant and order of reaction.
(h) Study the kinetics of the reaction between peroxydisulphate and potassium iodide and find the influence of ionic strength on the rate constant.
(i) Study the kinetics of the oxidation of ethanol by chromium (VI) and find the rate constant of the reaction. Also find the order of the reaction by half-life period method.

(j) Establish the order of reaction

$$K_2C_2O_4 + 2HgCl_2 \longrightarrow Hg_2Cl_2 + 2KCl + CO_2$$

by the method of ratio variation.

Unit 2: Conductometry

(a) Determine the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and hence find the degree of dissociation of the acid.

(b) Compare the relative strength of acetic acid and monochloroacetic acid by conductance measurement.

(c) Determine the solubility and the solubility product of a sparingly soluble salt like $PbSO_4$ or PBI_2 at room temperature by conductance measurement.

(d) Determine the degree of hydrolysis and the hydrolysis constant of aniline hydrochloride/sodium acetate.

(e) Determine the strength of the components of the following mixtures by conductometric titration.
(a) Hydrochloric acid and acetic acid.
(b) Sulphuric acid and copper sulphate.
(c) Hydrochloric acid and potassium chloride.

Unit 3: *pH*-metry and potentiometry

(a) Determine the dissociation constant of acetic acid/ oxalic acid by Albert-Serheart method, using Hendersen's equation.

(b) Find the amount of the components of the following mixtures using pH - metric titration-
i. Hydrochloric acid + acetic acid
ii. Hydrochloric acid + oxalic acid
iii. Potassium chloride + potassium bromide + potassium iodide

(c) Determine the apparent ionization constant of acetic acid by potentiometric titration of the acid against sodium hydroxide using quinhydrone electrode.

(d) Potentiometrically estimate strengths of solution of hydrochloric acid and acetic acid individually and a mixture of the two using standard sodium hydroxide solution.

(e) Titrate potentiometrically ferrous ammonium sulphate against potassium dichromate and determine the standard electrode potential of the ferrous/ferric system.

Unit 4: Spectrophotometry and refractometry

(a) Verify Beer's law and determine the concentration of solutions like $KMnO_4$ / $K_2Cr_2O_7$ / $CuSO_4$

(b) Determine the concentration of Chromium and Manganese in a mixture of dichromate and permanganate by spectrophotometric method.

(c) Determine the composition of iron-salicyclic acid complex spectrophotometrically by Job's method of continuous variation.

(d) Determine the refractive index of a liquid like carbon tetrachloride and hence find the radius of its molecule.

(e) Verify the mixture law refraction and draw the calibration curve for mixtures like glycerol/water, n-heptane/ n-hexane. Hence determine the composition of an unknown mixture of two components.

Unit 5: Miscellaneous experiments

(a) Determine the molar mass of a polymer by viscometric method.

(b) Study the variation of surface tension of a solution of n-propyl alcohol/ ethanol with concentration and determine the limiting cross-sectional area of the alcohol molecule.
(c) Determine the partial molar volume of methanol/ethanol/ formic acid by graphical method by determining the densities of solutions at different concentrations.
(d) Determine the influence of NaCl, naphthalene and succinic acid on the critical solution temperature of phenol-water system using 0.5, 1 and 1.5% concentrations.
(e) Study the complex formation between Cu2+ ion and ammonia by distribution method and find the composition of the complex.
(f) Perform theoretical calculations using a computer on-
(a) Least squares fitting and plotting linear and exponential graphs.
(b) Charge density distribution and shapes of *s* and *p* orbitals.
(c) Potential energy diagram of hydrogen molecule ion.

ELECTIVE PAPER
Credits: 3 (2+1+0)

One topic to be chosen by the Department from the list of Elective Papers given at the end of Semester- IV syllabus.

SEMESTER – IV

PHYSICAL CHEMISTRY SPECIAL GROUP

Physical special paper: CHM 1001C

ADVANCED QUANTUM CHEMISTRY
Credits: 4 (3+1+0)

Unit 1: Approximate methods of quantum mechanics

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

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

Unit 2: Electronic structure of Many-electron atoms

Product wave functions- complete many-electron wave functions including electron spin. Pauli's anti-symmetry and exclusion principles. Spin states of a two-electron system- singlet and triplet states.
Independent particle central field model of many-electron atoms- the helium atom. Atomic orbital theory- Slater type orbitals (STO); electron repulsion parameters (Racah and Condon-Shortly types). Spectroscopic term symbols for the s^1p^1, p^2 and d^2 configurations- splitting of term energies due to electron repulsion and magnetic effects- spin orbit coupling and Zeeman splitting.

Unit 3: General theorems in molecular quantum mechanics

(a) Born-Oppenheimer approximation, separation of electronic and nuclear motion.
(b) Hellmann-Feynman theorem and its chemical applications. The electrostatic theorem and the force

field concept in chemistry.

(c) Introduction to the molecular electronic virial theorem.

Unit 4: Semi-Empirical Theories

Huckel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MOPAC and AMI.

Unit 5: Density Functional Theory

Derivation of Hohenberg-Kohn theorem, Kohn-Sham formulation, N- and V-representabilities; review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory.

Physical special paper: CHM 1002C

CHEMICAL KINETICS AND ELECTROCHEMISTRY

Credits: 4 (3+1+0)

Unit 1: Chemical kinetics

(a) Study of fast reactions

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

(b) Theories of unimolecular reactions and reactions in solution

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

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

Unit 2: Photochemical reactions

(a) Photochemical reactions

Photophysical kinetics- state energy diagrams. Delayed fluorescence- the mechanism and kinetics of fluorescence quenching – Stern-Volmer equation.

(b) Chemical kinetics in the elucidation of reaction mechanism

Organic reactions: hydrolysis of lactones and aldol condensation.

Inorganic reactions: Thermal decomposition of nitrogen pentoxide- ligand replacement reactions of octahedral complexes.

Unit 3: Electrochemistry-I

Theories of electrical interface

Electrocapillary phenomena- Lippmann equation. Electron transfer at interfaces- polarisable and non-polarisable interfaces, Butler-Volmer equation, Tafel Plots.

