

Department of Chemistry
R. K. M. Residential College (Autonomous)
Narendrapur, Kolkata – 700103

M. Sc. Chemistry New Syllabi - 2015

All the units of Semesters I and II are compulsory. The first 1-6 units for Semester III and IV each carrying a total of 100 marks (2x18 + 4x16) are compulsory. Choose only 3 units out of the units 7-15 for Semester III and IV each carrying a total of 50 (1x18 + 2x16) marks. Marks distributions of the course are summarized below. In order to teach one unit, enrollment of 4 students is essential. If necessary number of students in any specialization will be restricted and it will be done on the basis of the theoretical marks obtained in the M. Sc. Semester-I Examination.

Sem I	Theoretical			Practical			Total Marks	
	Paper I (Organic)	Paper II (Inorganic)	Paper III (Physical)	Paper IV				
				Unit-1 (Org) 34 M	Unit-2 (Inorg) 33 M	Unit-3 (Phy) 33 M	250	
	50M	50M	50M	100M				
Sem II	Paper V (Organic)	Paper VI (Inorganic)	Paper VII (Physical)	Paper VIII			250	
				Unit-1 (Org) 34 M	Unit-2 (Inorg) 33 M	Unit-3 (Phy) 33 M		
	50M	50M	50M	100M				
Sem III	Paper IX&X (Advanced General Chemistry)	Paper XI (Organic or Inorganic or Physical Special or mixed)		Paper XII				250
				Unit-1 (Org) 25M	Unit-2 (Inorg) 25M	Unit-3 (Phy) 25M	Unit-4 (Computer) 25M	
	50M+50M	50M		100M				
Sem IV	Paper XIII&XIV (Advanced General Chemistry)	Paper XV (Organic or Inorganic or Physical Special or General)		Paper XVI			250	
				Unit-I (Grand Viva by External Experts on Specialization or General) 50M	Unit-II Practical (Inorg/Org/Physical) 25 M	Unit-III Projects/Review 25M		
	50M+50M	50M		100M				

Organic Specialization	Units 7, 8 and 9 of Semesters III & IV
Inorganic Specialization	Units 10, 11 and 12 of Semesters III & IV
Physical Specialization	Units 13, 14 and 15 of Semesters III & IV
M. Sc. (General)	Mixed units of Organic, Inorganic and Physical specialization

Sem-I (250 M)

Paper-I (Organic Chemistry)		50 M
Unit-1	Bonding in Organic Compounds: (20-22)L Qualitative M.O. approach to bonding in organic molecules, Huckel's rule and its applications to ethylene, cyclopentadiene, butadiene, cyclobutadiene. Walsh orbitals of cyclopropane. Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerene, tautomerism. Huckel's approach to conjugated systems, concept of aromaticity (η) in benzenoid and non benzenoid compounds, alternate and non-alternate hydrocarbons,. Energy level of pi-molecular orbitals; annulenes and heteroannulenes, fullerenes (C_{60}), antiaromaticity pseudo - aromaticity, homo aromaticity - PMO approach. Bonds weaker than covalent bond-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catanates and rotaxanes. Stability of carbocations, strained organic molecules, calculation of strain energies.	16
Unit-2	Stereochemistry and Conformational Analyses : (20-22)L Elements of symmetry, chirality, molecules with more than one chiral center, point groups, nomenclature: threo- and erythro- isomers, methods of resolution and optical purity, enantiotopic and diastereotopic atoms, groups and faces. Conformational analysis- acyclic systems up to 4 chiral centers, cyclohexane, cyclohexanone, cyclohexene; decalin, conformation of sugars. Effects of conformation on the reactivity of acyclic compounds and cyclohexanes. Stereochemistry of monocyclic, bicyclic and tricyclic systems (typical examples). Optical activity in absence of chiral carbon (biphenyls, allenes and spirans), chirality due to helical shape. Stereochemistry of organo nitrogen-, sulfur- and phosphorus- compounds.	16
Unit-3	Heterocyclic Chemistry; (20-22)L Synthesis and reactions of heteroaromatics containing one hetero atom. General approaches to heterocycle synthesis – cyclisation and cycloaddition routes. Umpolung, synthon approach; Stork annulation reactions and recent applications i.e. synthesis of Ranitidine, Omeprazole, Lansoprazole etc.	18
Paper-II (Inorganic Chemistry)		50 M
Unit-1	Chemical Bonding: (20-22)L LCAO-MO and VB treatments on H_2^+ , H_2 ; application to homo- and hetero- nuclear diatomic molecules/ ions of second period elements, Importance of bond order, MO's of diatomic and polyatomic molecules BeH_2 , H_2O , NH_3 , CH_4 .	18
Unit-2	Theory of Coordination Chemistry: (20-22)L <i>Crystal Field Theory:</i> Splitting of d orbitals in crystal fields of different symmetry for similar and dissimilar ligands (Octahedral, tetrahedral, Linear, trigonal planar, trigonal bipyramidal, square pyramid), crystal field stabilization energies (CFSE), spectrochemical series, octahedral site preference energy (OSPE) and their applications. Tetragonal distortion (John-Teller effect). Thermodynamic aspects of crystal field splitting (variation of ionic radii, lattice energy, hydration enthalpy and stability constants of complexes – Irving Williams order). Kinetic aspects of crystal field stabilization: crystal field activation energy, labile and inert complexes. Spin and orbital moments, spin-orbit coupling, quenching of orbital moment, spin only formula, temperature dependence of magnetic moment, Super exchange Phenomena, Diamagnetic Corrections. Dependence of Orbital contribution on the nature of the electronic ground state.	16

