Chemistry Honours : Scheme of the Syllabus

Course names and Marks distribution : CEMAT denotes Chemistry Hons Theory CEMAP denotes Chemistry Hons Practical

Code : First digit refers to year, second to paper, third letter to subject, fourth to part.

PART – I (1st Year), Total marks = 200 (Theory = 150, Practical = 50)

Paper I

CEMAT [11-IA+11-IB], each course 25 marks, Total marks = 50 (Inorganic)

CEMAT [11-0A+11-0B], each course 25 marks, Total marks = 50 (Organic)

Paper II

CEMAT [12-PA+12-PB], each course 25 marks, Total marks = 50 (Physical)

CEMAP [12 -PrA+12 PrB], each course 25 marks, Total marks = 50 (course 12-PrA – Organic, 12-PrB – Inorganic{Analytical})

Courses 11-IA, 11-IB, 11-OA, 11-OB, 12-PA, 12-PB each contains two units. Unit 1 : 12 marks, Unit 2 : 13 marks

PART – II (2nd Year), Total marks = 200 (Theory = 150, Practical = 50)

Paper III

CEMAT [23 -IA+23-IB], each course 25 marks, Total marks = 50 (Inorganic)

CEMAT [23 -0A+23-0B], each course 25 marks, Total marks = 50 (Organic)

Paper IV

CEMAT [24-PA+24-PB], each course 25 marks, Total marks = 50 (Physical)

CEMAP [24-PrA+24-PrB], each course 25 marks, Total marks = 50 (course 24-PrA – Physical, 24-PrB – Inorganic{Qualitative})

Courses 23-IA, 23-IB, 23-0A, 23-0B, 24-PA and 24-PB each contain two units. Unit 1 : 12 marks, Unit 2 : 13 marks

PART – III (3rd Year), Total marks = 400 (Theory = 200, Practical = 200)

Paper V

CEMAT [35-IA+35-IB], each course 25 marks, Total marks = 50 (Inorganic)

CEMAT [35-AA+35-AB], each course 25 marks, Total marks = 50 (Advanced Chemistry) {Course 35-AA – Bioinorganic + Material Chemistry Course 35-AB – Bioorganic + Biophysical}

Paper VI

CEMAT [36-OA+36-OB], each course 25 marks, Total marks = 50 (Organic)

CEMAT [36-PA+36-PB], each course 25 marks, Total marks = 50 (Physical)

Courses 35-IA, 35-IB, 35-AA, 35-AB, 36-OA, 36-OB, 36-PA and 36-PB each contain two units. {Unit 1 : 12 marks, Unit 2 : 13 marks}

Paper VII

CEMAP [37] Total marks = 100 Course 37-Pr Physical (50 marks) + Organic TLC etc (25 marks) + LNB-viva (25 marks)

Paper VIII CEMAP [38] Total marks = 100 Course 38-Pr Inorganic (50 marks) + Organic Preparation (25 marks) + LNB-viva (25 marks)

Notes:

1. Each Theory module of 25 marks contains units I (marks = 13) and II (marks = 12). 2. Number of class hours = 30-35 for a 25-mark Theory module, 70-80 for a 25-mark Practical module

Effective from academic session 2011-2012

B.Sc Part-I (1st Year) Chemistry (Honours)

Total Marks 200 (Theory = 150, Practical = 50)

Paper I Courses : CEMAT 11-IA, 11-IB, 11-OA, 11-0B (Each 25 marks : Total 100 marks)

CEMAT 11-IA Unit-I. Radioactivity and Atomic Structure

13 marks

Nuclear stability and nuclear binding energy. Nuclear forces: meson exchange theory. Nuclear models (elementary idea): Concept of nuclear quantum number, magic numbers. Nuclear Reactions: Artificial radioactivity, transmutation of elements, fission, fusion and spallation. Nuclear energy and power generation. Separation and uses of isotopes in tracer techniques. Radio chemical methods: principles of determination of age of rocks and minerals, age of earth, radio carbon dating, hazards of radiation and safety measures.

Bohr's theory to hydrogen-like atoms and ions; spectrum of hydrogen atom. Sommerfeld's theory (no derivation). Quantum numbers. Introduction to the concept of atomic orbitals; shapes, radial and angular probability diagrams of s, p and d orbitals (qualitative idea). Many electron atoms and ions: Pauli's exclusion principle, Hund's rule, exchange energy, Aufbau principle and its limitation. Electronic energy level diagram and electronic configurations of hydrogen-like and polyelectronic atoms and ions. Term symbols of atoms and ions for atomic numbers < 30.

Unit-II. Chemical periodicity I

12 marks

Periodic table, group trends and periodic trends in physical properties. Classification of elements on the basis of electronic configuration. Modern IUPAC Periodic table. General characteristic of s, p, d and f block elements. Position of hydrogen and noble gases in the periodic table.