Unit 4: Electrochemistry-II

Electrochemical methods used in electrode kinetics

Polarography- rotating disc electrode (RDE) – chronopotentiometric method, elucidation of mechanism of multi-step electrode reactions. Electrodeposition on metals, convective diffusion-

applications in electrode processes.

Physical special paper: CHM 1003C

HETEROGENEOUS CATALYSIS

Credits: 4 (3+1+0)

Unit 1: Kinetics of heterogeneous catalysis

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

Kinetics of heterogeneous catalysis, effect of temperature on rates of catalysed reactions, Langmuir, Hinselwood and Eley Redial models, mass transport limitation of catalysed reactions. Surface dependence of reaction rates, volcano principles.

Unit 2: Preparation and characterization of industrial catalysts

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

Electron microscopy, XPS and PES, ESCA, IR and magnetic resonance spectroscopy, temperature programmed desorption (TDP), and DTA and TGA.

Unit 3: Zeolite and clays

Zeolites (natural and systhetic)- shape selectivity properties- solid acids, acidity of zeolites and clays. Mesoporous materials, poorly crystalline silicates and aluminosilicates- MCM-41 type materials.

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

Unit 4: Catalysis in petroleum industry and environmental catalysts

Hydrodesulphurization, synthetic gas and production of chemicals from it. Bifunctional catalysts. Non-selective oxidation of hydrocarbon compounds. Manufacture and transformation of hydrocarbons- hydrogenation and isomerization. Catalytic deactivation and reactivation, control of pollution from automobile exhaust, catalytic converters. Abatement of nitrogen oxides and odours, cleaning of industrial effluents.

Physical special paper: CHM 1004C

LAB COURSE (ADVANCED PHYSICAL CHEMISTRY PRACTICAL & LITERATURE SURVEY)

Credits: 4 (0+0+4)

The students should perform at least 12 experiments, at least 3 experiments from each unit. Students are required to perform 3 experiments in the end-semester examination. The examination will be of 18 hours duration over 3 days.

Students will also be required to carry out a literature survey on a certain topic which must be presented in writing and orally in the end-semester examination.

Internal evaluation will have a weightage of 40 per cent.

Unit 1: Conductometry, Potentiometry and polarography

(a) Study the variation of solubility of potassium hydrogen tartrate (or any such sparingly soluble salt) / $Ca(IO_3)_2$ with ionic strength using solution of KCl at room temperature conductometrically. Hence determine the ionic activity coefficient.

(b) Determine the amount of each component of the following ternary mixture by conductometric titration.
(a) Hydrochloric acid, acetic acid and copper sulphate
(b) Hydrochloric acid, sodium chloride and ammonium chloride.

(c) Determine the basicity of a polybasic acid by potentiometric titration using NaOH solution and find out the dissociation constants.

(d) Study the thermodynamics of a Galvanic cell and determine ΔG, ΔS, and ΔH of a suitable reaction.

(e) Determine the transport number of Ag^+ and NO_3^- ions (or H^+ in HCl) by measuring emf of concentration cells with or without transference.

(f) Determine the instability constant of silver-ammonia complex and the stoichiometry of the complex potentiometrically.

(g) Determine the half-wave potential of Cadmium (II) ion in 1M potassium chloride solution and estimate the amount of cadmium ion in unknown solution containing 1M KCl.

(h) Determine the composition and stability constant of a metal complex like copper glycine/ lead oxalate.

Unit 2: Spectrophotometry, Computational analysis

(a) Determine the composition of iron-thiocyanate complex spectrophotometrically and hence find the stability constant of the complex at ionic strength of 1M.

(b) Study the kinetics of the reduction of methyl orange with stannous chloride catalysed by Cl^- ion spectrophotometrically under the following conditions:
(i) reaction pseudo first order with respect to methyl orange,
(ii) dependence of rate on Sn^{2+} ion concentration,
(iii) dependence of rate on Cl^- concentration.

(c) Determine spectrophotometrically the indicator constant of an indicator, (e.g. methyl red).

(d) Determine the composition of Cu (II) and Fe (III) in a mixed solution by spectrophotometric titration using EDTA.

(e) Rotational probability distribution for HCl at two different temperatures, comparision of its rotational partition function by direct calculations and by simple formula $q = T/\theta_{rot}$.

(f) (i) Drawing a moderately complex molecule (e.g. aniline/ pyridine/ furan/ ethylene diamine) using PC model, and obtaining its nuclear framework Z-matrix in usual MOPAC form.
(ii) Conversion of this Z-matrix to Cartesian coordinate from using MOPAC.

(g) Plots for Maxwell's speed distribution formula in speed and translational energy form, and calculation of the fraction of molecules in a given speed range by numerical integration.

(h) Justification of Job's method of continuous variation for determination of the formula of a complex using the ferric-thiocyanate complex example.

(i) Iterative evaluation of the Wein's displacement law constant b for a Black Body.

Unit 3: Miscellaneous experiments

(a) Study the ternary system of acetic acid-chloroform-water at room temperature and construct the phase diagram.

(b) Determine the apparent molar mass of a non-volatile solute like benzoic acid in benzene and find its degree of association by cryoscopic method.

(c) Study the following equilibrium: $I_2 + I^- \rightarrow I_3^-$ determine the value of the equilibrium constant of the reaction by distribution method.

(d) Compare the cleansing power of different samples (at least four) of soaps and detergents by surface tension measurement.

(e) Determine the transport number of Ag^+ and NO_3^-, or $Cu2^+$ and SO_4^{2-} ions by Hittorf's method. Or

determine the transport numbers of H^+ and Cl^- ions in HCl by the moving boundary method.

(f) Study the kinetic of decomposition of benzene diazonium chloride, determine the rate constant of the reaction at different temperatures and hence determine the activation energy of the reaction.
(g) Study the salt effect and the solvent effect on the rate law of alkaline hydrolysis of crystal violet.
(h) Determine the percentage of polymerisation of MMA or Styrene initiated by AIBN at 60° C by dilatometric method.
(i) Study the decomposition kinetics of oxalic acid solution photosensitized by uranyl sulphate.

