Structure of Postgraduate Chemistry Course

<table>
<tr><th rowspan="3">Semester</th><th colspan="7">Course Description with Marks</th></tr>
<tr><th colspan="6">Theory</th><th rowspan="2">Practical</th></tr>
<tr><th>Organic Chemistry</th><th>Inorganic Chemistry</th><th>Physical Chemistry</th><th>Common Paper</th><th>Special Paper (Organic/Inorganic /Physical)</th><th>Total</th></tr>
<tr><td>First</td><td>50
(CHEM 0701)</td><td>50
(CHEM 0702)</td><td>50
(CHEM 0703)</td><td>-</td><td>-</td><td>150</td><td>Inorganic: 50
(CHEM 0791)
Physical: 50
(CHEM 0792)</td></tr>
<tr><td>Second</td><td>50
(CHEM 0801)</td><td>50
(CHEM 0802)</td><td>50
(CHEM 0803)</td><td>-</td><td>-</td><td>150</td><td>Organic: 50
(CHEM 0891)
Computer Application: 50
(CHEM 0892)</td></tr>
<tr><td rowspan="3">Third</td><td rowspan="2">-</td><td rowspan="2">-</td><td rowspan="2">-</td><td>50
(CHEM 0901)</td><td>-</td><td rowspan="3">150</td><td rowspan="3">Practical: 50
(CHEM 0991)
Practical: 50
(CHEM 0992)</td></tr>
<tr><td>50
(CHEM 0902)</td><td>-</td></tr>
<tr><td>-</td><td>-</td><td>-</td><td>-</td><td>50
(CHEM 0903A/B/C)</td></tr>
<tr><td rowspan="3">Fourth</td><td rowspan="3">-</td><td rowspan="3">-</td><td rowspan="3">-</td><td rowspan="3">-</td><td>50 (CHEM 1001)</td><td rowspan="2">100</td><td rowspan="3">Project Work
(CHEM 1091 and CHEM 1092):
50 + 50</td></tr>
<tr><td>50 (CHEM 1002)</td></tr>
<tr><td>50 (CHEM 1003)
Seminar and Grand Viva</td><td>50</td></tr>
<tr><td colspan="7">600</td><td>400</td></tr>
</table>

FIRST SEMESTER

Course No. CHEM 0701 (FM = 50; C = 4)
Organic Chemistry-I

Unit 1: Stereochemistry (M = 15)

Static Aspects: Symmetry properties, point group; configuration – acyclic and cyclic systems; conformation – cyclic systems (cyclohexene, cyclohexanone, substituted cyclopentanes and cyclopentanones, medium rings, decalin and hydrindane systems).

Dynamic Aspects: cyclisation reactions, Baldwin's Rules; conformation and reactivity with reference to substitution, elimination, addition and rearrangement reactions.

Unit 2: Pericyclic reactions (M = 18)

Pericyclic reactions: Molecular orbitals for acyclic conjugated systems. Theory of pericyclic reactions – i) Frontier Molecular Orbital (FMO) approach ii) concept of aromaticity of transition states (Hückel / Möbius systems). The Woodward-Hoffmann selection rules and general rules.

General perturbation molecular orbital theory in cycloadditions: Symmetry principles in pericyclic reactions, orbital and state correlation diagram for electrocyclic and cycloaddition reactions. Reactivity, regioselectivity and periselectivity. Cycloaddition reactions: antarafacial and suprafacial additions, 4n and 4n+2 systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Ene reactions, group-transfer reactions and eliminations. Scope, reactivity and stereochemical features of electrocyclic reactions (4e, 6e and 8e neutral systems). Electrocyclic reactions of charged systems (cations and anions), Electrocyclic reactions: conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

Sigmatropic rearrangements: [1, j] shifts – [1, 5] and [1, 7] shifts in neutral systems and [1,4] shift in charged species: [i, j] shifts – [3, 3] shifts, Sommelet-Hauser, Cope, aza-Cope rearrangements, Fluxional tautomerism. Claisen rearrangements; [5, 5] shifts, [2, 3] shifts in ylids.

Unit 3: Spectroscopy (M = 17)

Review of UV and IR spectroscopy

^{1}H NMR Spectroscopy: Basic theory – phenomenon of energy absorptions (resonance) and relaxation, chemical shift, shielding and deshielding mechanisms, equivalence and nonequivalence of protons, spin-spin coupling – notation for spin systems, coupling constant and its variation with stereochemistry – Karplus equation. Structural application of ^{1}H NMR, aromaticity, antiaromaticity and homoaromaticity of organic molecules and related problems.

^{13}C NMR Spectroscopy: Principles; broad band decoupling, DEPT; structural applications of ^{13}C NMR.

Mass Spectrometry: Types of ionization techniques, basic principles of EI, fragmentation pattern of small molecules.

Problems incorporating spectroscopic data.

Course CHEM 0702 (FM = 50; C = 4)
Inorganic Chemistry-I

Unit 1 Coordination chemistry(I): Structure, stability and reactivity (M= 18)

Thermodynamic aspects of crystal field splitting, kinetics aspects of crystal field splitting, crystal field activation energy, labile and inert complexes. Single ion magnetic behavior, metal centered transitions.

Limitations of CFT, evidences of metal-ligand orbital overlap, nephelauxetic series; spectrochemical series. Free ion terms arising from d^n configuration and their splitting in Oh and Td fields – Orgel diagrams. Charge transfer spectra – LMCT and MLCT transition in O_h and T_d complexes.