Effective nuclear charges, screening effects, Slater's rules, atomic radii, ionic radii (Pauling's univalent), covalent radii. Ionization potential, electron affinity and electronegativity (Pauling's and Allred-Rochow's scales) and factors influencing these properties. Inert pair effect. Group trends and periodic trends in these properties in respect of s-, p- and d-block elements. Catenation property and its controlling factors.

CEMAT 11-IB

Unit-I. Chemical Bonding and structure

Ionic bonding: Size effects, radius ratio rules and their limitations. Packing of ions in crystals, lattice energy, Born-lande equation, Born-Mayer equation, Kapustinskii equation (no derivation) and applications, Born-Haber cycle and its applications. Solvation energy, polarizing power and polarizability, ionic potential, Fajan's rules. Defects in solids (elementary idea).

Covalent bonding: Lewis structures, formal charge. Valence Bond Theory, directional character of covalent bonds, hybridizations, equivalent and non-equivalent hybrid orbitals, Bent's rule, VSEPR theory, Failure of VSEPR theory-to explain [e.g., TeCl_6^{2-} , TeBr_6^{2-} and SbBr_6^{3-} in $(\text{NH}_4)_4(\text{SbBr}_6)_2$] shapes of molecules and ions containing lone pairs and bond pairs (examples from main groups chemistry), importance of π -bonding particularly in the '2p' sublevel- and its effect on – structure (dimerization, polymerization etc.), bonding and reactivity e.g. acid base and redox properties (application to different groups.). Partial ionic Character of covalent bonds, bond moment, dipole moment and electronegativity differences. Concept of resonance, resonance energy, resonance structures. Effect of $3d^{10}$ configuration on the chemistry of non metals e.g. As, Se, and Br particularly on the acidic and redox properties of compounds.

Unit-II. Acid-Base reactions

Acid-Base concept: Arrhenius concept, theory of solvent system (in H_2O , NH_3 , SO_2 and HF), Bronsted-Lowry's concept, relative strength of acids, Pauling rules. Amphoterism. Lux-Flood concept, Lewis concept. Superacids, HSAB principle. Acid-base equilibria in aqueous solution and pH. Acid-base neutralisation curves; indicator, choice of indicators. Buffer solution, composition, buffer capacity.

CEMAT 11-OA

<u>Unit I</u>

Nomenclature (trivial and IUPAC), DBE, hybridization(spⁿ, n = 1,2,3) of C, N, O, halogens, bond distance, bond angles, VSEPR, shapes of molecules, inductive and field effects, bond energy, bond polarity and polarisability, dipole moment, resonance, resonance energy, steric inhibition of resonance, hyperconjugation, π M.O diagrams of ethylene, butadiene, 1,3,5-hexatriene, allyl cation, allyl anion, allyl radical, HOMO and LUMO in ground and excited states, orbital pictures of allene, carbene(singlet and triplet), vinyl cyanide, Huckel's rule for aromaticity and antiaromaticity (neutral systems 4,6,8,10 annulene, charged systems 3,4,5,7 rings, homoaromaticity, Frost-diagram, melting point, boiling point, heat of hydrogenation, heat of combustion, hydrogen bonding (intra- and inter-molecular), crown-ether, concepts of acidity, basicity and nucleophilicity.

13 marks

13 marks

<u>Unit II</u>

Stereochemistry of acyclic compounds: representation of molecules in Fischer, flyingwedge, Sawhorse and Newman formula and their translations, chirality, elements of symmetry, simple axis (Cn), plane of symmetry(σ), centre of symmetry(i), alternating axis of symmetry(Sn), asymmetry and dissymmetry, optical activity, specific rotation, molar rotation, specific rotation of mixture, Biot's law.

Stereoisomerism: enantiomerism, diastereoisomerism, stereogenic centre, systems with chiral centres, stereogenic centres involving C=C, C=N, D/L, R/S, E/Z, syn/anti, cis/trans, meso/dl, threo/erythro nomenclature.

Conformation: conformational nomenclature; eclipsed, staggered, gauche and anti, dihedral angle, torsional angle, Klyne-Prelog terminology, energy barrier of rotation, relative stability of conformers on the basis of steric effect, dipole-dipole interaction, hydrogen bonding, conformational analysis of ethane, propane, n-butane, 1,2-dihaloethane, 2-methylbutane, 1.2-glycols, invertomerism of trialkyl amines.

Stereochemistry of carbocation, carbanion, radical, thermodynamic requirements of reaction, Δ H, Δ G, Δ S, dependence of Δ H on bond energy, equilibrium controlled changes, relative ease of intermolecular versus intramolecular reactions.