Unit-3	Chemistry of d- and f- Block Elements: (Comparison) (20-22)L Electronic configuration, oxidation states; aqueous, redox and complex chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d,4d, and 5d elements with references to Ti-Zr- Hf, Cr- Mo- W, Mn-Tc-Re and Pt group metals. Occurrence and isolation in respect of Mo, W, Re, Pt. Synthesis, properties, reactions, structure and bonding as applicable in respect of: Mo-blue, W-blue, Pt-blue, W-bronze, Ru-red, Creutz- Traube complexes, Vaska's complexes. <i>Lanthanide and Actinide Elements</i> ; Nuclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox- and complex- chemistry; electronic spectra and magnetic properties. Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples).	16
Paper-III (Physical Chemistry)		50 M
Unit-1	Thermodynamics: (20-22)L <i>Classical Thermodynamics</i> ; Brief resume of the laws of thermodynamics, of concepts of enthalpy, free energy, chemical potential and entropies. Gibbs- Helmholtz equation. Chemical equilibrium: free energy and entropy of mixing. Partial molar properties: partial molar free energy, partial molar volume, partial molar heat content and their significances. Gibbs-Duhem equation. <i>Statistical Thermodynamics</i> ; Thermodynamic probability and entropy, Maxwell-Boltzman, Partition function: rotational, translational, vibrational and electronic partition functions of diatomic molecules, calculation of thermodynamic functions and equilibrium constants. Theories of heat capacities of solids. Concept of ensemble and ergodic hypothesis phase space. Microcanonical ensemble, Canonical ensemble distribution probability partition function, its relation with different thermodynamic state functions. Gibb's paradox and Sackur- Tetrode equation. Concept of thermal wave length. Equipartition theorem and its validity. Chemical potential and chemical equilibrium. Heat capacity of solids.	18
Unit-2	Surface Chemistry and dielectric Behavior: (20-22)L <i>Surface phenomena</i> : Vapour pressure over curved surface, the Young- Laplace equation, vapour pressure of droplets (Kelvin equation). The adsorption isotherms (Gibbs, Langmuir), BET equation, estimation of surface area. Surface active agents and their classification, Surface films on liquids, micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles. Study of surface phenomena by photoelectron spectroscopy, ESCA and Auger spectroscopy. Catalytic activity at surfaces. <i>Dielectric Behaviour</i> : Dielectric polarization and solvent effect, polar molecules, Mossotti-Clausius relation and its limitations, Debye equation. Dipole moment and molecular structure. Intermolecular forces: attraction and repulsion potentials, van der Waals, Keesom, Debye and London forces and their relative contributions. Onsager reaction field, dielectric effects on absorption and emission spectra.	16
Unit-3	Molecular Spectroscopy: (20-22)L The rigid diatomic rotor, energy eigenvalues and eigenstates, selection rules, intensity of rotational transitions, the role of rotational level degeneracy, the role of nuclear spin in determining allowed rotational energy levels. Classification of polyatomic rotors and the non-rigid rotor. Vibrational spectroscopy, harmonic and anharmonic oscillators, Morse potential, mechanical and electrical anharmonicity, selection rules. The determination of anharmonicity constant and equilibrium vibrational frequency from fundamental and overtones. Normal modes of vibration, G and F matrices, internal and symmetry coordinates. Raman spectroscopy, polarizability and selection rules for rotation and vibrational Raman spectra.	16

Paper-IV (Practical)		100 M
Unit-1	<p>Organic: 20 + 5 (LNB) + 5 (Viva)+4 (IAs) Examination: 6 hr</p> <p>Experiment-1: Chemical separation of organic compounds and Identification. Experiment-2: Separation, purification and identification of organic compounds in binary mixtures (two solids, one solid + one liquid) using TLC, PC, column chromatography, chemical tests, UV-, IR- spectral measurements as required.</p>	34
Unit-2	<p>Inorganic: 20 + 5 (LNB) + 5 (Viva)+3 (IAs) Examination: 6 hr</p> <p>Spectrophotometric Estimations: (i) Fe^{III} as [Fe^{III}(SCN)²⁺] complex (ii) Mn as MnO₄⁻ (iii) Phosphate as phosphomolybdate blue complex (iv) Fe^{III} and Fe^{II} in mixture as [Fe^{II}(1,10-phenanthroline)₃²⁺] complex. Estimations based on ion-exchange separation, acid-base, complexometric and argentimetric titrations. Hardness of water, separation of (i) Zn^{II} + Mg^{II} (ii) Cl⁻ + Br⁻ mixtures.</p>	33
Unit-3	<p>Physical: 20 + 5 (LNB) + 5 (Viva)+3 (IAs) Examination: 6 hr</p> <p>Student will practice six experiments taking at least one from each group:</p> <p>Group-a: Phase-rule; 1. Determination of critical solution temperature (system: phenol-water) 2. To construct the phase diagram of a three component system: (i).Chloroform-acetic acid-water (ii). Benzene-acetic acid-water (iii). Nitrobenzene-acetic acid-water Group-b: Adsorption; 3. To study the surface tension – concentration relationship of solutions (Gibbs equation) Group-c: Kinetics; 4. Determination of rate constant of reactions: (i). Iodination of acetone (zero order) (ii). Decomposition of H₂O₂ (first order) (iii). Oxidation of iodide ion by bromate ion (second order) 5. Determination of rate constant of oxidation of iodide by H₂O₂ and to study the kinetics of iodine-clock reaction Group-d: Thermodynamics & Equilibrium; 6. Determination of exchange capacities of ion-exchange resins and studies on ion-exchange equilibria. 7. Determination of solubility and solubility product of salts (systems: PbI₂, Potassium hydrogen tartarate) 8. Determination of partition coefficients of a solute between two immiscible solvents (systems: benzoic acid between benzene and water) 9. Determination of composition of complexes formed in solution (systems: Cu²⁺ - NH₃, Ag⁺ - NH₃). 10. Determination of equilibrium constant of hydrolysis of an ester. 11. Determination of isoelectric point by viscosity measurement</p>	33