Structural and stereoisomerism of coordination compounds, optically active coordination compounds and their resolution procedures, absolute configuration of enantiomers.

Unit 2 Chemistry of elements: Special features (M = 16)

Structure and bonding of higher boranes, Lipscomb's tropological diagrams and Wade's rules. Metal-metal bonded complexes of transition metals (structure and bonding): dirhenium complexes, molybdenum blue, tungsten blue, tungsten bronze, ruthenium red, Creutz-Taube complex, transition metal dioxygen and dinitrogen complexes (structure, bonding and reactivity), Vaska's complex.Alkali metal complexes with macrocyclic ligands, crown ether and cryptate complexes. Chlorophyll-Mg complex (active centre).

Unit 3 Chemistry of f-block elements: Comparative study with d-block elements (M =16)

Lanthanide and actinide elements: terrestrial abundance and distribution, relativistic effect, variation of atomic and ionic radius, ionization energy, electronic configuration and oxidation states, magnetic properties, electronic spectra, aqueous and complex chemistry in different oxidation states, comparison with those of d-block elements; organometallic compounds, use of lanthanide compounds as NMR-shift reagent and others. Super heavy elements. Production, properties and uses of Ce, Gd, Pu and Pt- metals and their compounds.

Course No. CHEM 0703 (FM = 50; C = 4)
Physical Chemistry-I

Unit 1 Thermodynamics and surface phenomena (M = 14)

Recapitulation of 1st and 2nd law of thermodynamics, Mathematical theorems on Pfaffian equations, Caratheodory's theorem, entropy in the light of caratheodory's principle, Nernst heat theorem, the third law of thermodynamics, entropy determination. Excess function, fugacity, activity and activity coefficients, Concept of standard state. Thermodynamics of polymer solution: entropy, heat and free-energy of mixing.

Vapour pressure over curved surface, the Young-Laplace eqution, the Kelvin equation, Interfacial region, adsorption on solid, the adsorption isotherms (Langmuir, BET – with derivation). Surface active agents, micelles, reverse micelles, solubilisation, and micro-emulsion.

Unit 2 Statistical mechanics- l (M = 12)

Probability, thermodynamic probability and entropy, Maxwell-Boltzman statistics, Partition function: translational (for ideal gas - concept of thermal wavelength), rotational, vibrational and electronic partition functions (diatomic molecule); molecular and molar partition function, Qualitative idea of Quantum statistics (Bose-Einstein, Fermi-Dirac statistics): Thermodynamic probability and distribution formula (without derivation), comparison with classical statistics - distinguishability and indistinguishability of identical particles.

Application: Theory of specific heat of solids – Einstein's and Debye's pictures.

Unit 3 Electrochemistry (M = 09)

Debye-Hückel theory of strong electrolytes, concept of ionic atmosphere. Debye-Hückel limiting law for single ionic activity coefficient and mean activity coefficient (with derivation), its relation to ionic strength.

Bjerrum model for ion association: Formation of ion pairs, derivation of ion-association constant.

Unit 4 Kinetics-l (M = 15)

Collision theory: Lines of centre model. Introduction of potential energy surface and contour, internal coordinates and reaction coordinates, reaction path – valley and saddle point; saddle point – activation energy, classical trajectory, and theory of absolute rate. Comparison of collision and absolute rate theory. Fast reaction - relaxation methods. Branching chain reactions and explosion. Oscillatory reactions: Lotka-Volterra model and its applications.

Rate equation for electrode process. Butler-Volmer equation, High Field approximation, Tafel equation, Low field approximation, kinetic derivation of Nernst equation, exchange current density and polarizability of interfaces, concept of overvoltage.

Course No. CHEM 0791 (FM = 50; C = 4)
Inorganic Practical

Part-I

Qualitative analysis of mixture of compounds containing two rare elements and insoluble

Rare elements: Ti, V, Mo, W, Zr, Ce, U

Insoluble Samples: $PbSO_4$, $BaSO_4$, $SrSO_4$, Fe_2O_3, CaF_2, Cr_2O_3, Al_2O_3, SiO_2, SnO_2, TiO_2, ZrO_2, CeO_2

Part II (any three)

1. Determination of the amount of calcium in milk powder by EDTA complexometry
2. Potassium trioxaltoferrate III: Sythesis, analysis and photochemistry.
3. Analysis of kidney stones by permanganometric titration
4. Preparation of $[Ni(NH3)_6]^{2+}$ and its analysis by different methods
5. Estimation of iodine in iodized common salt using iodometry
6. Estimation of phosphoric acid in cola drinks by molybdenum blue method
7. Paper and column chromatography of plant pigments

Course No. CHEM 0792 (FM = 50; C = 4)
Physical Practical

1. Spectrophotometric experiment - determination of composition of a complex (Job's method)
2. Determination of cmc of surfactants: conductometry and spectrophotometry.
3. Determination of molecular weight of macromolecules by viscometry.
4. Determination of dipole moment.
5. Analytical experiments: Study of distribution of an organic acid in an organic solvent and water – determination of association constant (with the help of Nernst distribution law), determination of van't Hoff factor.
6. Determination of transport number.
7. Molecular structure determination – gas phase vibrational rotational spectra of HCl/DCl.

SECOND SEMESTER
Course No. CHEM 0801 (FM = 50; C = 4)
Organic Chemistry-II

Unit 1: Synthetic methodology and Synthetic strategy (M = 17)

Synthetic methodology: The roles of boron, phosphorus, sulfur and silicon in organic synthesis. Stereoselective hydroboration, hydrogenation, epoxidation and hydroxylation.