Reaction kinetic; rate equations, transition-state theory and ΔG_{\star}^{*} , free energy profile for one step and two steps reactions, Hammond postulate, kinetically and thermodynamically controlled reactions, kinetic studies, studies of intermediates, cross-over experiments, stereochemical proof, isotope labeling (kinetic and non-kinetic), primary kinetic isotope effect (K_H/K_D only),

CEMAT 11-OB

<u>Unit I</u>

13 marks

Addition to C=C and C=C bonds, halogenation, oxidation, epoxidation, hydroxylation, ozonolysis, carbene addition, oxymercuration-demercuration, peroxide effect, conjugated dienes, 1,2- vs 1,4- addition, Birch reduction of alkadienes and alkynes, regio and stereo selectivity.

Nucleophilic substitution and elimination reactions: SN_1 , SN_2 , SN_i , NGP, E_1 , E_2 , E_1CB mechanism, elimination vs substitution, Sayetzeff and Hoffman rules, 1,1-elimination.

Alcohol and ethers: synthesis and reactivity including pinacol-pinacolone rearrangement.

Unit II

12 marks

Aromatic electrophilic substitution: π -complex, σ -complex, ipso-substition, activating and deactivating groups, orienting influence of groups, activated aromatic nucleophilic substitution, cine- substitution.

Alkanes: synthesis and reactivity, reactivity of radicals, carbene, nitrene: generation and stability, definition and examples of ylide and zwitterions.

Paper II

Courses : CEMAT 12-PA, 12-PB, CEMAP 12-PrA, 12-PrB (Each 25 marks : Total 100 marks)

CEMAT 12-PA

Unit -I : Kinetic Theory of Gas

13 marks

Concept of pressure and temperature. Nature of the distribution of velocities in one dimension (with derivation), extension to two and three dimensions (without derivation, expression by induction). Maxwell's distribution of speeds. Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case ; calculation of the number of molecules having energy $\geq \varepsilon$. Principle of the equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases.

Collision of gas molecules; collision diameter; collision number and mean free path; frequency of binary collisions (similar and different molecules); wall collision and rate of effusion. Viscosity of gases from kinetic theory of gas.

Unit-II : Real gas and Liquid State

12 marks

Deviation of gases from ideal behaviour; Compressibility factor; Andrew's and Amagot's plots; van der Waals equation and its characteristic features. Existence of critical state. Critical constants in terms of van der Waals constants. Law of corresponding state and significance of second virial coefficient. Boyle temperature. Intermolecular forces; Lennard-Jones potential.

Nature of the liquid state (short range order and long range disorder). Vapor pressure. Surface tension, surface energy, excess pressure, capillary rise and measurement of surface tension (relative and absolute methods). Work of cohesion and adhesion, spreading of a liquid over other surface. Vapour pressure over curved surface. Temperature dependence of surface tension.

General features of fluid flow (streamline flow and turbulent flow). Reynold number, nature of viscous drag for streamline motion, Newton' equation, viscosity coefficient. Poiseuille's equation (with derivation), temperature dependence of viscosity of liquid and its difference from gas, principle of determination of viscosity coefficient of liquids by the falling sphere method.

CEMAT 12-PB

Unit-I : Thermodynamics-I

Definition of thermodynamic terms : intensive and extensive variables, isolated, open and closed systems, concept of heat and work, thermodynamic processes : cyclic, reversible, irreversible, isothermal, adiabatic processes, thermodynamic functions and their differentials, zeroth law of thermodynamics; first law of thermodynamics, internal energy (U), Joule's experiment and its consequences, Joule-Thomson experiment and its consequences, enthalpy (H), relation between Cp and Cv, calculation of work (w), quantity of heat (q), ΔU and ΔH for expansion of ideal and van der Waals gases, gas under isothermal and adiabatic conditions for reversible and irreversible processes including free expansion. Heat changes during various physico-chemical processes at constant pressure / constant volume, Hess's law, Kirchoff's relation, concept of standard state, bond dissociation energy, Born-Haber cycle for calculation of lattice energy.

Spontaneous process, heat engine, Carnot cycle and its efficiency, statements of second law, refrigeration cycle, thermodynamic scale of temperature, entropy as a state function, Clausius inequality, calculation of entropy changes in different processes, molecular interpretation of entropy. Maxwell relations.

Unit-II : Chemical Kinetics

12 marks

Introduction of reaction rate in terms of extent of reaction (degree of advancement); rate constants, order and molecularity of reactions. Reactions of zero order, first order, second order and fractional order. Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate). Determination of the order of a reaction by half-life and differential method, integrated rate equation and isolation method. Rate-determining and steady-state approximation – explanation with suitable examples.

Opposing reactions, consecutive reactions and parallel reactions (with explanation of kinetic and thermodynamic control of products; all steps first order).

Temperature dependence of rate constant: Arrhenius equation, energy of activation. Collision theory (detailed treatment); outline of Transition State theory. Primary kinetic salt effect. Lindemann theory of unimolecular reaction. Homogeneous catalysis with reference to acid-base catalysis.