Sem-II (250 M)

Paper-V (Organic Chemistry)		50 M
Unit-1	Pericyclic Reactions: (20-22)L Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams. FMO and PMO approach, concept of aromaticity of pericyclic transition states. Selection rules and stereochemical aspects of electrocyclic reactions, cycloaddition and sigmatropic shifts. Electrocyclic reactions: conrotatory and disrotatory motions, $4n$, $4n+2$ and allyl systems. Cycloaddition reactions: antarafacial and suprafacial additions, $4n$ and $4n+2$ systems; 2,2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements. Sommelet-Hauser, Cope, Claisen, and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.	18
Unit-2	Organic Reaction Mechanism: (20-22)L <i>Addition to C-C multiple bonds</i> : Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Hydrogenation of double and triple bonds and aromatic rings. Hydroboration reaction, Sharpless asymmetric epoxidation. <i>Addition to Carbon- Hetero Multiple Bonds</i> : Mechanism of metal hydride reaction of substituted and unsubstituted carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organo-Zn and organo-Li and organo Si reagents to saturated and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation involving enolates:	16
Unit-3	Chemistry of Natural Products-I (20-22)L Structural types; Biogenesis; Structure Elucidation and chemistry of representative examples of the following classes of natural products. Alkaloids- Structural types- General introduction to phenylethylamine, pyrrolidine, pyridine, indole, isoquinoline type alkaloids. Structure elucidation (by chemical and spectroscopical methods), synthesis, biogenesis, biosynthesis, biological activity of atropine, nicotine, coniine and papaverine. Terpenoids – Isoprene rule; structure elucidation (by chemical and spectroscopical methods), synthesis, biogenesis, biosynthesis of representative examples of acyclic, monocyclic and bicyclic monoterpenes. Structural types – general introduction to sesqui-, di-, and tri-terpenes.	16
Paper-VI (Inorganic Chemistry)		50 M
Unit-1	Organometallics: (20-22)L Classification, synthesis, reactions, structure and bonding and applications with typical examples. Application of 18- electron and 16- electron rules to transition metal organometallics, structure, bonding (pictorial MO-approach) and reactions of η^2 - ethylenic, η^3 -allylic and η^5 - cyclopentadienyl compounds: $K [Pt (\eta^2 -C_2 H_4)Cl_3]$, $[(\eta^3 - C_3H_5) Pd Cl]_2$, $(\eta^5 - C_5H_5)_2 Fe$; carbene and carbyne complexes. Stereochemical non-rigidity and fluxional behavior of organometallic compounds with typical examples. Metal-metal single and multiple bonding (pictorial MO –approach). Bond orders, bonding in dirhenium compounds. Isolobal and isoelectronic relationships. Organometallic catalysts.	18
Unit-2	Molecular Clusters: (20-22)L Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the <i>closo</i> -, <i>nido</i> -, <i>arachno</i> -borane structural paradigm, styx No. of neutral and	16

	boron hydrides, Wade-Mingos and Jemmis electron counting rules, clusters with nuclearity 4-12 and beyond 12. Structure, synthesis and reactivity. Transition-metal clusters: Capping rules, metal-ligand complexes vs heteronuclear cluster. Main-group-Transition-metal clusters: Isolobal analogs of p-block and d-block clusters, limitations and exceptions. Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters. Metal-carbonyl clusters, structures, capping and electron counting. Molecular clusters in catalysis, clusters to materials, boron-carbides and metal-borides. Illustrative examples from recent literature.	
Unit-3	Inorganic Analyses: (20-22)L Basic principle, instrumentation, special features and applications in inorganic analysis (qualitative/ quantitative as applicable) of the following techniques. <i>Electro analytical methods</i> : Polarography: Ilkovic equation, half wave potential and its significance; amperometric, titrations, coulometry, cyclic voltametry, ion-selective electrode. <i>Thermo analytical methods</i> : TGA, DTA and DSC, thermometric titrations. <i>Flame photometric techniques</i> : AAS, AES, and atomic fluorescence methods, ICP techniques, Fluorimetric analysis. <i>UV-VIS-spectrophotometric methods</i> : Photometric titration, derivative spectrophotometry, simultaneous determination of two components in a mixture.	16
Paper-VII (Physical Chemistry)		50 M
Unit-1	Quantum Mechanics-I: Principles (20-22)L Wave particle duality, Heisenberg's microscope uncertainty principle. Genesis of Schrodinger wave equation, probability concept, concept of stationary state. Linear operators in quantum mechanics, Eigen value equation. Hermitian operator, commutation relation, expectation value, Ehrenfest's theorem. Elementary applications: free particle, potential barrier problems particle in a box, simple harmonic oscillator (wave function and operator method), variation method and their simple applications.	18
Unit-2	Quantum Mechanics-II: Applications (20-22)L The Rigid Rotor and the Hydrogen Atom Problem Cartesian and polar coordinates. Center of mass and relative coordinates. Spherical harmonics. Real and complex orbitals. Energy states. Zeeman effect, Fine structure, spin orbit interaction, effect of high magnetic field, Stern – Gerlach experiment, spin quantum number, magnetic quantum number. Lande's g factor, Atomic terms.	16
Unit-3	Chemical Kinetics and Reaction Dynamics: (20-22)L <i>Reaction Dynamics</i> : Rates and mechanisms of photochemical, chain and oscillatory reactions (hydrogen-bromine, hydrogen – chlorine reactions, pyrolysis of acetaldehyde, decomposition of ethane and Belousov-Zhabotinsky reaction as examples), dynamics of barrier less chemical reactions in solutions, dynamics of uni molecular reactions (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories). <i>Fast Reactions</i> : Luminescence and energy transfer processes. Study of kinetics by stopped-flow and relaxation methods, flash photolysis and magnetic resonance method. Statistical formulation of chemical kinetics reaction dynamics: Intermolecular collision and its consequence. Role of intermolecular potential, elastic and inelastic collision. Thermodynamics of reaction rates. Activation energy- Experimental and zero point activation energy. Rate constant expression for chemical reaction based on Eyring equation with examples. Physical rate processes –viscosity and diffusion.	16