Synthetic strategy: Retrosynthetic analysis, disconnection, typical examples to illustrate the disconnection approach to organic synthesis.

Unit 2: Heterocyclic Chemistry (M = 17)

Systematic nomenclature (Hantzsch – Widman system) for monocycle and fused heterocycles.

General approach to heterocyclic synthesis – cyclisation and cycloaddition routes. Heterocycles in organic synthesis – masked functionalities, umpolung, Stork annulation reaction and applications (synthesis of testosterone, estrone, progesterone, ranitidine, lansoprazole and/or recently discovered molecules etc. Rearrangement and ring transformation involving 5- and 6-membered heterocycles with one heteroatom.

Unit 3: Natural products (M = 16)

Structural types; structure elucidation, reactions and synthesis of representative examples of (i) Alkaloids (ii) Terpenoids. Stereochemistry, reactions and synthesis of terpenoids and carotenoids: zingiberine, santonin, abietic acid, β-carotene. Stereochemistry, reactions and synthesis of alkaloids: quinine, morphine, camptothecin and recently discovered bioactive natural products.

Course No. CHEM 0802 (FM = 50; C = 4)
Inorganic Chemistry-II

Unit 1 Aspects of Chemical Bonding (M = 16)

LCAO-MO and VB treatments on H_2^+, H_2: Valence bond theory (VBT), resonance in VBT, VBT of homonuclear diatomic molecules, sigma and pi bonds, VBT of heteronuclear diatomic molecules, inadequacies of the simple VBT. Hybridization, participation of d orbitals in hybridization in polyatomic species. Molecular orbital theory (MOT), linear combination of atomic orbitals (LCAO), criteria for the formation of stable MOs. Sigma, Pi and Delta molecular orbitals. Homonuclear and heteronuclear diatomic molecules and ions. MO theory of polyatomic molecules and ions. MO theory of π bonding and multi-centre bonding. MO concept of metal-ligand bonding (pictorial approach)

Unit 2 Organometallic Chemistry (M = 17)

Preliminary idea and applications of 16 and 18 electrons rule for organometallic compounds. Reaction of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands. Stereochemical non-rigidity and fluxional behaviour of organometallic compounds, catalysis by organometallic compounds: Wilkinson's catalyst, Tolman's catalytic loops; synthesis gas, water gas shift reaction, synthesis of methanol, hydroformylation (oxo process), hydrogenation of unsaturated compounds, Masanto acetic acid process, Waker process, synthetic gasoline, Fischer-Tropsch process and mobil process; Polymerisation, oligomerisation and metathesis reactions of alkenes and alkynes; Zieglar-Natta catalysis.

Unit 3 Principle of symmetry in Chemistry (M = 17)

Concept of symmetry in molecules, symmetry elements and symmetry operations, combining symmetry operations. Multiplication Table by stereographic projection technique. Elements of Group Theory, Sub groups and classes of group elements. Symmetry point groups of molecules, systematic classification of molecular point groups, Application of symmetry in identifying polar and chiral molecules. Symmetry and stereo-isomerism. Unit vector transformation and interpretation of character table. Identification of symmetry label of MO in a molecule. Construction of MO on the basis of Symmetry of the molecules (H_2O, NH_3, B_2H_6, CH_4). Two dimensional space group.

Course No. CHEM 0803 (FM = 50; C = 4)

Physical Chemistry-ll

Unit 1 Quantum mechanics - l (M = 17)

Introductory ideas of classical mechanics – Equation of motion: Newtonian mechanics, Lagrangian mechanics, Hamiltonian mechanics, Classical mechanical Poisson bracket.

Identification of classical and quantum systems, Bohr's correspondence principle with examples; Double slit experiment. Uncertainty principle. Plausibility arguments leading to Schrödinger equation, Probability concept. Continuity equation. Elementary applications – different potential problems: free particle, confined particle in a box, step potential barrier problem: tunnelling and its applications.

Linear operators in quantum mechanics. Eigen value equation. Hermitian operator, Heisenberg equation of motion, constant of motion, Ehrenfest's theorem. Commutator and relationship with Poisson bracket, non compatibility and uncertainty; Formal derivation of Heisenberg uncertainty principle: commutability and compatibility.

Simple harmonic oscillator (operator method).

Approximate method: Elementary perturbation theory, Variation theorem, Simple applications.

Unit 2 Atomic structure (M = 16)

Motion under central force: Conservation of angular momentum and its consequence. Motion of angular momentum under magnetic field. Larmor prescision. Quantization rule and quantum numbers. Zeeman effect. Stern-Gerlach experiment. Spin-orbit interaction, conservation of total angular momentum J, Vector atom model. Anomalous Zeeman effect, Paschen-Beck effect. Multielectron system- Pauli exclusion principle. Term symbols for simple multi-electron system. Magnetic moment and Lande's g factor.

Schrödinger equation for hydrogen atom (only qualitative idea), separation of radial and angular part. Orbits and Orbitals. Shape of orbitals.

Unit 3 Molecular spectroscopy, structure and properties (M = 17)

Molecular spectroscopy: Introduction, elementary idea about spectroscopic instrumentation, spectral broadening. Electromagnetic spectrum and molecular processes associated with the regions. Rotational spectra of polyatomic molecules: classification of molecules into spherical, symmetric and asymmetric tops; linear triatomic molecules, Non-rigid rotor. Elementary idea of Stark effect. Anharmonic oscillator and dissociation. Elementary idea of Born-Oppenheimer approximation. Vibration rotation spectra for diatomic molecule, Rotational-vibrational coupling. Raman spectra: classical theory of Raman scattering, concept of polarizability ellipsoid.