CEMAP 12-PrA

Practical Organic	
Experiment	20M
1 Molting point determination	1 M
1. Melting point determination	
2. Detection of special elements (N, Cl, Br, I, S) by Lassigne's test	3M
3. Solubility and classification.	2 + 1 = 3M
(Solvents: water, 5% HCl, 5% NaHCO ₃ , 5% NaOH)	
4. Detection of the following functional groups by systematic chemical analysis:	
	9x1=9M
Aromatic amino(NH ₂), anilido, amido, aromatic nitro, C=C, phenolic OH	, ester,
carboxylic acid, carbonyl(aldehyde and ketone distinction), only one test	for each
functional group is to be reported.	
5a. Preparation of suitable derivative	3M
1 I	-
b. M.P. of derivative	1M
NOTE: Each student during laboratory session is required to carry out qu	alitative chem

NOTE: Each student during laboratory session is required to carry out qualitative chemical test for all special elements and functional groups in known and unknown (at least six) organic compounds. In practical examination, one unknown solid organic compound containing not more than two of the above functional groups (5) shall be assigned to a candidate through a single draw lottery

b) Laboratory records & viva:

CEMAP 12-PrB

Practical Inorganic

- 1) Determination of hardness of water (by EDTA).
- 2) Estimation of vitamin-C (Iodometry).
- 3) Determination of strength of H_2O_2 (Permanganometry).
- 4) Estimation of i) NH_4^+ ii) H_3BO_3 (any one).
- 5) Estimation of available oxygen in pyrolusite.
- 6) Estimation of Cu(II) iodometric.
- 7) Estimation of Fe(III) after reduction (Dichromatometry).

** If NH_4HF_2 is used in place of H_3PO_4 titration should be carried out in 100 ml. 2(N) H_2SO_4 solution for better result.

25 marks

25 marks

2.5x2 = 5M

B.Sc Part-II (2nd Year) Chemistry (Honours)

Total Marks 200 (Theory = 150, Practical = 50)

Paper III Courses : CEMAT 23-IA, 23-IB, 23-OA, 23-0B (Each 25 marks : Total 100 marks)

CEMAT 23-IA

Unit I. Chemical Periodicity II

13 marks

General trends of variation of electronic configuration, elemental forms, metallic nature, magnetic properties (if any), catenation and catalytic properties (if any), oxidation states, inert pair effect (if any), aqueous and redox chemistry in common oxidation states, properties and reactions of important compounds such hydrides, halides, oxides, oxy-acids (if any), complex chemistry (if any) in respect of the following elements:

(i) s-block elements: Li-Na-K, Be-Mg-Ca-Sr-Ba.

(ii) p-block elements: B-Al-Ga-In-Tl, C-Si-Ge-Sn-Pb, N-P-As-Sb-Bi, O-S-Se-Te, F-Cl-Br-I, He-Ne-Ar-Kr-Xe

Unit II. Other Types of Bonding

12 marks

Molecular orbital concept of bonding (elementary pictorial approach) :sigma and pi-bonds, multiple bonding, MO diagrams of H₂, F₂, O₂, C₂, B₂, CO, NO, CN⁻, HF, and HF₂⁻ ion, BeH₂, CO₂, magnetic properties, bond orders, bond lengths. Coordinate bonding: Lewis acid-base adducts (examples), double salts and complex salts, Werner theory of coordination compounds. Ambidentate and polydentate ligands, chelate complexes, inermetallic complexes(formation as a function of pH and effect of entropy and ring size). IUPAC nomenclature of coordination compounds (up to two metal centers). Coordination numbers, constitutional isomerism. Stereoisomerism in square planar and octahedral complexes.

Hydrogen bonding and its effects on the physical properties and chemical properties of compounds of the main group elements.

Metallic bonding: qualitative idea of band theory, conducting, semi conducting and insulating properties with examples from main group elements.

CEMAT 23-IB

Unit I. Chemistry of s- and p-block Elements

(i) Structure, bonding and reactivity of B_2H_6 ; $(SN)_X$ with x = 2, 4; phosphazines; interhalogens; XeF₆. (ii) Structure of borates, polyphosphates, borazole, boron nitride, silicones, thionic acids (iii) Reactivity of polyhalides, pseudo halides, fluorocarbons, freons and NO_x with environmental effects, (iv) Chemistry of hydrazine, hydroxylamine, N₃⁻, thio-and per-sulphates.

Noble gases: oxides, fluorides and oxofluorides of xenon; chemical and photochemical reactions of ozone.