Physical Chemistry special group
ELECTIVE PAPER
Credits: 3 (2+1+0)

One topic to be chosen by the Department from the list of Elective Papers given in the end of Semester- IV syllabus.

SEMESTER – IV

ORGANIC CHEMISTRY SPECIAL GROUP

Organic chemistry special paper: CHM 1031C
NATURAL PRODUCTS CHEMISTRY
Credits: 4 (3+1+0)

Unit 1: Chemistry of carbohydrates

Disaccharides- Ring structure of sucrose, maltose, lactose and their hydrolysis.

Polysaccharides- Representative structure of starch, glycogen and cellulose.

Introduction to deoxysugars, glycosides, glycals, glycosamines and glycosans.

Unit 2: Chemistry of Terpenoids, Steroids and Alkaloids

Chemistry of the following compounds- caryophyllene, α-santonin, abietic acid, gibberellic acid, longifolene; biogenetic pathway of mono- and sesquiterpenes.
Introduction and general reactions; introduction to steroids, cholesterol, ergosterol, oestrogens, prosgesterone and corticosteroids, vitamin D_1 and D_2; introduction to sex hormones.

Unit 3: Chemistry of alkaloids

Chemistry of reserpine, nicotine and atropine, including structural determinations and medicinal uses.

Unit 4: Chemistry of vitamins

Carotenoids- classification, chemistry of β-carotene, lycopene and canthaxanthin. Synthesis of β-carotene, provitamin A, singlet oxygen quenching and food coloring properties of carotenes.
Classification and functional role in biological systems; chemistry of thiamine, riboflavin, retinol, tocopherols, vitamin C and pyridoxine.

Organic chemistry special paper: CHM 1032C

ORGANIC SYNTHESIS

Credits: 4 (3+1+0)

Unit 1: Organic photochemistry

Photochemistry carbonyl compounds- representation of the excited states of ketones, photolysis of saturated and β, γ- unsaturated ketones. Photoreduction of saturated arylalkyl and α, β – unsaturated ketones and ρ – benzoquinone. Patterno-Buchi reaction, |2+2|-cycloaddition, reactions of singlet oxygen- photooxidation, ene reaction, synthetic applications of singlet oxygen.

Olefinic photochemistry- photostereomutation of cis-trans isomers, optical pumping, |2+2|-cycloaddition,. Photochemistry of conjugated polyenes- cycloaddition and dimerization of 1, 2-butadiene, photochemistry of vision.

Photoarrangements- di-π-methane rearrangement, photo-Fries rearrangement and photorearrangement of cyclohexadienones, Barton rearrangement.

Unit 2: Formation of carbon-carbon single bonds

Alkylation- importance of enolate anions, aklylation of activated methylene groups, dianion in synthesis, alkylation of ketones, enamine and related reactions; alkylation of thio- and selenocarbanions; allylic alkylation of alkenes, Michael addition (conjugated addition).

Aldol reaction- use of boron and silyl enolates; directed aldol reaction.

Synthetic applications of carbene and carbenoids; formation of carbon-carbon bond by addition of free radicals to alkenes; photocyclization reactions.

Unit 3: Formation of carbon-carbon double bonds

Pyrolytic syn elimination- pyrolyses of carboxylic esters and xanthates (Chugaev reaction) and amine oxides (Cope reaction).
Wittig and related reactions- use of stabilized and unstabilized phosphorus ylides, Peterson reaction;
Stereoselective synthesis of tri and tetra-substituted alkenes.

Unit 4: Pericyclic reactions

Sigmatropic rearrangement- |m+n| sigmatropic rearrangements of hydrogen and chiral alkyl group; divinylcyclopropane rearrangements.
Electrocyclic reactions and cyclo reversions – stereoselectivity of the reactions.
Cheletropic reactions- linear and non-linear cheletropic rearrangement; theories of cheletropic reactions, stereoselectivity of the reactions.
The ene reactions- ene reactions of 1, 7-dienes, carbonyl enophiles; simple problems.

Unit 5: Synthetic application of Organometallics and activation of C-H bonds

Preparation, stability, reactivity and synthetic applications of organo-lithium, tin, copper, zinc and palladium reagents. Hofmann- Loeffler- Freytag reactions, cyclisation reactions of nitrenes, Barton reaction and related processes, photolysis of hypohalides, reactions of monohydric alcohols with lead tetraacetate.

Unit 6: Designing Organic synthesis

Rectosynthesis- disconnection approach, synthons and synthetic equivalents; retrons transform, umpolung; Functional Group Interconversions (FGI); Functional Group Protections- protection and deprotection of hydroxy, dihydroxy, carbonyl, carboxyl and amino groups; retrosynthesis of some

simple compounds.

Organic chemistry special paper: CHM 1033C

BIO-ORGANIC AND MEDICINAL CHEMISTRY

Credits: 4 (3+1+0)

Unit 1: Bio-organic chemistry

(a) **Metabolism of carbohydrates**
Glycolysis and gluconeogenesis; fate of pyruvic acid and Krebs cycle; biosynthesis of fatty acids, triacylglycerols, phospholipids, cholesterol and related steroids; nucleic acids- DNA replication and RNA transcription.

(b) **Biochemistry of lipids**
Biosynthesis of fatty acids, triacylglycerols, phospholipids.

(c) **Proteins**
Primary, secondary, tertiary and quaternary structure of proteins; biosynthesis of aminoacids, tRNA, ribosomes, mRNA, mechanism of transcription and translation; sequencing of aminoacids in polypeptides.

(d) **Nucleic acids**
Classification; nucleosides, nucleotides, their structures and functions; DNA replication.

Unit 2: Medicinal Chemistry

(a) **Introduction to basic concepts**
Definition of drugs and factors affecting their bioactivity; definition chemotherapeutic index and therapeutic index; theoritical aspects of drug-receptor interaction, the two-state Model of Receptor Theory; QSAR, drug agonist and antagonist; pharmaco-kinetics and pharmacodynamics; mechanism of drug action.
Lead compound, molecular modification; elementary idea of molecular modelling of drug; introduction to combinatorial library of drugs

(b) **Antibiotics**
Introduction and classification. β- Lactarn antibiotics- Natural and semisynthetic penicillins, their structure-action relationship and chemical modification, penicillin sensitive and resistant to penicillinase; mode of action of β- Lactarn antibiotics.