Paper-VIII (Practical)		100 M
Unit-1	<p>Organic: 20 + 5 (LNB) + 5 (Viva)+4 (IAs) Examination: 6 hr</p> <p>Preparation of organic compounds by typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PC, determination of R_f value as required, m.p/b.p. , UV, IR spectra (as applicable)]: <i>Oxidation</i>: Adipic acid from cyclohexanol (by chromic acid oxidation). <i>Grignard reaction</i>: Triphenylcarbinol from benzoic acid. <i>Aldol condensation</i>: Dibenzal acetone from acetone and benzaldehyde. <i>Sandmeyer reaction</i>: <i>p</i>-Chlorotoluene from <i>p</i>-toluidine. <i>Cannizzro reaction</i>: Using <i>p</i>-chlorobenzaldehyde as the substrate. <i>Fridel-Craft reaction</i>: β-Benzoylpropeonic acid from succinic anhydride and benzene. <i>Acetoacetic ester condensation</i>: Ethyl <i>n</i>-butylacetoacetate from ethylacetoacetate. <i>Aromatic electrophilic substitution</i>: <i>p</i>-Nitroaniline from <i>p</i>-bromoaniline. <i>Parikin reaction</i>: Cinnamic acid from benzaldehyde and potassium acetate.</p>	34
Unit-2	<p>Inorganic: 20 + 5 (LNB) + 5 (Viva)+3 (IAs) Examination: 6 hr</p> <p>Semi-Micro Qualitative Inorganic Analysis of Complex Inorganic Mixtures containing not more than six (6) inorganic radicals from the lists : (a) Cation Radicals derived from: Pb, Bi, Cu, Sb, Sn, Fe, Al, Cr, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, Na, K and NH_4^+ ion. (b) Anion Radicals: F^-, Cl^-, Br^-, I^-, BrO_3^-, IO_3^-, SCN^-, S^{2-}, $\text{S}_2\text{O}_3^{2-}$, SO_3^{2-}, SO_4^{2-}, NO_2^-, NO_3^-, PO_4^{3-}, BO_3^{3-}, H_3BO_3, SiO_4^{2-}, CrO_4^{2-}, $\text{Cr}_2\text{O}_7^{2-}$, $[\text{Fe}(\text{CN})_6]^{4-}$, $[\text{Fe}(\text{CN})_6]^{3-}$. (c) Insoluble Materials: PbSO_4, BaSO_4, SrSO_4, PbCrO_4, CaF_2, SiO_2 and various silicates, SnO_2, Al_2O_3, Fe_2O_3, Cr_2O_3, AgCl, AgBr, AgI. (d) Cation radicals, anion radicals and insoluble materials derived from the following rare Elements: V, Mo, W, U, Ti, Zr, Ce, Th and Be.</p>	33
Unit-3	<p>Physical: 20 + 5 (LNB) + 5 (Viva)+3 (IAs) Examination: 6 hr</p> <p>(a) Conductometry: 1. Determination of strengths of strong and weak acids in a mixture conductometrically 2. Determination of strengths of halides in a mixture conductometrically by precipitation titrations 3. Determination of concentrations of halides and halogen acids in a mixture conductometrically by precipitation titrations (system: $\text{HCl} + \text{KCl}$ mixture by titration with standard NaOH and standard AgNO_3 solutions 4. Verification of Ostwald's dilution law conductometrically 5. Determination of critical micelle concentration (CMC) of a surfactant by conductometric method (b) Potentiometry / pH-metry: 6. Determination of strengths of strong and weak acids in a mixture potentiometrically / pH-metrically (system: acetic acid + HCl) 7. Determination E° value of redox couples (i). Quinhydrone electrode (ii). Ferricyanide- ferrocyanide couple (iii). $\text{Ag} \text{Cl} / \text{Ag}$ electrode 8. Determination of strengths of halides in a mixture potentiometrically by precipitation titrations ($0.02\text{N KBr} + 0.02\text{N KI}$ mixture with standard 0.1N AgNO_3) 9. Determination of concentration by potentiometric / pH- metric titrations: (i). Acid-base titration (standard oxalic acid vs. NaOH, acetic acid vs. NaOH) (ii). Determination of ferrocyanide ion using standard bromate solution (iii). Determination of iodide ion by differential redox titration using standard bromate solution (iv) Determination of composition of zinc-ferrocyanide complex by potentiometric titration (c) Colourimetry: 11. Determination of pK_a of an indicator by colourimetric method (systems: methyl red, methyl orange, alizarin red -S in aqueous solution) 12. Kinetic studies on iodination of aniline (d) Polarimetry: 13. Determination of specific rotation and molar rotation of dextro-tartaric acid 14. Polarimetric determination of rate constant of reactions: (i). Inversion of sucrose (ii). Mutarotation of glucose (determination catalytic coefficients: k_{H^+} and $k_{\text{H}_2\text{O}}$)</p>	33