Unit II. Precipitation and Redox Reactions

Solubility product principle, common ion effect and their applications to the precipitation and separation of common metallic ions as hydroxides, sulfides, phosphates, carbonates, sulfates and halides. Ion-electron method of balancing equation of redox reaction. Elementary idea on standard redox potentials with sign conventions, Nernst equation. Influence of complex formation, precipitation and change of pH and ionic strength on redox potentials; formal potential. Feasibility of a redox titration, redox potential at the equivalence point, redox indicators. Redox potential diagram (Latimer, Frost, Ellingham diagrams) of common elements and their applications. Disproportionation and comproportionation reactions (typical examples), Choice of redox indicators.

CEMAT 23-OA

<u>Unit-I</u>

UV: Electronic transitions (σ - σ *, n- σ *, π - π *, n- π *),

Factor influencing the relative position of λ max (conjugative effect, steric effect, solvent effect, conformational effect, effect of pH), relative intensity of absorption of allowed transition, transition moment, effective chromophor concentration, red shift (bathochromic shift), blue shift (hypsochromic shift), hyperchromic shift, hypochromic shift (typical examples).

IR: Modes of molecular vibration, application of Hook's law, force constant, factor influencing stretching frequency (H-bonding, mass, electronic factors, bond multiplicity, ring size, solvent effect, bond coupling), Fermi resonance, characteristic and diagnostic stretching frequencies of O-H, N-H, C-H, C-D, C=C, C=N, C=O, C=C, C=N functions.

¹**H-NMR:** Nuclear spin, NMR active nuclei, principle of proton magnetic resonance, equivalent and non-equivalent protons, chemical shift(δ), shielding and deshielding of protons, upfield and downfield shift, NMR peak area, spin-spin coupling(simple type), ¹H-NMR spectra of toluene, nitrobenzene, benzaldehyde, o-,m-,p-dichlorobenzene,

13 marks

13 marks

dinitrobenzene, CH₃CH₂Br, CH₃CHBr₂, CH₂BrCH₂Br, CHBr₂CH₂Br, CH₃CH₂OH (ordinary and pure), *E*- and *Z*- 2-butene, ethylene and acetylene, *E*- and *Z*- 1-Bromo-2-chloroethene. Mass: Basic principle of mass spectroscopy

<u>Unit II</u>

12 marks

Phenol, ambident nucleophile: C- substitution versus O-substitution, reaction of phenols: Reimer-Tiemann reaction, Kolbe's reaction, Manasse reaction, alkylation, acetylation, Fries rearrangement, Claisen rearrangement, nitration, sulphonation, halogenation, oxidation (aerial), oxidative coupling by Fe³⁺, Dakin reaction, Cumene-phenol rearrangement.

Organometallic compounds: Preparation and synthetic applications of organomagnesium, organolithium, organozinc, organocopper, use of TMSCI, TMSI, TMSCN.

Stereochemistry: cumulene with odd and even number of C=C, axial chirality (allene, spiro compound, alkylidene cycloalkanes, biphenyls (atropisomerism)), and R/S nomenclature, resolution of racemic acids, bases, and alcohols, optical purity/enantiomeric excess, topicity(topic attribute-chirotopic, achirotopic,; topic relationship-homotopic, enantitopic, diastereotopic), prochirality, Pro-r, Pro-s and re/si descriptor.

CEMAT 23-OB

<u>Unit I</u>

13 marks

Chemistry of carbonyl compounds: Nucleophilic addition to C=O, reactivity of carbonyl compounds, relative stability of acetal, ketal, thioacetal, thioketal and cyanohydrin, reductions (using LiAlH₄, NaBH₄, electrolytic reduction, reductive coupling, MPV reduction), Cannizzaro reaction, benzil-benzilic acid rearrangement, Tischenko reaction, nucleophilic addition to α,β -unsaturated carbonyl compounds, reaction of benzoquinone, Wolf-Kishner reduction, aldol condensation, Claisen-Schimdt reaction, Wittig reaction, enamine reaction, Eschweiler-Clarke methylation, Darzen's reaction, Perkin reaction, benzoin condensation, electrophilic substitution at α position of carbonyl compounds (D-exchange, nitrosation, halogenation, haloform reaction, SeO₂ oxidation), Baeyer-Villiger oxidation, concept of umpulong.

Carboxylic acids and their derivatives: Nucleophilic substitution at the acyl carbon of acyl halide, anhydride, ester, carboxylic acid, amide, esterification of carboxylic acids and hydrolysis of ester-AAc², AAc¹, AAl¹, BAc², BAc¹, BAl¹ mechanisms, HVZ reaction, Claisen ester condensation, Bouveault Blanc reduction, decarboxylation reaction, Hunsdiecker reaction, action of heat on hydroxy acid.

<u>Unit II</u>

Organonitrogen compounds: synthesis and reactions of nitroalkanes, alkylnitrites, alkyl cyanides and isocyanides, aliphatic amines, aromatic nitro, amines and diazo compounds, distinction and separation of 1^{0} , 2^{0} , 3^{0} amines, diazomethane, diazoacetic ester-preparation and synthetic applications.