Aminoglycoside antibiotics-
Streptomycin, gentamycin, kanamycin, neomycin and their mode of action.

Tetracyclines
Structure-action relationship and therapeutic uses.

Chloramphenicol
Synthesis and characterization, mode of action, macrolide and peptide antibiotics.

Organic chemistry special paper: CHM 1034C

LAB COURSE (ADVANCED ORGANIC CHEMISTRY PRACTICAL)

Credits: 4 (3+1+0)

Students are to perform experiments from each unit. The end semester examination will be of 18 hours

duration, extending over three days. There should be at least one experiment from each unit in the end-semester examination. The total number of experiments will be decided by the examiner.

Unit 1: Three step preparation: Spectroscopic identification of intermediates and final products should be emphasized.

(a) 1,3,5-Tribromobenzene from nitrobenzene via aniline and 2,4,6-tribromoaniline.
(b) m-Nitrophenol from nitrobenzene via m-dinitrobenzene and m-nitroaniline.
(c) Benzidine from nitrobenzene via azobenzene and hydrazobenzene.
(d) Acridone from anthranilic acid via o-chlorobenzoic acid and N-phenylbenzoic acid.
(e) Benzanilide from benzene via benzopheene and benzophenone oxime.
(f) Pivalic acid from acetone via pinacol and pinacone.
(g) Tritylchloride from bromobenzene via phenylmagnesiumbromide and triphenyl carbinol.
(h) Anthranilic acid from phthalic acid via phthalic anhydride and phthalimide.
(i) 2,4-dinitrophenylhydrazine from aniline via chlorobenzene and 2,4-dinitrochlorobenzene.
(j) Phenyl-p-totylthiourea from aniline via thiocarbanilide and phenylisothiocyanate.

Unit 2: Estimations

(a) Number of hydoxy groups in an organic compound by acetylation method.
(b) Estimation of formaldehyde by iodometry.
(c) Equivalent weight of carboxylic acids by – (a) volumetric and (b) gravimetric [Ag-salt] method.
(d) Percentage purity of carbonyl compounds by gravimetric method (with DNP).
(e) Nitro group by reduction with titanous salts.
(f) Unsaturated compounds by bromination method.
(g) Iodine value, saponification value, and RM value of fats.
(h) Molecular weight determination of organic compounds by Rast's camphor method.
(i) Estimation of azobenzene by UV-Visible spectroscopy.

Unit 3: Separation and identification (by comparision of Rτ value) of organic compounds in a ternary mixture by-

(a) Paper chromatography
(b) Thin layer chromatography and
(c) Column chromatography

Students are required to carry out a literature survey. It is to be presented in the end-semester examination both in writing and orally.

Organic chemistry special group

ELECTIVE PAPER

Credits: 3 (2+1+0)

One topic to be chosen by the Department from the list of Elective Papers given in the end of Semester- IV syllabus.

SEMESTER -IV

INORGANIC CHEMISTRY SPECIAL GROUP

Inorganic chemistry special paper: CHM 1061C

MATERIAL CHEMISTRY

Credits: 4 (3+1+0)

Unit 1: Glasses, Ceramics, Composites and Nanomaterials

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical

properties, clay products. Refractories, characterizations, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.

Unit 2: Thin Films and Langmuir -Blodgett Films

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

Unit 3: Liquid Crystals

Mesmorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

Unit 4: Organic Solids, Fullerenes, Molecular Devices

Conducting organics, organic superconductors, magnetism in organic materials.
Fullerenes —doped, fullerenes as superconductors.
Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches -sensors.
Nonlinear optical materials: nonlinear optical effects, second and third order - molecular hyperpolarisability and second order electric susceptibility - materials for second and third harmonic generation.

Inorganic chemistry special paper: CHM 1062C

BIO-INORGANIC CHEMISTRY

Credits: 4 (3+1+0)

Unit 1: Metal Storage Transport and Biomineralization

Ferritin, transferrin, and siderophores.

Unit 2: Calcium in Biology

Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins.

Unit 3: Metalloenzymes

Zinc enzymes —- carboxypeptidase and carbonic anhydrase. Iron enzymes — catalase, peroxidase and cytochrome P-450. Copper enzymes — superoxide dismutase.
Molybdenum oxatransferase enzymes — xanthine oxidase. Coenzyme vitamin B_{12}.

Unit 4: Metals in Medicine

Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

Inorganic chemistry special paper: CHM 1063C

ORGANO-METALLIC CHEMISTRY & CATALYSTS

Credits: 4 (3+1+0)

Unit 1: Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

Unit 2: Compounds of Transition Metal-Carbon Multiple Bonds

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

Unit 3: Transition Metal Compounds with Bonds to Hydrogen

Transition metal compounds with bonds to hydrogen.

Unit 4: Homogeneous Catalysis

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions, activation of C-H bond.

Inorganic chemistry special paper: CHM 1064C

LAB COURSE (ADVANCED INORGANIC CHEMISTRY PRACTICAL)

Credits: 4 (3+1+0)

Students should do experiments from each Unit. The end-semester examination will be of 18 hours duration, extending over three days. Number of experiments in the end semester examination shall be decided by the examiners. Internal evaluation will have a weightage of 40 per cent.

Unit 1: Chromatography

Separation of cations and anions by
(a) Paper chromatography
(b) Column chromatography – ion exchange.

Unit 2: Preparation and characterizations

Preparation of selected inorganic compounds and their physico-chemical characterization by elemental analysis, IR and electronic spectrophotometry, magnetic susceptibility measurements as well as cyclic voltammetric measurements, powder XRD measurements wherever appropriate and possible. Handling of air and moisture sensitive compounds.

(a) $M(acac)_3$, M = Mn, Co
(b) Prussian Blue, Turnbull's Blue
(c) $Co(en)_2Cl_2$, $Co(en)_2(NO_2)_2$ and study of their isomerization by electronic spectroscopy
(d) $[Fe(phen)_3](ClO_4)_2$

Unit 3: Other experiments

(a) Preparation of an optically active Co(III) complex and its optical activity measurement [Ref: H.R. Hunt, Jr., *J. Chem. Educ*., **54** (1977)711].