Sem-III		Sem-IV	
Paper-IX (Six units, 100 M)	4 hr Exam	Paper-XII (Six units, 100 M)	4 hr Exam
Unit-1	<p>Principles of NMR/EPR/ Mossbauer Spectra and FT Spectroscopy (20-22)L: 18 M</p> <p><i>Nuclear Magnetic Resonance (NMR) Spectroscopy:</i> Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift, and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant J. Classification of molecules: (ABX, AMX, ABC, A₂B₂, etc. types), spin decoupling. FT-NMR (qualitative idea) and its advantages, Applications of NMR in medical diagnosis.</p> <p><i>Electron Spin Resonance (ESR) Spectroscopy:</i> Basic principles, zero field splitting, and Kramer's degeneracy, factors affecting the g value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship</p> <p><i>Nuclear Quadruple Resonance (NQR) Spectroscopy:</i> Qudrupole nuclei, qudrupole moments, electric field gradient, coupling constant, splitting and simple applications.</p> <p><i>Mössbauer (MB) Spectroscopy:</i> Basic principle, instrumentation, spectral parameters and spectrum display, center shift, qudrupole and magnetic interactions.</p>	<p>Applications of NMR/EPR/Mossbauer Spectra (14-16 L): 18M</p> <p>NMR phenomenon, spin $\frac{1}{2}$ nuclei, (¹H, ¹³C, ³¹P and ¹⁹F), ¹H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Multinuclear NMR of B, Al, Si, F and P nuclei; structure and dynamics of representative inorganic molecules, deriving activation and thermodynamic parameters;</p> <p>EPR: hyperfine splitting in various systems, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, nuclear quadrupole interactions, Application.</p> <p>Mössbauer: Gamma ray emission and absorption by nuclei, Mössbauer effect, Isomer shift, quadrupole splitting, Application to the elucidation of structure and bonding of Fe^{III} and Fe^{II}, Sn^{IV} and Sn^{II} compounds, detection of oxidation states and inequivalent MB atoms.</p>	
Unit-2	<p>Photochemistry: (20-22)L 16M</p> <p>Jablonski diagram, Fluorescence and phosphorescence, Delayed fluorescence, quantum yield, Mechanism and decay kinetics of photophysical processes. Fluorescence quenching (dynamic and static), Stern - Volmer equation. Energy transfer (Forster's dipole coupling), Electron Transfer phenomenon (Marcus theory, Rehm Weller theory), Proton transfer phenomenon, complex formation phenomenon (excimer, exciplex).</p> <p>Interaction of electromagnetic radiation with matter, Transition probabilities, Transition moment integral and its applications. Electric and magnetic dipole moments. Selection rules. Violation of Franck Condon principle, oscillator strength. Nature of transitions (e.g., $n-\pi^*$, $\pi-\pi^*$, d-d, charge transfer) solvent effect on absorption and emission spectra, Stoke's shift. Properties of electronically excited molecules: Life-time, redox potential, dipole moment, pK values. Potential energy diagram for donor acceptor system, Polarized luminescence.</p> <p>Nonradiative intramolecular electronic transition; internal conversion, inter-system</p>	<p>Solid State Structure:(14-16)L 16M</p> <p>Crystalline solid – single crystal and polycrystal (twining problem); lattice; unit cell – primitive and non-primitive unit cells</p> <p>Unit cell parameters and crystal systems</p> <p>Crystal symmetry – (i) point group elements and (ii) space group elements; 32 crystal classes, HM notations, distribution in different systems and stereographic projections.</p> <p>Space group – HM notation, space groups in triclinic and monoclinic systems</p> <p>Indexing of lattice planes; Miller indices</p> <p>X-ray, Cu Kα and Mo Kα radiation; X-ray diffraction; Bragg equation; Reciprocal lattice and its relation to direct lattice; Bragg reflection in terms of reciprocal lattice – sphere of reflection and limiting sphere; relation between d_{hkl} and lattice parameters.</p>	