Paper IV Courses : CEMAT 24-PA, 24-PB, CEMAP 24-PrA, 24-PrB (Each 25 marks : Total 100 marks)

CEMAT 24-PA

Unit-I : Quantum Chemistry I

13 marks

Black body radiation: Rayleigh-Jeans and Planck's energy distribution law, Planck's theory, Wave-particle duality, light as particles: photoelectric and Compton effects; electrons as waves (electron diffraction experiment) and the de Broglie hypothesis.

Elementary concepts of operators, eigenfunctions and eigenvalues. Linear operators. Commutation of operators, fundamental commutator and uncertainty relation (without proof). Expectation value. Hermitian operator. Schrödinger time-dependent and time-independent equation: nature of the equation, acceptability conditions imposed on the wave functions and probability interpretations of wave function, postulates of quantum mechanics.

Particle in a box: setting up of Schrodinger equation for one-dimensional box and its solution. Comparison with free particle eigenfunctions and eigenvalues. Properties of PB wave functions (normalisation, orthogonality, probability distribution). Expectation values of x, x^2 , p_x and p_x^2 and their significance in relation to the uncertainty principle. Extension of the particle in a one-dimensional problem to two and three dimensions and the concept of degenerate energy levels.

Simple Harmonic Oscillator: setting up of the Schrodinger equation, energy expression (without derivation), expression of wave function for n = 0 and n = 1 (without derivation) and their characteristic features.

Unit-II : Quantum Chemistry II and Photochemistry12 marks

Stationary Schrodinger equation for the H-atom in polar coordinates, separation of radial and angular (θ , ϕ) parts. Solution of ϕ -part and emergence of quantum number 'm'; energy expression (without derivation), degeneracy. Hydrogenic wave functions up to n = 2 (expression only); real wave function. Concept of orbitals and shapes of s and p orbitals.

Potential energy curves (diatomic molecules), Qualitative idea of Born Oppenheimer approximation and Franck-Condon principle, vibrational structure of electronic spectra. Bond dissociation and principle of determination of dissociation energy (ground state). Decay of excited states by radiative and non-radiative processes. Fluorescence and phosphorescence, Jablonsky diagram.

Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence and Lambert-Beer's law; quantum yield and its measurement for a

photochemical process, actinometry. Photostationary state. Photosensitized reactions. Kinetics of HI decomposition, H_2 -Br₂ reaction, dimerisation of anthracene.

CEMAT 24-PB

Unit-I : Thermodynamics(II) and Chemical Equilibrium13 marks

Gibbs function (G) and Helmholtz function (A), criteria of thermodynamic equilibria and spontaneity, Maxwell's relations, variation of G and A with P, V and T, Thermodynamic equation of state, Clausius-Clapeyron equation, equilibrium between different phases, system of variable composition, partial molar quantities, chemical potential of a component in an ideal mixture, thermodynamic functions of mixing of ideal gases, Gibbs-Duhem equation, variation of chemical potential with T, P and mole fraction, thermodynamics of real gases – fugacity and activity determination.

Equilibrium constant and standard Gibbs free energy change. Definitions of KP, KC and Kx; van't Hoff's reaction isotherm, isobar and isochore from different standard states. Shifting of equilibrium due to change in external parameters e.g. temperature and pressure. Le Chatelier's principle and degree of advancement.

<u>Unit -II : Electrochemistry(Conductance, EMF and Ionic Equilibrium)</u> 12 marks

Conductance and measurement of conductance, cell constant, specific conductance and molar conductance. Variation of specific and equivalent conductance with dilution for strong and weak electrolytes. Kohlrausch's law of independent migration of ions, ion conductance and ionic mobility. Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes. Ostwald's dilution law. Debye-Huckel model (physical idea only). Application of conductance measurement (determination of solubility product and ionic product of water). Conductometric titrations. Determination of transport number by moving boundary method.

Types of electrochemical cells and examples, cell reactions, emf and change in free energy, ΔH and ΔS of cell reactions from emf measurements. Thermodynamic derivation of Nernst equation. Standard cells. Half-cells/electrodes, different types of electrodes (with examples). Standard electrode potential (IUPAC convention) and principles of its determination. Types of concentration cells. Liquid junction potential and its minimization. Glass electrode and determination of pH of a solution. Potentiometric titrations: acid-base and redox.

Activity and activity coefficients of electrolyte/ion in solution. Debye-Huckel limiting law (statement and applications only). Solubility equilibrium and influence of common ions and indifferent ions thereon. pH, buffer solution, buffer capacity, salt hydrolysis (detailed treatment).

CEMAP 24-PrA

Experiments:

1. Determination of surface tension of a given solution by the drop weight method using a stalagmometer, considering aqueous solutions of NaCl, acetic acid, ethanol etc, as systems.