(b) Preparation of the fac and mer isomers of $Co(NH_3)_3(NO_2)_3$ [Ref: M. Liang, *J.Chem.Educ.,* **62** (1985) 707].
(c) Determination of composition of and Fe-SCN complex by Job's method of continuous variation [Ref: W.R. Carmody, *J.Chem.Educ.,* **41** (1964) 615].
(d) A preparation in a non-aqueous medium.
(e) A preparation in a solid state compounds at high temperature.

Inorganic chemistry special group

ELECTIVE PAPER

Credits: 3 (2+1+0)

One topic to be chosen by the Department from the list of Elective Papers given in the end of Semester- IV syllabus.

ELECTIVE PAPERS

Credits: 3 (2+1+0)

Department will offer at least one elective paper each semester (except in the 2nd Semester) from the following list of elective papers.

1. Organotransition Metal Chemistry (CHM 1201E)
2. Bioinorganic and Supramolecular Chemistry (CHM 1202E)
3. Photoinorganic Chemistry (CHM 1203E)

4. Analytical Chemistry (CHM 1204E)
5. Organic Synthesis-I (CHM 1205E)
6. Organic Synthesis-II (CHM 1206E)
7. Heterocyclic Chemistry (CHM 1207E)
8. Chemistry of Natural Products (CHM 1208E)
9. Medicinal Chemistry (CHM 1209E)
10. Physical Organic Chemistry (CHM 1210E)
11. Chemistry of materials (CHM 1211E)
12. Computational Chemistry (CHM 1212E)
13. Computational Quantum Chemistry (CHM 1213E)
14. Liquid State (CHM 1214E)
15. Polymers (CHM 1215E)
16. Nanochemistry (CHM 1216E)

ELECTIVE PAPER (CHM 1201E)

This elective is not meant for students who specialize in Inorganic Chemistry in the fourth semester. Units 1, 2 and 3 are compulsory, and one Unit from the remaining ones may be chosen.

ORGANOTRANSITION METAL CHEMISTRY (Paper Code: CHM 1201E)

1. **Alkyls and Aryls of Transition Metals**
   Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

2. **Compounds of Transition Metal-Carbon Multiple Bonds**
   Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

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

4. **Transition Metal Compounds with Bonds to Hydrogen**
   Transition metal compounds with bonds to hydrogen.

5. **Homogeneous Catalysis**
   Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions, activation of C-H bond.

6. **Fluxional Organometallic Compounds**
   Fluxionality and dynamic equilibria in compounds such as 112- olefin, 113- allyl and dienyl complexes.

Books Suggested

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and F-LG. Finke, University Science Books.

2. The Organometallic Chemistry of the Transition Metals, FLH. Crabtree, John Wiley
3. Metallo-organic Chemistry, A.Ji Pearson, Wiley.
4. Organornetallic Chemistry, Fl.C. Mehrotra and A. Singh, New Age international

ELECTIVE PAPER (CHM 1202E)

Four of the five units may be chosen for the course by the teacher.

BIOINORGANIC CHEMISTRY (Paper Code: CHM 1202E)

1. **Metal Storage Transport and Biomineralization**
   Ferritin, transferrin, and siderophores.

2. **Calcium in Biology**
   Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins.

3. **Metalloenzymes**
   Zinc enzymes —- carboxypeptidase and carbonic anhydrase. Iron enzymes — catalase, peroxidase and cytochrome P-450. Copper enzymes — superoxide dismutase.
   Molybdenum oxatransferase enzymes — xanthine oxidase. Coenzyme vitamin B_{12}.

4. **Metal—Nucleic Acid Interactions**
   Metal ions and metal complex interactions. Metal complexes - nucleic acids.

5. **Metals in Medicine**
   Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

Books Suggested

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and ll. ed. G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley.
5. Supramolecular Chemistry, J.M. Lehn, VCH.

ELECTIVE PAPER (CHM 1203E)

PHOTOINORGANIC CHEMISTRY (Paper Code: CHM 1203E)

1. **Basics of Photochemistry**
   Absorption, excitation, photochemical laws, quantum yield, electronically excited states-life times-measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages — primary and secondary processes.

2. **Properties of Excited States**
   Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics-calculation of rates of radiative processes. Bimolecular deactivation — quenching

3. **Excited States of Metal Complexes**
   Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for

obtaining charge-transfer spectra.

4. **Redox Reactions by Excited Metal Complexes**
   Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10-phenonthroline complexes), illustration of reducing and oxidising character of Ruthenium^{2+}(bipyridal complex, comparision with $Fe(bipy)_3$; role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.

Books Suggested

1. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley.
2. Inorganic Photochemistry, J. Chem. Educ.. vol. 60, no. 10, 1983.
3. Progress in Inorganic Chemistry, vol. 30, ed. S.J. Lippard, Wiley.
4. Coordination Chem. Revs., 1981, voi. 39, 121, 131; 1975, 15, 321; 1990, 97, 313.
5. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press
6. Elements of Inorganic Photochemistry, G. J. Ferraudi, Wiley.

ELECTIVE PAPER (CHM 1204E)

Units 1 and 2, and any two of the remaining units.

ANALYTICAL CHEMISTRY (Paper Code: CHM 1204E)

1. **Introduction**
   Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations - dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

2. **Errors and Evaluation**
   Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data-determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics.

3. **Food Analysis**
   Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

4. **Analysis of Water Pollution**
   Origin of waste water, types, water pollutants and their effects. Sources of water pollution-domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis.

Water pollution laws and standards

5. Analysis of Soil, Fuel, Body Fluids and Drugs

(a) Analysis of soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

(b) Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating values-grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.

(c) Clinical chemistry: Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (FHA) and applications. The blood gas analysis- trace elements in the body.

Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

Books Suggested

1. Analytical Chemistry, G.D. Christian, J. Wiley.
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W. B. Saunders.
3. Analytical Chemistry-Principles, J.H. Kennedy, W. B. Saunders.
4. Analytical Chemistry-Principles and Techniques, L.G. Hargis, Prentice Hall.
5. Principles ol Instrumental Analysis, D.A. Skoog and J.L. Loary, W. B. Saunders.
6. Principles of instrumental Analysis, D.A. Skoog, W. B. Saunders.
7. Quantitative Analysis, Fl.A. Day, Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern
9. Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern
10. Handbook oi instrumental Techniques for Analytica Chemistry, F. Settle, Prentice Hall.

ELECTIVE PAPER (CHM 1205E)

ORGANIC SYNTHESIS I (Paper Code: CHM 1205E)

1. **Organometallic Reagents**

Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details

Group I and ll metal organic compounds: Li, Mg, Hg, Cd, Zn and Ce compounds.

Transition metals: Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti compounds.

Other elements: S, Si, B and I compounds.

2. **Oxidation**

Introduction. Different oxidative processes.

Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated).

Alcohols, diols, aldehydes, ketones, ketals and carboxyalic acids.

Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (lll) nitrate.

3. **Reduction**

Introduction. Different reductive processes.

Hydrocarbons— alkanes, alkenes, alkynes and aromatic rings.

Carbonyl compounds — aldehydes, ketones, acids and their derivatives. Epoxides.

Nitro, nitroso, azo and oxime groups.

Hydrogenolysis.

4. **Rearrangements**

General mechanistic considerations - nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements-

Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert

synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Baeyer-Villiger, Shapiroreaction.

Books Suggested
1. Modern Synthetic Reactions, H.O.House, W. A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
4. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B, F. A. Carey and R. J. Sundberg, Plenum Press.
6. Rodd's Chemistry oi Carbon Compounds, Ed. S. Coffey, Elsevler.

ELECTIVE PAPER (CHM 1206E)

ORGANIC SYNTHESIS II (Paper Code: CHM 1206E)

1. **Disconnection Approach**
   An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C—X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

2. **Protecting Groups**
   Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

3. **One Group C-C Disconnections**
   Alcohols and carbonyl compounds, regioselectiviity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

4. **Two Group C-C Disconnections**
   Diels-Alder reaction, 1,3—difunctionalised compounds, α, B-unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Michael addition and Robinson annelation.

Books Suggested
1. Designing Organic Synthesis, S. Warren, Wiley.
2. Organic Synthesis- Concept, Methods and Starting Materials, J.Fuhrhop and G. Penzillin, Verlage VCH.
3. Some Modern Methods of Organic Synthesis. W. Carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions, H.O.House, W. A. Benjamin,
5. Advanced Organic Chemistry: Reactions, Mechanisms and Structure, J. March, Wiley.
6. Principles of Organic Synthesis, Fl. Norman and J. M. Coxon, Blackie Academic & Professional.
7. Advanced Organic Chemistry Pan B, F. A. Carey and H. J. Sundberg, Plenum Press.

ELECTIVE PAPER (CHM 1207E)

HETEROCYCLIC CHEMISTRY (Paper Code: CHM 1207E)

1. **Nomenclature of Heterocycles**
   Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles.

2. **Aromatic Heterocycles**
   General chemical behaviour of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in ^{1}H NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations).

Heteroaromatic reactivity and tautcmerism in aromatic heterocycles.

3. **Non-aromatic Heterocycles**
   Strain -bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction.
   Stereo~electronic effects - anomeric and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic- electrophilic interactions.
4. **Heterocyclic Synthesis**
   Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes.
   Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.
5. **Benzo-Fused Five-Membered Heterocycles**
   Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes.
6. **Six-Membered Heterocycles with Two or More Heteroatoms**
   Synthesis and reactions of diazines, triazines, tetrazines and thiazines.

Books Suggested

1. Heterocyclic Chemistry Vol.1-3, Ft. Ft. Gupta, M. Kumar and V.Gupta, Springer Verlag.
2. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemisiry.T.L Gilchrist,Longman Scietitic Techinal
4. Contemporary Heterocyclic Chemistry, G. Fl. Newkome and W. W. Paudler, Wiley-Inter Science.
5. An Introduction to the Heterocyclic Compounds, Ft. M. Acheson, JohnWiley.
6. Comprehensive Heterocyclic Chemistiy, A. Fl. Katritzky and C. W. Rees, eds. Pergamon Press.

ELECTIVE PAPER (CHM 1208E)

CHEMISTRY OF NATURAL PRODUCTS (Paper Code: CHM 1208E)

1. **Terpenoids and Carotenoids**
   Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule.
   Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geranlol, or-Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abietic acid and β-Carotene.
2. **Alkaloids**
   Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants.
   Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+)- Coniine, Nicotine, Atropine, Ouinine and Morphine.
3. **Steroids**
   Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progestrone, Aldosterone.
   Biosynthesis of steroids.
4. **Prostaglandins**
   Occurrence, nomenclature, classification, biogenesis and physiological effects.
   Synthesis of PGE_2 and $PGF_{2\alpha}$

Books Suggested
1. Natural Products: Chemistry and Biological Significance, J. Mann, Fl.S.Davidson, J.B.Hobbs, D.V. Banthrope and J. B. Harborne, Longman,Essex.
2. Organic Chemistry, Vol 2, LL. Finar, ELBS.
3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed.Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
7. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.l. Choudhary, Harwood Academic Publishers.
8. lnsectcides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

ELECTIVE PAPER (CHM 1209E)

Students should be taught Units 1, 2 and 3, and any one of the units from 4 to 8.

MEDICINAL CHEMISTRY (Paper Code: CHM 1209E)

1. **Drug Design**
   Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).

2. **Pharmacokinetics**
   Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

3. **Pharmacodynamics**
   Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotranstormation, significance of drug metabolism in medicinal chemistry.

4. **Antineoplastic Agents**
   Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors.
   Synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards, and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

5. **Cardiovascular Drugs**
   Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators.
   Synthesis of amyl nitrate, sorbitrate, dlltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenolol.

6. **Local Antiinfective Drugs**
   Introduction and general mode of action.
   Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprotloxacin, nortloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econozole, griseotulvin, chloroquin and primaquin.

7. **Psychoactive Drugs- The Chemotherapy of Mind**
   Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs - the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis ot diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximde, trimethadione, barbiturates, thiopental sodium, glutethimide.