	crossing. Crossing of potential energy surface (Franck-Condon factor). Adiabatic and non-adiabatic cross over. Kasha's rule.	
Unit-3	<p>Bioinorganic Chemistry:(20-22)L 16M</p> <p>Essential and trace elements in the biological systems, metal of life, basic reactions in the biological systems and the roles of metal ions in biological process. Ion transport (active) across biological membrane and its significance, mechanism of Na^+K^+ -ion pump. Transport and storage of dioxygen: Active site structures and bio functions of O_2-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes.</p> <p>Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome <i>c</i>; iron-sulfur proteins (ferredoxines). cytochrome <i>c</i> oxidase. Toxic effects of metal ions, detoxification by chelation therapy, metal dependent diseases and metal complexes as drugs- Pt, Ru Rh and Au drugs.</p>	<p>Medicinal Chemistry:(14-16)L 16M</p> <p>Pharmakodynamics and pharmakokinetics and Drug design and synthesis of drugs, synthesis and chemistry of vitamins.</p> <p>Drugs: Introduction, Classification of drugs, brief discussion of drug targets, Drugs based on enzyme inhibition: Sulfa drugs, penicillin antibiotics and fluorouracil (Mechanism of drug action). Drug targets on nucleic acids (Alkylating agents and intercalating agents). Definition of antagonist, agonist, prodrugs, pharmacokinetics and pharmacodynamics, concept of structure-activity relationship (SAR) and quantitative structure and relationship (QSAR).</p>
Unit-4	<p>Symmetry Elements and Point Group: (20-22)L 18M</p> <p>Symmetry in nature, symmetry elements and symmetry operations. Symmetry properties of atomic orbitals. Elements of group theory. Elements of group theory: groups, subgroups, classes and characters, classes of symmetry operations, symmetry point groups; representation of groups by matrices. Representation of symmetry operator-transformation of basis vector, Symmetry transformation of operators The Great Orthogonality Theorem (without proof) and its consequences; construction and applications of character tables, representation of cyclic groups. direct product and projection operator and their applications; symmetry adapted linear combination(SALC)s.</p>	<p>Group Theory-Applications:(14-16)L 18M</p> <p><i>Simple applications of symmetry and group theory:</i> Bonding and Geometry of AB_n ($n = 1-6$) molecules; LCAO approximation, Huckel's theory of pi-electrons, LCAO-mo-pi-bonding, three center bonding (open and closed); Crystal field splitting of free ion terms in weak and strong crystal fields (Oh and Td), energy level diagrams and symmetries and multiplicities of energy levels, effect of lowering symmetry on the d-orbital energy levels, selection rules for electronic transitions, vibronic coupling and vibronic polarization, electronically allowed transitions (Laporte selection rule); construction of MO diagrams of polyatomic molecules including coordination complexes (Oh and Td), Symmetry of normal vibrations, normal mode analysis, selection rules for vibration and Raman spectra. Correlation diagrams, Walsh diagram & its application towards molecular geometry.</p>
Unit-5	<p>Principles and use of Mass/IR/UV-vis Spectra:(20-22)L 16 M</p> <p><i>UV-VIS Spectroscopy:</i> Various electronic transitions (185-800 nm), effect of solvent, Lambert-Beer law; uv-bands of saturated and unsaturated carbonyl compounds, -dienes, -conjugated polyenes, Fieser-Woodward rules; uv- spectra of aromatic and heterocyclic compounds; steric effects in biphenyls. <i>IR Spectroscopy:</i> Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic and heterocyclic compounds, ethers,</p>	<p>Electrochemistry:(14-16)L 16M</p> <p>Ion Solvent interactions: Concept, experimental determination, application to equilibria, kinetics, universal scales of potential acidity and basicity in different solvents. Born Model & Eley-Evans model, Absolute heats of hydration (Halliwell & Nyburg Method). Solvation number and its determination. Ion-solvent-non-electrolyte interactions: Salting-in and salting-out phenomena.</p> <p>Ion-Association: Bjerrum and Fuoss equation for ion-pair formation. Conductance minima, Ion-</p>

	<p>phenols and amines, carbonyl compounds (aldehydes, ketones, esters, carboxylic acids, amides, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effects of solvent, hydrogen bonding on vibrational frequencies, overtones, combination bands and Fermi resonance, FT IR. <i>Mass Spectrometry</i>: Basic instrumentation, ion production - EI, CI, FD and FAB techniques, Mass spectral fragmentation of typical organic compounds, common functional groups.</p>	<p>triplet, Ion-quadruplets; Walden's empirical rule and Fuoss treatment of conductance minima. Fuoss Shedlovsky's method of determination of association constant.</p> <p><i>Ion-transport in solution:</i> Limiting Debye Huckel-Onsager Expression. (Electrophoretic effect, Relaxation effect and time of relaxation). Transport number as a function of concentration. Wien Effect, Debye-Falkenhagen effect, Nernst Hartley Expression, Viscosity B-Coefficients.</p>
Unit-6	<p>Biochemistry:(20-22)L 16M</p> <p>Proteins: Classification, Amino acid, property, primary, secondary, tertiary and quaternary structure of protein .Determination of primary structure.</p> <p>Enzyme: Classification, nomenclature, Kinetic of enzyme action, comparative, uncooperative and non comparative inhibition, allo enzyme, isozymes.</p> <p>Vitamins and Hormones: Fat soluble and water soluble vitamins .Vitamins as co-enzymes and co-factor.NAD, FAD, TPP, Folic acid, Vit.B₆, Vit.B₂, Lipoic acid, Co ASH, Epinephrine, nor epinephrine, Steroid hormones.</p> <p>Chemistry of lipids: Structure and function of bio membranes. Structure and function of lipids.</p> <p>Chemistry of carbohydrates: Classification and importance constitution plants and bacterial cell wall. Animal cell coat.</p> <p>Bioenergetics: The ATP cycle.</p> <p>Nucleic Acids: DNA and RNA. Type of RNA and their function. Property of DNA in solution. Watson - Crick Model of DNA structure. Replication, Transcription and translation, (in detail). Regulation of gene expression</p>	<p>Supramolecular Chemistry:(14-16)L 16M</p> <p>Origin of supramolecular chemistry- "Chemistry beyond the molecules". Concepts and terminology of supramolecular chemistry.</p> <p>Nature and types of supramolecular interactions (Hydrogen bonding, van derWaal interactions, π-stacking, C-H...π interactions etc.)</p> <p>Molecular recognition- Information and complementarity. Different types of receptors with special reference of Crown ethers, cryptates and Calix[4]arene. Anion recognition and anion coordination chemistry. Molecular self-assembly-formation and examples.</p> <p>Supramolecular chemistry of life, application of supramolecular chemistry in drug design. Application in material science-molecular machines.</p>