2. Determination of viscosity coefficient of a given solution with Ostwald's viscometer considering aqueous solutions of cane-sugar, glycerol, ethanol, etc.

3. Determination of solubility of sparingly soluble salts in water and various Electrolyte medium by titrimetric method. KHTa as sparingly soluble salt in water, KCl, NaNO₃ may be used.

4. Determination of partition coefficient of Iodine or Acetic acid in water and an immiscible organic solvent.

5. Determination of the rate constant for the first order acid catalyzed hydrolysis of an ester (V_0 and V_{∞} to be supplied)

6. Determination of rate constant of decomposition of H_2O_2 by acidified KI solution using clock reactions.

7. Determination of the equilibrium constant of the reaction $KI + I_2 = KI_3$ by partition method (partition coefficient to be supplied).

8. Determination of pH of an unknown buffer solution by colour matching.

A separate laboratory workbook should be maintained for these experiments.

CEMAP 24-PrB

25 marks

<u>Qualitative inorganic analysis of mixtures containing not more than 4 radicals from the following:</u>

Cation Radicals: Na⁺, K⁺, NH₄⁺, Ca⁺², Sr⁺², Ba⁺², Al⁺³, Mg⁺², Cr⁺³, Mn⁺², Fe⁺², Fe⁺³, Sn²⁺,
Co⁺², Ni⁺², Cu⁺², Zn⁺², Sb⁺³.Anion Radicals: F⁻, Cl⁻, Br⁻, BrO₃⁻, I⁻, SCN⁻, S²⁻, SO₃²⁻, SO₄²⁻ S₂O₃²⁻, NO₃⁻, NO₂⁻, PO₄³⁻,
BO₃³⁻ CrO₄²⁻/Cr₂O₇²⁻, Fe(CN)₆⁴⁻, Fe(CN)₆³⁻. IO₃⁻Insoluble Materials: Al₂O₃, Fe₂O₃, Cr₂O₃; SnO₂, SrSO₄, BaSO₄, CaF₂.

Detection of toxic metal ions and radicals (*under special supervision*): As^{3+} , AsO_4^{3-} , Bi^{3+} , Pb^{2+} , Hg_2^{2+} , Hg^{2+} , Cd^{2+} ,.

Analysis of the sample with confirmation avoiding interference including special tests (dry/wet) taking different extracts [e.g. (i) aqueous; (ii) HCl extract; (iii) HNO₃ extract; (iv) NaOH extract (after fusion) or from the residue left after Na_2CO_3 extract for basic radicals] or by the usual procedure as follows:

1.	Reporting of radicals including charges	4 x 0.5 = 2
2.	Dry tests for radicals	4 x 1 = 4
3.	Wet tests for radicals	4 x 1 = 4
4.	Confirmation of radicals	4 x 1.5 = 6
5.	Probable composition with appropriate logic	4
6.	Laboratory note book	3
7.	Viva voce	2

Note: Students will be allowed to sit for practical examination provided they submit the Laboratory Note book containing at least six unknown sample analysis, duly signed by the concerned teacher.

Oxide, hydroxide, carbonate and bicarbonate should not be reported as radicals.

B.Sc Part-III (3rd Year) Chemistry (Honours)

Total Marks 400 (Theory = 200, Practical = 200)

Paper V Courses : CEMAT 35-IA, 35-IB, 35-AA, 35-AB (Each 25 marks : Total 100 marks)

CEMAT 35-IA

Unit I. Chemistry of coordination compounds

13 marks

Isomerism, reactivity and stability: Determination of configuration of cis- and trans- isomers by chemical methods. Labile and inert complexes (application of CFAE), substitution reaction on square planer complexes, trans effect (example and applications). Stability constants of coordination compounds and their importance in inorganic analysis.

Structure and bonding: EAN rule, VB description and its limitations. Elementary Crystal Field Theory: splitting of dⁿ configurations in octahedral, square planar and tetrahedral fields, crystal field stabilization energy in weak and strong fields; pairing energy, evidence and application of crystal field (lattice energy, ionic radius, hydration energy, redox pot, spinel), Jahn-Teller distortion(static and dynamic),evidence from stability constant and vis-spectra. Metal-ligand bonding (MO concept, elementary idea), sigma- and pi-bonding in octahedral complexes (qualitative pictorial approach) and their effects on the oxidation states of transitional metals (examples).

Magnetism and Colour: Orbital and spin magnetic moments, spin only moments of d^n ions and their correlation with effective magnetic moments, including orbital contribution; quenching of magnetic moment: super exchange and antiferromagnetic interactions (elementary idea with examples only); d-d transitions; L-S coupling, Hole formalism principle; qualitative Orgel diagrams for $3d^1-3d^9$ ions and their spectroscopic ground states; selection rules for electronic spectral transitions; spectrochemical series of ligands; Nephelauxetic parameter charge transfer spectra, different types (elementary idea with examples).