8. **Antibiotics**
   Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin.

Books Suggested

1. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F.Dorge.
3. An Introduction to Drug Design, S. S. Pandeya and J. Fl. Dimmock, New Age International.
4. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch-14). Ed. M. E. Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis oi Therapeutics, McGraw-Hill.
6. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press.
7. Strategies for Organic Drug Synthesis and Design, D. Lednicer. John Wiley.

ELECTIVE PAPER (CHM 1210E)

PHYSICAL ORGANIC CHEMISTRY

SUPRAMOLECULAR CHEMISTRY (Paper Code: CHM 1210E)

1. **Supramolecular Chemistry - I**
   Properties of covalent bonds - bond length, inter~bond angles, force constant, bond and molecular dipole moments. Molecular and bond polarizability, bond dissociation enthalpy, entropy. intermolecular forces, hydrophobic effects. Electrostatic, induction, dispersion and resonance energy. magnetic interactions, magnitude of interaction energy, forces between macroscopic bodies, medium effects.Hydrogen bond.
   Principles of molecular association and organization as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles. Molecular receptors and design principles. Cryptands, cyclophanes, calixeranes, cyclodextrines.
   Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

2. **Supramolecular Chemistry - II**
   (a) Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition.
   (b) Supramolecular reactivity and catalysis.
   (c) Transport processes and carrier design.
   (d) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices.

3. **Dendrimers**
   (a) Introduction, synthesis and characterization of macromolecular materials, including linear, branched, dedrimetric and star polymers.
   (b) Synthetic strategies and stuctural variations
   Mechanical and physiochemical properties of polymer types,
   Kinetics of living polymerization; applications to nanostructures, templates and advanced devices
   (c) Host-guest assembly and supramolecular assembly

(d) Competitive binding of guest molecules on the surface or in the interior of dendrimers
(e) Supramolecular structure of dendrimer/surfactant aggregates
(f) Biomedical applications, biosensing, photodynamic theory, dendrimer-based MRI contrasts

Books Suggested

1. Molecular Mechanics, U. Burkertand NA L. Allinger, ACS Monograph 177, 1982.
2. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
3. The Physical Basis of Organic Chemistry, H. Maskill,Oxford University Press.
4. Supramolecular Chemistry, J. Steed and J.L. Atwood (Wiley, 2nd Edn 2009)
5. Dendrimer Chemistry, F. Vogtle, G. Richardt, N. Werner, A.J. Rackstraw, Wiley-VCH, 2009.

ELECTIVE PAPER (CHM 1211E)

Not meant for students who are specializing in Inorganic Chemistry in the fourth semester. Any four of the units may be taught.

CHEMISTRY OF MATERIALS (Paper Code: CHM 1211E)

1. **Multiphase Materials**
   Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non'-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.
2. **Glasses, Ceramics, Composites and Nanomaterials**
   Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties, applications.
1. **Thin films and Langmuir-Blodgett films**
   Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film; growth techniques; photolithography; properties and applications of thin and LB films.
3. **Liquid Crystals**
   Mesmorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature-homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals.Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.
4. **Polymeric Materials**
   Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric polymers.
5. **Inonic Conductors**
   Types of ionic conductors, mechanism of ionic conduction, interstital jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.
6. **High Tc materials**
   Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence

length; elastic constants, position lifetimes, microwave absorption pairing and multigap structure in high Tc materials, appplications of high Tc materials

7. **Materials for solid state devices**
   Rectifiers, transistors, capacitors -IV-V compounds, low-dimensional quantum structures; optical properties.

5. **Organic Solids, Fullerenes, Molecular Devices**
   Conducting organics, organic superconductors, magnetism in organic materials.
   Fullerenes —doped, iullerenes as superconductors.
   Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches -sensors.
   Nonlinear optical materials: nonlinear optical effects, second and third order - molecular hyperpolarisability and second order electric susceptibility - materials for second and third harmonic generation.

Books Suggested

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D.Callister, Wiley.
3. Principles of the Solid State, H.V. Keer, Wiley Eastern.
4. Materials Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings,ELBS
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Wiley.
6. Handbook oi Liquid Crystals, Kelker and Hatz, Chemie Verlag.

ELECTIVE PAPER (CHM 1212E)

COMPUTATIONAL CHEMISTRY (Paper Code: CHM 1212E)

1. **Fortran/ C Programming and Numerical Methods**
   Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc.

   a. Solution of Equations
   Bisection, regular falsi, Newton -Flaphson and related methods for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning.

   b. Linear Simultaneous Equations
   Gaussian elimination, Gauss -Seidel method, Gauss-Jordan method. Pivoting strategy. Errors and ill conditioning.

   c. Eigenvalues and Matrix Diagonalization
   Jacobi and Householder methods, analysis or errors.

   d. Interpolation
   Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. Polynomial wiggle problem.

   e. Numerical Differentiation
   Solution of simple differential equations by Taylor series and Runge-Kutta methods.

   f. Numerical Integration
   Newton-Cotes formulae, Romberg integration, errors in integration formulae.

The students should develop computer programs for some of the above numerical methods.

2. **Running of Advanced Scientific Packages**
   The students are expected to get hands on experience of running a few selected advanced level scientific software packages after a brief introduction to the basic theory and methodology. *ab initio* quantum chemical packages such as GAUSSIAN/GAMES with carefully designed exercises for illustrating various features of the packages. Semi-empirical/Dynamics/Simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design etc.

Books Suggested

1. Computational Chemistry, A.C. Norris, John Wiley.
2. Computer Programming in FORTRAN 77, Fl. Rajaraman, Prentice Hall.
3. Numerical Analysis, C. E. Frogberg, Macmillan.
4. Numerical Analysis - A Practical Approach, M.J. Maron, John Wiley.
5. Numerical Methods for Scientists and Engineers, H. M. Antia, Tata McGraw Hill.

