SEMESTER – I

General (G) Course: Hard Core / Compulsory

Marks – 400

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

SEMESTER – I

Paper: CHEM-G11

Unit 1: Coordination Chemistry I

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

Unit 2: Theories of Bonding

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

Unit 3: Metal – ligand Equilibria in Solution

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

Unit 4: Bioinorganic Chemistry I

Principles of coordination chemistry related to bioinorganic chemistry, Essential and trace metal ions in biological systems, Porphyrin and related ligands, ATP as energy source, oxidative phosphorylation and phosphorylation of glucose. Transport and storage of dioxygen: Structure and function of hemoglobin, myoglobin, hemocyanin and hemerythrin. Synthetic oxygen carriers.

Unit 5: Electrochemical Analyses

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

CHEM – G12

Unit 1: Stereochemistry

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

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

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

Unit 2: Organic Reaction Mechanism

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

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

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

Unit 3: Fundamentals of Organic Synthesis

(a) Introduction to synthons, retrons, and chirons

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

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

(d) Protection and deprotection reactions.

Unit 4: Oxidising and reducing agents in organic synthesis

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

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

Unit – 5: Natural Products (Terpenoids and Alkaloids)

(a) Terpenoids: Introduction, isoprene rule, general methods of isolation, structure elucidation and synthesis of some representative members of mono and sesquiterpenes.

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

CHEM G – 13

Unit 1: Quantum Chemistry I

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

Unit 2: Introduction to Biophysical Chemistry

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

Unit 3: Symmetry & Group Theory

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

Unit 4: Kinetics I

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

Unit 5: Spectroscopy I

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

CHEM G – 14 (Practical)

Unit 1: Quantitative estimations and inorganic preparations

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

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