Dielectric polarization. Mossotti-Clausius relation, polar molecule. Debye equation. Dipole moment and molecular structure. Intermolecular forces. Attraction and repulsion potentials: van der Waals forces, Keesom, Debye and London forces, their relative contribution; Lennard-Jones potential.

Course No. CHEM 0891 (FM = 50; C = 4)
Organic Practical

Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components by chemical and spectroscopic methods.

Course No. CHEM 0892 (FM = 50; C = 4)
Computer Application

Introduction to programming languages; basic numerical analysis: solution of nonlinear equations using Newton-Raphson method (e.g. finding the roots of a cubic equation – vander Waals equation), solution of linear systems using Gaussian elimination, interpolation, numerical integration (trapezoidal and Simpson's $1/3^{rd}$ rule), numerical solution of differential equations (Euler and Runge-Kutta method). Fourier transformations and applications in spectroscopy.

Use of molecular geometry optimisation software (Gaussian 09); construction of z-matrix and concept of force field.

Classical Molecular Dynamics (MD) simulation and application to simple systems like Lennard-Jones fluids.

[Effort should be made to reproduce data reported in the literature using the above mentioned numerical methods wherever possible.]

THIRD SEMESTER
Course No. CHEM 0901 (FM = 50; C = 4)
(Common Paper)

Unit 1 Elementary Group Theory and Application of Symmetry (M = 20)

Introduction, symmetry elements and group theory, group theory and quantum mechanics (elementary ideas), elementary ideas of representation theory, irreducible representations of point group, definitions of classes and character, statement of grand orthogonality theorem, orthogonality theorem for characters, character tables, concept of character projection operator.

Selection rules in molecular spectroscopy, electronic spectroscopy and crystal field theory. SALC – Hückel, Hybridization. Vibration of polyatomic molecules – normal modes, their symmetry properties and IR activity.

Unit 2 Materials Chemistry (M = 08)

Classification of polymers, kinetics of two dimensional polymerization, condensation and addition polymerizations; initiation, propagation and termination; chain transfer, co-polymerization; molecular weight of polymers; determination of molecular weights.

Unit 3 Biophysical Chemistry (M = 07)

Structure of Biomolecules: Protein structure – building blocks, peptide bond, levels of structure; Biomolecular complexes: protein-ligand, enzyme-substrate.

Techniques for study of biomolecular structure and function- optical techniques: CD, ORD: Cotton effect, Faraday effect. Fluorescence anisotropy for biomolecular structure determination.

Unit 4 Spin Magnetic Resonance Spectroscopy (M = 15)

Magnetic resonance spectroscopy – introduction, basis features of spectroscopy, relaxation processes: spin-spin and spin-lattice.

NMR: chemical shift and spin-spin coupling; chemical shielding – elementary idea of diamagnetic and paramagnetic shielding.

ESR: ESR spectrometer, line width, hyper-fine splitting, ESR of triplet state, applications.

Course No. CHEM 0902 (FM = 50; C = 4)
(Common Paper)

Unit 1 FT NMR, FT IR, 2D NMR, Mass spectrometry (M = 18)

Fourier transformations, time domain versus frequency domain. Principles of FT NMR, instrumentation, the rotating frame of reference, simple 1D experiments. FT IR – principles and instrumentation.

Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE, INDOR, INEPT for simple compounds and problems. Applications of multinuclear NMR in inorganic compounds – Examples from ^{1}H, ^{11}B, ^{13}C, ^{19}F, ^{31}P. NMR of paramagnetic molecules – Lanthanide shift.

Mass spectrometry: Fragmentation processes and structural analysis; ESI, GC/MS, LC/MS and MS/MS techniques. Interpretation of spectroscopic (NMR, IR and mass) data, as applied to organic, inorganic and biological systems.

Unit 2 Electronic Spectroscopy (Absorption and Emission) (M = 15)

Qualitative treatment of Born-Oppenheimer separation, Frank-Condon principle, selection rules, characteristics of π-π*, n-π*, d-d transitions and their intensities. Apparent violation of selection rule (vibrational and spin-orbit couplings). Potential energy curves, mirror-image symmetry, deactivation – internal conversion and intersystem crossing, radiationless deactivation, fluorescence and phosphorescence. Quenching of fluorescence, Life-time variation in presence of quencher. Excimers and exciplexes. Intermolecular energy transfer (FRET). Energy transfer and conformation distributions of biopolymers, protein fluorescence. Excited state proton transfer. Einstein theory – A, B coefficients, Principles of LASER and characteristic features.

Unit 3 Supramolecular Chemistry (M = 09)

Introduction, Origins and Concept. Molecular recognition. Host-guest complex. supramolecular orbitals, non-covalent forces: soft interactions, Supramolecular reactivity and catalysis. Self-assembly and self-organisation, Liquid crystals and supramolecuar polymers, polymer-surfactant interaction. Nanoparticles and nanomaterials, elementary idea of synthesis, nano-composites, applications (special attention in drug design). Molecular sensors and supramolecular devices. Microporous materials, microgels, bioconjugate polymers, Nanoencapsulation.

Unit 4 Mossbauer spectroscopy, PES, XPS and Applications (M = 08)

Principles of Mossbauer spectroscopy: experiments, center shift, quadrouple interaction, magnetic interaction. PES - photoexcitation and photoionisation; XPS - principle and applications.