Paper-X (Three Units, 50 M) 2 hr Exam (To teach one unit 4 students are required)		Paper-XIII (Three Units, 50 M) 2 hr Exam (To teach one unit 4 students are required)	
Organic: Paper-X(Org) 50 M		Organic: Paper-XIII(Org) 50 M	
Unit-7	<p>Dynamic Aspects of Stereochemistry: (20-22)L 18M</p> <p>Stereoselective and stereospecific synthesis, enantio- and diastereo- selective synthesis; π-facial selectivity, Cieplak model.</p> <p><i>Diastereoselective reactions:</i> Addition to prochiral and chiral carbonyl compounds; reactions of chiral enolates; α-substitution of prochiral ketones (RAMP/SAMP and related methodologies); aldol reactions; addition to C=C bonds, conjugate addition.</p> <p><i>Enantioselective reactions:</i> Chiral catalysis; Sharpless epoxidation and dihydroxylation; asymmetric cyclopropanation; asymmetric hydrogenation, CBS reduction; baker's yeast mediated reduction; enzyme mediated hydrolysis/esterification of <i>meso</i> compounds</p>	<p>Advanced Heterocyclic Chemistry : (14 – 16)L 18M</p> <p>Synthesis, reactions and their mechanisms of aziridine, azetidine; pyrazines and their analogues; oxazole, thiazole, imidazole, iso-oxazole, isothiazole and corresponding fused systems; pteridines, folic acid. Nomenclature of bicyclic and tricyclic fused system. Introduction to chemistry of azepins, oxepins, thiepins and their aza –analogues; phosphorous- containing and selenium containing heterocycles.</p>	
Unit-8	<p>Advanced Organic Syntheses: (20-22)L 16M</p> <p>Common named reactions and rearrangements – applications in organic syntheses. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.</p> <p>Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.</p> <p>Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction –substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic</p>	<p>Syntheses of Selectives Drugs (14-16)L 16M</p> <p>Synthesis of different types of Antibiotics: Penicilines, tetracyclines, newer generation of antibiotics like Norfloxacin, ofloxacin and levofloxacin, vitamins: vitamin B complex, vitamin c, hormones, Prostaglandins-Structure and synthesis. Drugs for metabolic diseases and Endocrine function and psychopharmacological agents.</p>	
Unit-9	<p>Chemistry of Natural Products II : (20-22L) 16M</p> <p>Isolation, synthesis, biosynthesis/ biogenesis (where applicable), general method of structure determination (with spectral parameters), stereochemistry / biological roles/technical applications (where applicable) in respect of following type natural products:(i) Alkaloids:Quinine, morphine, yohimbine, reserpine, strychnine, ellipticine, lysergic acid and their uses. (ii) <i>Steoroids</i>: Cholesterol, bile acids, androsterone, testosteron, estone, progesterone, aldosteron.</p>	<p>Organometallic Reagents in organic syntheses and Structure Determination of Organic Compounds: (14-16L) 16M</p> <p>(a) Use of Si, S, B, Cr, Ti, Co, Rh, Pd, Cu, Ni, Fe and Ce in organic syntheses.</p> <p>(b) Elucidation of the structures of the organic molecules by spectra (IR, UV-vis, NMR and Mass)</p>	

Inorganic: Paper-X(Inorg)	50M	Inorganic: Paper-XIII(Inorg)	50 M
Unit-10	<p>Electronic Spectra (d-block and f-block Elements): (20-22)L 18M</p> <p>Term symbols (R-S Coupling), Microstates, ground and excited state terms of d^n ions; splitting of d^n terms in octahedral and tetrahedral fields, Hole formalism, inversion and equivalence reactions; selection rules for spectral transitions, $d-d$ spectra of d^n ions and crystal field parameters, nephelauxetic series. Orgel and Tanabe-Sugano diagrams. Term symbols and Electronic spectral features of f-block elements. Comparison with d-block elements. Charge Transfer Spectra-MLCT, LMCT, LLCT, and MMCT with molecular orbital approaches.</p>	<p>Advanced Bioinorganic Chemistry: (14-16)L 18M</p> <p>Redox enzymes: Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and abiological nitrogen fixing systems. Molybdo enzymes: nitrate reductases, sulfite oxidase. Bioinorganic chemistry of human iron metabolism: ferritin and transferrin. Transition metal radical complexes.</p> <p>Vitamins and coenzymes: Vitamin B₆ and vitamin B₁₂ coenzymes, model systems.</p>	
Unit-11	<p>Inorganic Reaction Kinetics: (20-22)L 16M</p> <p><i>Substitution reaction:</i></p> <p>(i) Mechanistic labels - A, D, I, I_a, I_d, comparison with S_N1, S_N2.</p> <p>(ii) Tools of the trade: Rate law, activation parameters etc.</p> <p>(iii) Studies on Octahedral complexes of Co(III), Cr(III), Rh(III)-aquation, anation, pseudo substitution acid catalysed aquation, base hydrolysis, Isomerisation and racemisation reaction- the Ray-Dutta twist and Bailier twist mechanism: Square planar complexes of Pt(II); the trans-effect.</p>	<p>Magnetochemistry: (14-16)L 16M</p> <p>Types of magnetic materials. Magnetic susceptibility and its determination: Gouy, Faraday and Evans methods, vibrating sample magnetometer, SQUID and NMR methods. Magnetic anisotropy, diamagnetism in atoms and polyatomic systems, Pascal's constants. Spin and orbital moments, spin-orbit coupling, Lande interval rule, energies of J states. Curie equation, Curies law and Curie-Weiss law. First order and second order Zeeman effects, temperature independent para magnetism, simplification and application of Van Vleck susceptibility equation. Quenching of magnetic moments of transition metal compounds in cubic and axially symmetric crystal fields, low spin- high spin crosser. Magnetic behaviour of Lanthanides and actinides; magnetic exchange interactions, magnetic materials</p>	
Unit-12	<p>Complex Equilibria: (20-22)L 16M</p> <p>Stability constants of metal-ligand complexes (definitions). Determination of composition and stability constants of complexes by spectrophotometric-, pH-metric and polarographic-methods. Conditional stability constants and their importance in complexometric EDTA titration of metal ions. Statistical and non - statistical factors affecting stability of complexes in solution. Stability of mixed-ligand complexes. Solubility equilibria: Quantitativeness of precipitation, separation of metals by precipitation of metal -hydroxides, -sulfides and-chelate complexes.</p>	<p>Inorganic Photochemistry: (14-16)L 16M</p> <p>Introduction to Inorganic Photochemistry, photophysical and photochemical processes, characteristics of the electronically excited states of inorganic compounds-ligand field states, charge transfer states, Frank-Condon, and thexi states, kinetics of photochemical process, reactivities of transition metal complexes in the ligand field and charge transfer excited states, photoelectrochemistry of excited state redox reactions, photosensitization, selective inorganic photochemistry using laser beams, Relevance of ruthenium polypyridine complexes in solar energy conversion and storage, photo splitting of water, Inorganic photochemistry in biological processes and their model studies.</p>	