ELECTIVE PAPER (CHM 1213E)

COMPUTATIONAL QUANTUM CHEMISTRY (Paper Code: CHM 1213E)

(Pre-requisite: Mathematics at least up to First Year B.Sc. level is necessary. At least one PC among 4 students should be available)

1. **Chemical Bonding**
   (a) The hydrogen molecule ion: linear combination of atomic orbital (LCAO)- molecular orbital (MO) theory- ground and excited electronic states.
   (b) The hydrogen molecule: LCAO-MO and valence bond (VB) treatments. Equivalence of the MO and VB methods.
   (c) Extension of the LCAO-MO method to homo- and heteronuclear diatomics- inclusion of hybridization.
   (d) Term symbols for molecular electronic states, their symmetry classification. Correlation diagrams and the non-crossing rule.
   (e) LCAO-MO theory of simple polyatomic molecules (e.g., the H_2O molecule).
   (f) ´ -electron theory: Hückel molecular orbital (HMO) method for unsaturated carbon compounds showing chain and ring structures; introduction to extended Hückel theory.

2. **Quantum Computational Treatment of Atoms and Molecules, *Ab Initio* SCF Theories**
   (a) Review of the principles of quantum mechanics, Born-Oppenheimer approximation, Slater-Condon rules.
   (b) The self consistent field method, Hartree-Fock theory of closed shell electronic configurations of atoms and molecules. Coulomb and exchange integrals, canonical Hartree-Fock equations, Koopman's theorem without derivation. Gaussian basis sets.
   (c) SCF LCAO-MO theory of molecules- Roothan equation.

3. **Configuration Interaction and MC-SCF**
   Introduction to Cl; full and truncated Cl theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods.

4. **Computer-Based Experiments**
   Computer experiments using quantum chemistry - software packages such as GAUSSIAN/GAMESS/MOPAC and modelling software e.g. Avogadro/ArgusLab etc.

Books Suggested

1. Modern Quantum Chemistry, N.S. Ostlund and A. Szabo, McGraw Hill.

2. Methods of Molecular Quantum Mechanics, Ft. McWeeny and B.T. Sutcliife, Academic Press.
3. Exploring Chemistry with Electron Structure Methods, J. B. Foresman and E. Frish, Goussian Inc.
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ELECTIVE PAPER (CHM 1214E)

LIQUID STATE (Paper Code: CHM 1214E)

1. **General Properties of Liquids**
   a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations, internal pressure and its significance in liquids. Equations of state, critical constants.
   Different types of intermolecular forces in liquids, different potential functions for liquids, additivity of pair potential approximation.

   b) A classical partition function for liquids, correspondence principle, configuration integral, configuration properties.

2. **Theory of Liquids**
   Theory of liquids, partition function method or model approach; single cell models, communal energy and entropy, LJD model, significant structure model.

3. **Distribution Function and Related Equations**
   Radial distribution function method, equation of state in terms of RDF. Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion.
4. **Methods for Structure Determination and Computational Techniques**
   Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy.
   Computation Techniques—Monte Carlo and molecular dynamics methods.

5. **Supercooled and ionic Liquids**
   Supercooled and ionic liquids, theories of transport properties; non Arrhenius behaviour of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in supercooled liquids.

Books Suggested
1. An introduction to Liquid State, P.A. Egelstaft, Academic Press.
2. The Dynamic Liquid State, A.F.M. Barton, Longman.
3. Introduction to Statistical Thermodynamics, T.L. Hill, Addison Wiley.
4. The Liquid State, J.A. Pryde.
5. Significant Liquid Structures, H. Eyring and MS. John.

ELECTIVE PAPER (CHM 1215E)

POLYMERS (Paper Code: CHM 1215E)

1. **Basics**
   Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers.
   Polymerization: condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

2. **Polymer Characterization**
   Polydispersion-average molecular weight concept. Number, weight and viscocity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscocity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers-chemicai analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance. Hardness and abrasion resistance.

3. **Structure and Properties**
   Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point Tm - melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg-Relationship between Tm and Tg, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

4. **Polymer Processing**
   Plastics, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

5. **Properties of Commerical Polymers**
   Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers - Fire retarding polymers and electrically conducting polymers. Biomedical polymers -contact lens, dental polymers, artificial heart kidney, skin and blood cells.

Books Suggested

1. Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley.
2. Polymer Science, VH. Gowarlker, N.V. Viswanalhan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K4 Takemolo, Y. lnaki and RM. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R, Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.

ELECTIVE PAPER (CHM 1216E)

NANOCHEMISTRY (Paper Code: CHM 1216E)

1. **Introduction:**
   History, scope and perspectives of nanochemistry.

2. **Synthesis and Stabilisation of Nanoparticles:**
   Chemical Reduction; Reactions in Micelles, Emulsions, Dendrimers; Photochemical and Radiation Chemical Reduction; Cryochemical Synthesis: Physical Methods; Particles of various shapes and films.

3. **Experimental Techniques:**
   Electron Microscopy; Transmission Electron Microscopy; Probe Microscopy. Diffraction Techniques: X-ray Diffraction. Miscellaneous Techniques: Comparision of Spectral techniques used for elemental analysis.

4. **Size Effects in Nanochemistry:**
   Models of reactions of metal atoms in matrices; Melting Point; Optical Spectra; Kinetic pecularities of chemical processes on the surface of nanoparticles; Thermodynamic features of nanoparticles.

5. **Applications of Nanoparticle** in various fundamental research, industries, medical fields and environmental fields. Toxicity, Biosafety and Ethical issues in application of nanoparticles.

Books Suggested

(a) Nanomaterilas and Nanochemistry, Bréchignac C., Houdy., and Lahmani M. (Eds.) Springer Berlin Heidelberg New York, 2007.

(b) Nanoparticle Technology Handbook, Hosokawa M., Nogi K., Naito M and Yokoyama T., (Eds.) First Edition 2007, Elsevier.

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14. *Modern Electrochemistry*, Bokris and Reddy, Vols. 1&2 (Butterworth)
15. *Chemical Kinetics*, K.J. Laidler
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19. *Principles of the Solid States,* H.V. Keer
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22. *Chemical Thermodynamics*, E.N. Yeremin
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32. *Principles of Biochemistry*, A. Lehninger
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5. *Chemical Hardness* by R.G. Pearson, Wiley-VCH
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29. *Organic Chemistry* by Gilman (four volumes)
30. *Natural Products* by Nakanishi
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