Course No. CHEM 0903A (FM = 50; C = 4)
(Organic Special)

Unit 1: Stereochemistry of polycyclic system (M = 14)

Conformation and reactivity of fused polycyclic systems – perhydrophenanthrenes, perhydroanthracenes, steroids; Stereochemistry of reactions – nucleophilic additions to cyclic ketones, Cieplak model; directed nucleophilic additions.

Unit 2 Organic Photochemistry and Radical Reactions (M = 18)

Photochemistry: Photolysis of carbonyl compounds and nitrites: Norrish Type I and Type II processes, β-cleavage, Barton reaction. Photoreduction and Photoexcitation; Photorearrangements in cyclohexanones and cyclohexadienone systems; Photorearrangements of α-tropolone methyl ether, di-π-methane rearrangement (cyclic system) Photochemistry of organic compounds: photoisomerisation, phodimerisation, cycloadditions of benzene and its derivatives.

Radical Chemistry: Generation and detection of radicals, radical initiators, reactivity pattern of radicals, substitution, addition and cyclization reactions; Radical cations and radical anions, single electron transfer reactions.

Unit 3: Chemistry of Natural Products (Synthesis and Biosynthesis) (M = 18)

Introduction: Primary and secondary metabolites, biogenetic hypothesis, elucidation of biosynthetic pathways; Biosynthesis of terpenoids and steroids; Shikimic acid pathway: Biosynthesis of flavonoids; Biosynthesis of alkaloids; Synthesis and biosynthesis of polyketides, fatty acids and prostaglandins; Reactions and synthesis of steroids: cholesterol, bile acid, testosterone, estrone, progesterone; Structure and synthesis of porphyrins: haemoglobin, chlorophyll.

Course No. CHEM 0903B (FM = 50; C = 4)
(Inorganic Special)

Unit 1 Chemical Application of Group Theory (M = 17)
Importance of group theory in inorganic chemistry, splitting of orbital and free ion terms in crystal fields, quantitative relationship between Oh & Td splittings, construction of energy level in infinitely strong crystal field, the effect of distortion on d-energy levels, vibronic coupling and vibronic polarization, utilization of symmetry and group theory in constructing the MO diagrams of polyatomic molecules, coordination complexes including metallocene complexes. Symmetry of normal vibration, normal mode analysis, selection rules for IR and Raman transitions.

Unit 2 Magnetochemistry (M = 18)
Definition of magnetic properties, types of magnetic bodies, Curie equation, Curie's law and Curie-Weiss law. Anisotropy in magnetic susceptibility, diamagnetism in atoms and polyatomic system, Pascal's constants, two sources of paramagnetism, spin and orbital effects, spin-orbit coupling, Lande interval rule, energies of J levels, first order and second order Zeeman effects, temperature independent paramagnetism, simplification and application of van Vleck susceptibility equation, quenching of orbital moment, magnetic properties of transition metal complexes, low spin, high-spin crossover, magnetic behavior of lanthanides and actinides, magnetic exchange interactions. Experimental arrangements for determination of magnetic susceptibility: Gouy method, Faraday method, Evans method, SQUID.

Unit 3 Solid state chemistry and X-ray crystallography (M = 15)

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap, metal and semi-conductors – intrinsic and extrinsic semiconductors; semiconductor/metal transition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory. Dia-, para- and ferromagnetism. Defects in solids.

The geometry of crystalline state; Nature and generation of X-rays, Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals, Bragg's law, 1, 2 and 3 dimensional Laue equations, atomic scattering factor, structure factor, systematic absences, Determination of space groups and crystal structures.

Course No. CHEM 0903C (FM = 50; C = 4)
(Physical Special)

Unit 1 Statistical mechanics- II (M = 15)

Introduction: Concept of ensemble and ergodic hypothesis, phase space; microcanonical ensemble, temperature; canonical ensemble distribution, probability distribution function, its relation with different thermodynamic state functions; Gibbs paradox and Sackur-Tetrode equation; Chemical equilibrium and equilibrium constant in terms of partition functions, equipartition theorem and its validity; chemical potential and chemical equilibrium – Saha ionization formula; system of interacting molecules – imperfect gas. Grand canonical ensemble – nature of quantum particles; Bose-Einstein and Fermi-Dirac distributions; black body radiation and photon gas, Bose-Einstein condensation.

Unit 2 Dielectric behaviour and solvent effect (M = 10)

Dielectric behaviour and solvent effects: Limitation of Mossotti-Clausius, Debye equation, deviation from Debye's theory; Onsager reaction field; dielectric relaxation, frequency dependent dielectric property, relaxation time, Debye semicircle; Solvent effect on the emission and absorption spectra - non-specific and specific interactions (H-bonding and charge transfer). Characteristics of CT interaction; Lippert equation; time resolved spectroscopy and the dielectric relaxation effect.

Unit 3 Solid state chemistry and X-ray crystallography (M = 15)

Bonding in metal crystals: free electron theory, electrical conductivity, band theory, band gap, metal and semi-conductors – intrinsic and extrinsic semiconductors; semiconductor/metal transition, p-n junctions, superconductivity, Bardeen, Cooper and Schriefer (BCS) theory. Dia-, para- and ferromagnetism. Defects in solids.

The geometry of crystalline state; Nature and generation of X-rays, Production of monochromatic X-rays, Scattering of X-rays, Diffraction of X-rays by crystals, Bragg's law, 1, 2 and 3 dimensional Laue equations, atomic scattering factor, structure factor, systematic absences, Determination of space groups and crystal structures.