	Physical: Paper-X(Phy) 50 M	Physical: Paper-XIII(Phy) 50 M
Unit-13	<p>Statistical Mechanics-I: (20-22)L 18 M</p> <p><i>Imperfect gases:</i> Virial equation of state from grand partition function; second and third virial coefficients. Classical monatomic liquids-radial distribution function (RDF); Relating RDF with the thermodynamic properties; Integral equations; Potential of mean force; The direct correlation function</p> <p><i>Statistical mechanical perturbation theory of liquids:</i> Theory and its application to derive van der Waals equation of state.</p>	<p>Non-Equilibrium Thermodynamics and Quantum Statistics: (14-16)L 18M</p> <p>Microscopic reversibility, Entropy production in irreversible processes. Different types of forces and fluxes, coupling of irreversible processes, phenomenological eqns. Onsager's law, Stationary states, Principle of minimum entropy production; membrane permeability, ionic conductance. Diffusion and sedimentation potentials, electrokinetic phenomena. Thermoelectric and Thermochemical effects; Membrane transport involving biochemical reaction. Active transport.</p> <p><i>Quantum Statistics:</i> Liouville theorem and its consequences, its quantum version. Fermi-Dirac and Bose-Einstein distribution; their Classical limits; Application of the quantum statistics for deriving thermodynamic properties of ideal BE and FD systems (Specific heat of electron, black-body radiation, Bose Einstein condensation); density matrix.</p>
Unit-14	<p>Quantum Mechanics-III: (20-22)L 16 M</p> <p><i>General Theory:</i> Vector space formulations of Quantum Mechanics; measurements and Heisenberg's uncertainty principle, matrix Eigenvalue and Diagonalization problem. Coordinate representation. Schrödinger and Heisenberg pictures; Constants of motion: Parity and Angular momentum.</p>	<p>Quantum Mechanics-V: (14-16)L 16 M</p> <p>Theoretical Treatments for Many-electron systems:</p> <p>(a) <i>Variation Method:</i> Variation theorem; application to ground states of different systems; extension to excited states; linear variation;</p> <p>(b) <i>Many-electron-atoms:</i> Many electron wave function including spin eigen functions of S^2, S_z, L^2, L_z operators, Hartree self consistent field (SCF) Method, Hatree-Fock SCF Method, Multi-configuration SCF Method, Configuration Interaction (CI) Method and Density Functional Theory (DFT).</p> <p>(c) <i>Molecular Systems:</i> (i) <i>Forces in molecules:</i> Virial theorem, Hellman-Feynman theorem applications. (ii) Hückel's theory with application to simple molecular systems.</p>
Unit-15	<p>Quantum Mechanics-IV: (20-22)L 16 M</p> <p><i>Perturbation Theory:</i></p> <p>(i) Time independent formalism: Rayleigh-Schrödinger theory for nondegenerate systems; Perturbation treatment in He atom; degenerate perturbation theory, Stark and Zeeman effects.</p> <p>(ii) Time dependent formalism: Transition probability; Fermi Golden Rule; Einstein transition probabilities; spontaneous and induced emission.</p> <p>Derivation of spectroscopic selection rules.</p>	<p>Statistical Mechanics-III: (14-16)L 16 M</p> <p><i>Non-equilibrium Statistical Mechanics:</i></p> <p>Random processes; Time-correlation functions; Brownian motion; Langevin equation for random motion; Random walk in one dimension; Time dependence of fluctuation; Fluctuation-dissipation theorem; Fokker-Planck equation.</p>

Marks	Theory 150 M	Theory 150 M
Paper-XI (Practical)		Paper-XIV (Grand Viva, Practical & Project/ Review)
Unit-1	Organic: 15 + 5 (LNB) + 5 (V) 25 M Advanced Organic Syntheses and Characterizations (6 hr Examination)	Grand Viva (on specialization) by External Experts 50 M
Unit-2	Inorganic: 15 + 5 (LNB) + 5 (V) 25 M Inorganic Syntheses and Characterizations (6 hr Examination)	Practical (Spl): 15 + 5 (LNB) + 5 (V) 25 M Organic/ Inorganic/Physical Characterization/Isolation and Characterization of Natural Products/Syntheses of Inorganic Functional Molecules/ Advanced Physicochemical Experiments
Unit-3	Physical: 15 + 5 (LNB) + 5 (V) 25 M Advanced Physicochemical Experiments (6 hr Examination)	Project/Review 25 M
Unit-4	Computer Application 25 M (6 hr Examination)	
	Total Marks: 250 M	Total Marks: 250 M