Unit 4 Kinetics - II (M = 10)

(a) Rate constant expression for chemical reaction based on Eyring equation with one example.

(b) Physical rate processes – viscosity and diffusion.

(c) Non- equilibrium formulation: Passage to statistical approach – energy redistribution in activated complex, Lindemann collision, Hinshelwood suggestion, Rice-Ramsperger-Kassel (RRK) theory.

(d) Reaction in solution. Diffusion-controlled reactions.

Course No. CHEM 0991A (FM = 50; C = 4)
Organic Special Practical-I

Preparation of organic compounds by typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PC, determination of Rf value as required, m.p/b.p.].

Characterization of organic compounds by spectroscopic means.

Course No. CHEM 0992A (FM = 50; C = 4)
Organic Special Practical-II

Multistep Organic Preparation. Extraction and Purification of Natural Products and Biomolecules.

Course No. CHEM 0991B (FM = 50; C = 4)
Inorganic Special Practical-I

(a) Quantitative estimation of inorganic ions by colorimetry/ion-exchange method

i) Separation and estimation of the following binary mixtures: Mg^{2+} - Zn^{2+}; Zn^{2+} - Cd^{2+}

ii) Colorimetric determination of 1) Fe^{3+} as sulphosalicylate complex 2) Fe^{2+} as phenanthroline complex 3)Manganese as MnO_4^- 4) Chromium as $Cr_2O_7^{2-}$ (any two).

(iii) Quantitative analysis of complex inorganic materials *viz.* ores, minerals and alloys etc. by conventional method. (any one)

(b) Physicochemical Experiments:

i) Determination of composition of complexes by continuous variation/ Mole-Ratio / Slope ratio method of the following systems: Fe (III) – sulphosalicylate complex; Fe (II) - phenanthroline complex

ii) A conductance study of the kinetics on inorganic reaction.

iii) A colorimetric study of the kinetics on inorganic reaction.

Course No. CHEM 0992B (FM = 50; C = 4)
Inorganic Special Practical-II

Synthesis and characterization of Inorganic Compound

Preparation of transition metal complexes and their characterization

Course No. CHEM 0991C (FM = 50; C = 4)
Physical Special Practical – I

1. Principle of Sensors – colour, current, pressure, light.
2. Signal amplification and Computer interfacing.

Course No. CHEM 0992C (FM = 50; C = 4)
Physical Special Practical – II

1. Kinetic experiments- study of primary kinetic salt effect, Oscillatory reaction, study of the effect of temperature.
2. Spectrofluorimetric experiments - study of quenching, energy transfer.
3. Fabrication of a spectrophotometer: LED, photodiode, signal transfer to a computer – use in conjugated polyenes, 1D box problem, chemical kinetics.

FOURTH SEMESTER
Course No. CHEM 1001A (FM = 50; C = 4)
Organic Special-I

Unit 1: Organotransition Metal Chemistry: Applications to Organic Synthesis (M = 17)

Electron counting, bonding, organometallic reaction mechanism; Homogeneous hydrogenation; Organometallics as electrophiles; Synthetic applications of transition metal alkene complexes: Wacker oxidation. Synthetic applications of complexes containing metal – carbon σ bonds: Heck and related reactions, carbonylation reactions; Synthetic applications of transition metal carbene complexes: Fischer carbene, Schrock carbene, metathesis processes, Tebbe's reagent, Zieglar – Natta reaction; Synthetic applications of transition metal alkyne complexes: Pauson – Khand reaction, cyclooligomerisation; Applications of transition metal complexes in the synthesis of: cyclic enediynes, estrone by Volhardt, clavicipitic acid by Hegedus.

Unit 2: Asymmetric Synthesis (M = 16)

Principles; Addition to carbonyl compounds: use of chiral substrate, chiral reagent, chiral catalyst; Stereoselective reactions of carbonyl compounds: enolate formation, alkylation, asymmetric aldol reactions; Stereoselective reactions of alkenes: Diels-Alder reaction, sigmatropic rearrangement, stereoseletive hydrogenation, epoxidation, hydroxylation, aminohydroxylation, cyclopropanation; Kinetic resolution; Asymmetric synthesis of menthol (Takasago), crixivan (Merck)

Unit 3: Synthesis of complex and biologically important molecules Applying Modern reagents and methodologies (M = 17)

A. **Organic synthesis**: (i) Target-oriented synthesis – natural products, designed molecules (ii) Method-oriented synthesis – reagents, catalysts, synthetic strategies and tactics. Retrosynthetic analysis: Selected total synthesis of natural products like Taxol, Tetracycline antibiotics etc.

B. **Synthetic methodology and strategy of few compounds**: (i) cationic cyclisations: progesterone (Johnson) (ii) radical cyclisations: synthesis of hirsutene (Curran) (iii) pericyclic reactions: endiandric acids (Nicolaou); (iv) Photochemical reactions: strained compounds (isocomene by Pirrung) (v) aldol reactions: Prelog-Djerassi lactone; (vi) carbene reactions: making cyclopropanes (vii) biomimetic strategy: carpanone (Chapman) (viii) solid-supported reagents, solid phase synthesis: plicamine (Ley) (ix) combinatorial synthesis etc.

Course No. CHEM 1001B (FM = 50; C = 4)
Inorganic Special-I

Unit 1 Spectroscopy - Applications to Inorganic Systems (M = 20)

Electronic spectroscopy: Orgel diagrams, correlation between weak field and strong field terms. Tanabe-Sugano diagram, bonding parameters and structural evidences from electronic spectra of d-metal complexes, f-f transition, lanthanide and actinide spectra. Applications of IR, Raman, ESR and Mossbauer spectroscopy to inorganic and bioinorganic systems, NMR spectra: ^{11}B, ^{13}C, ^{19}F, ^{27}Al, ^{31}P NMR spectroscopy with typical examples, ^{1}HNMR spectra of coordination compounds of paramagnetic metal ions, dipolar and contact shifts, magnetic susceptibility and resonance shift. NQR spectroscopy: Principle, nuclear quadruple coupling constants, structural information from NQR spectra. Applications of CD and MCD; stereoselective and stereospecific effects.

Unit 2 Nuclear Chemistry & Radiochemical Analysis (M = 15)

Nuclear models – Nuclear forces, liquid drop model, Fermigas model, Shell model. Magic numbers. Nuclear spin and nuclear isomerism. Nuclear reactor and particle accelerators. Interaction of radiation with matter. Detection and measurement of radiation – proportional
counter, scintilater and detector. Radiation dosimetry. Chemical effects of nucleartransmutation (elementary idea), radiolysis of water. Application of radioactivity in geochemistry and cosmochemistry, methods of age determination, radioactive analysis. Tracer techniques: study of chemical reactions, isotopic exchange reactions, kinetic isotope effect. Radiation chemistry, carrier free tracers. Radiation hazards.

Unit 3 Inorganic Rings, Cages & Clusters (M = 15)

Metal-metal bonding (MO approach), metal-metal single and multiple bonded compounds involving transition and nontransition metals, Zintl ions, bridging and semi-bridging carbonyls. Low nuclearity and high nuclearity carbonyl clusters: Skeletal electron counting, Wade- Mingos-Lamther rule, application of isoelectronic and isolobal relationships, caping rules; carbide, nitride, chalcogenide and halide containing clusters; Nb, Ta and Mo clusters; one dimensional solids, solid state extended arrays, Chevrel phases. Cluster compounds in catalysis.

Course No. CHEM 1001C (FM = 50; C = 4)

Physical Special - I

Unit l Quantum Mechanics - II (M = 10)

Vector space, matrix representation of operators, Hermitian operators and matrices, Virial theorem, parity, time reversal symmetry; angular momentum operator – commutation relation, set-up and set-down operators, angular momentum operators in polar coordinates, angular momentum eigenfunctions: solutions from corresponding eigenvalue equation.

Many electron Hamiltonian, its communication with composite L^2 and L_z; spin operator and Pauli spin matrices; many electron atom and construction of wavefunction representing spectroscopic state; projection operators and their properties – projection operator technique and angular momentum.

Unit 2 Non-equilibrium phenomena (M = 15)

(a) Einstein's theory of Brownian motion; Langevin's description of Brownian motion; Brownian motion in velocity space and the Fokker-Planck equation; elements of Kramers' theory.

(b) Equation of continuity and conservation laws (Liouville's equation), Mathematical details of Gauss theorem, Properties of thermodynamic fluctuations, regression of fluctuation and laws of irreversible thermodynamics and their application, Linear response theory.

Unit 3 Molecular Reaction Dynamics (M = 10)

Reaction dynamics: Introduction, molecular dynamics – intermolecular collision and its consequence; role of intermolecular potential, reaction cross-section, energy threshold, reaction probability; angular distribution in relative collision; scattering in velocity space; electronic energy transfer; experimental methods in connection with molecular dynamics; chemiluminescence; chemical laser; crossed molecular beam; photofragmentation spectroscopy.

Unit 4 Advanced Electrochemistry (M = 15)

Limitation of Debye-Hückel limiting law and its extension; Pitzer ion-interaction approach. Debye-Hückel-Onsagar (DHO) theory of electrical conduction of electrolytes, electrophoretic and relaxation effects, Wien effect,

Debye-Falkenhagen effect, application of DHO theory. Limitation of DHO equation and Shedlovsky approach.
Double layer studies: nature of the double layer across electrode-solution interface, polarizable and non-polarizable electrodes, electrocapilarity (EC) – nature of EC curves, its thermodynamics, Lipmann equation, Helmholtz, Guoy-Chapman and Stern double layer models. Electron transfer reactions; fuel cells.

Course No. CHEM 1002A (FM = 50; C = 4)
Organic Special-II

Unit 1: Advanced Heterocyclic Chemistry (Two and more heteroatom)

(M = 17)

Synthesis and reactivity of 5,6-membered rings containing two heteroatoms, pyrimidines and purines. Introduction to chemistry of azepins, oxepins, thiepins and their analogues; phosphorous and selenium containing heterocycles with the use of modern reagents. ANRORC and Vicarious nucleophilic substitutions in heterocycles.

Unit 2: The molecules of life (M = 16)

Introduction: The molecules of life – nucleic acids, proteins and enzymes, carbohydrates, lipids. Mechanism in biological chemistry: (i) Mechanism of enzyme action, examples of enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A (ii) Enzyme catalysed reactions – examples of nucleophilic displacement on a phosphorus atom, coupling of ATP cleavage to endergonic processes, proton transfer reactions to and from carbon (iii) Mechanism of reactions catalysed by cofactors including coenzyme A, NAD^+, NADH, FAD and thiamine pyrophosphate; Chemical synthesis of peptides and proteins; Use of enzymes in organic synthesis; Structural analysis of proteins; Protein folding; Biotechnological applications of enzymes: Enzyme purification, immobilization of enzymes, enzyme therapy, enzyme and recombinant DNA technology.

Unit 3: Chemistry of Medicinally Important Molecules (M = 17)

Bacterial and animal cells, antibacterial agents – mechanism with reference to β-lactam antibiotics; General method of synthesis of β-lactam ring: synthesis of penicillin, 6-APA, cephalosporin, 7-ACA; Morin – Jackson rearrangement; Structure-activity relationship of penicillin. New generation antibiotics / antibacterial agents: Synthesis and mechanism of action of (i) fluoroquinolones – norfloxacin, ciprofloxacin, levofloxacin (ii) anti AIDS drugs – AZT, lamivadine (iii) antihypertensive agent – captopril (iv) calcium channel blocker – amlodipine (v) gastric secretion inhibitor – omeprazole (vi) drug for impotency – sildenafil etc.

Course No. CHEM 1002B (FM = 50; C = 4)

Inorganic Special-II

Unit 1 Inorganic Reaction Mechanism (M = 18)

Mechanism of substitution reactions: Solvent exchange, aquation, anation, base hydrolysis, acid catalysed aquation, pseudo-substitution. Four board classes of mechanism of substitution – 'D', 'A', 'Ia' and 'Id' Mechanism of isomerisation reaction–linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racemisation, Ray– Dutta and Bailar twist mechanisms. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, selfexchange reactions. Outer sphere and inner sphere reactions, applications of Marcus expression (simple form), redox catalysed substitution reactions.

Inorganic Photochemistry: Excitation modes in transition metal complexes, fate of photo excited species; photochemical processes: Photosubstitution and photoelectron transfer reactions in Co, Cr and Rh-complexes.

Unit 2 Chemistry of Complex Equilibria (M = 16)

Characteisation of stability of mononuclear, polynuclear and mixed –ligand complexes in solution, determination of composition and stability constants of complexes by pH metric, spectrophotometric and polarographic methods, DTA, TGA. Conditional stability constants and their importance in complexometric (EDTA) titrations and solvent extraction of metal ions. Statistical and non-statistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes. Soluility Equilibria – quantitativeness of precipitation (of metal hydroxides, sulphides and chelates).

Unit 3 Bioinorganic Chemistry (M = 16)

Uniqueness of metal ion as bioelements. Interaction of metal ions with biomolecules, Metal ion in metabolic energy transfer and ATP hydrolysis; Genetic information transfer; replication, transcription and translation processes. Metalloproteins and metalloenzymes Oxygen uptake proteins:- hemoglobin and myoglobin; Electron transport proteins: – cytochromes (specially cytochrome C), ferridoxins; metalloenzymes: – catalase, peroxidase, urease, superoxide dismutase (SOD), cytochrome P 450, cytochrome C oxidase, carbonic anhydrase, carboxypeptidase; molybdoenzymes; respiratory electron transport chain and photosynthetic electron transport chain, Toxic metal ions and their effects, chelation therapy, Pt and Au complexes as drugs, metal dependent diseases.

Course No. CHEM 1002C (FM = 50; C = 4)
Physical Special-II

Unit 1 Quantum mechanics - III (M = 15)

Perterbation theory (PT) – Rayleigh-Schrödinger PT for non-degenerate states theorem, some simple applications: expression for polarizability, ground state of helium atom; degenerate state PT – Stark effect, lifting of degeneracy by application of a magnetic field (e.g. , the $^{1}P_{1}$ state of helium atom) variation method – Euler variation, principle and Rayleigh-Ritz variation theorem, applications.

Quantum chemistry: Born-Oppenheimer approximation, theories of valence, the MO and VB methods for H_2 molecule – their relative merits, dissociation curve, excited state, configuration interaction.

Many electron systems – its charectaristics, independent particle model (IPM), Hartree and Hartree-Fock methods for closed shell (elementary ideas).

Unit 2 Quantum mechanics and spectroscopy (M = 20)

Time dependent perturbation theory – semiclassical treatment of interaction of matter with radiation, first and second order effects, Fermi golden rule, selection rule, selection rule for vibrational spectra, anharmonicity correction by perturbation – appearance of overtones; selection rule for rotational spectra, nucleur spin and rotational energy levels, stark effect revisited.

Raman scattering: selection rule for rotational and vibrational raman spectroscopy.

Quantum mechanical theory of magnetic resonance; Bloch equations and their solutions; theories of shielding – diamagnetic and paramagnetic shielding.

Unit 3 Advanced Group theory (M = 15)

Representation of symmetry operator – transformation of basis vector, general vector and functions under symmetry operations; symmetry transformation of operators and operator equation; invariance of the Hamiltonian under symmetry operation; vector space and representation theory, reducible and irreducible representations, concepts of classes and character; Wave functions as the basis of irreducible representations..

Great orthogonality and related theorems, construction of character table, reduction formula and projection operators, direct product representation, theorem on vanishing marix elements; applications of the projection operator technique and the direct product representation.

Course No. CHEM 1003 (FM = 50; C = 4)
Seminar/Review and Grand Viva

1. Seminar/Review (M = 30)
2. Grand viva (M = 20)

Course No. CHEM 1091 & CHEM 1092 (FM = 50 + 50)
Project Work

1. Project dissertation and presentation
2. Project viva
3. Project based Course work

Alternate proposal

Course No. CHEM 1091 (FM=50)
Project dissertation and presentation

CHEM 1092 (FM=50)
1. Project viva
2. Project based Course work/lit. survey