Unit II. Chemistry of d- and f- block elements

12 marks

General comparison of 3d, 4d and 5d elements in term of electronic configuration, elemental forms, metallic nature, atomization energy, oxidation states, redox properties, coordination chemistry, spectral and magnetic properties.

f-block elements: electronic configuration, ionization energies, oxidation states, variation in atomic and ionic (3+) radii, magnetic and spectral properties of lanthanides, comparison between lanthanide and actinides, separation of lanthanides (by ion-exchange method).

Chemistry of some representative compounds: K₂Cr₂O₇, KMnO₄, K₄[Fe(CN)₆], K₂[Ni(CN)₄], H₂PtCl₆, Na₂[Fe(CN)₅NO].

CEMAT 35-IB

Unit I. Organometallic Compounds

18-electron rule and its applications to carbonyls (including carbonyl hydrides and carbonylates), nitrosyls, cyanides, and nature of bonding involved therein. Simple examples of metal-metal bonded compounds and metal clusters. Metal-olefin complexes: zeises salt (preparation, structure and bonding), Ferrocene (preparation, structure and reactions). Hapticity(n) of organometallic ligands, examples of mono tri and penta-hapto cyclopentadienyl complexes. Simple examples of fluxional molecules. Coordinative unsaturation: oxidative addition and insertion reactions. Homogeneous catalysis by organometallic compounds: hydrogenation, hydroformylation and polymerization of alkenes (Ziegler-Natta catalysis).

Unit II: Gravimetric and tritimetric methods of analysis

Requirements of gravimetry: properties of precipitates and precipitating regents, particle size and filterability of precipitates, colloidal and crystalline precipitates coprecipitation and post-precipitation drying and ignition of precipitates, principles of gravimetric estimation of chloride, phosphate, zinc, iron, aluminum and magnesium singly. Primary and secondary standard substances in acid-base, redox, complexometric (EDTA) and argentometric titrations. Principle and application of redox tritimetric estimation based on the

use of the following reagents: $KMnO_4$, $K_2Cr_2O_7$, I_2 , $Na_2S_2O_3.5H_2O$, $KH(IO_3)_2$ and $KBrO_3$. Principle of argentimetric estimation of chloride using adsorption indicators.

Principle of complexometric EDTA titration, metal ion indicators (examples), masking and demasking reactions, estimation of Cu-Zn, Fe-Al and Ca-Mg mixture by EDTA titration methods.

Dissolution, scheme of analysis and principles of estimation of the constituents of the following materials: dolomite, pyrolusite, chalchopyrites, Portland cement, basic slag, brass, steel and type metal.

13 marks

CEMAT 35-AA

Unit I. Bioinorganic Chemistry

Elements of life: essential major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na⁺, K⁺, Mg²⁺, Ca²⁺, Fe^{3+/2+}, Cu^{2+/+}, and Zn²⁺).Metal ion transport across biological membrane Na⁺-ion pump, ionophores. Biological functions of hemoglobin and myoglobin, cytochromes and ferredoxins, carbonate bicarbonate buffering system and carbonicanhydrase. Biological nitrogen fixation, Photosynthesis: Photosystem-I and Photosystem-II. Toxic metal ions and their effects, chelation therapy (examples only), Pt and Au complexes as drugs (examples only), metal dependent diseases.

Unit II. Material Chemistry

Silicate minerals (Quartz) Zeolite: structure, accommodation of 'guest ions'.

Nanomaterials: (Definition and properties). Carbon nano particles (Buckmister Fullerence C_{60}), Gold nano particles

Metal clusture structure i) carbonyl ii) oxide, Metal surface catalysis (NH₃ products, Haber process).

Polymer: definition, classification, different types of molecular weight and their determination (viscosity average and weight average method).

CEMAT 35-AB

Unit I : Bioorganic Chemistry

Secondary, tertiary and quaternary structure of proteins, classification of enzymes and coenzymes (simple examples), nucleic acids: structure of nucleosides and nucleotides, DNA, RNA, complementary base pairings, elementary idea of double helical structure of DNA [Watson-Crick model, Houg-Steen model (for adenine only)], naturation and denaturation of protein.

Unit-II : Biophysical Chemistry

Colloids and their stability, elementary idea of electrical double layer and its protective role in the stability of colloids, isoelectric point, Autocatalysis, Enzyme catalysis, Michaelis-Menten equation, Lineweaver-Burk plot, turnover number and catalytic efficiency of enzymes, Mechanisms of enzyme inhibition, pH-dependence of enzyme activity, Electrophoresis, elementary idea of gel electrophoresis, polyacrylamide gel electrophoresis (PAGE) and SDS-PAGE, Isoelectric focusing.

13 marks

13 marks

12 marks

Paper VI Courses : CEMAT 36-OA, 36-OB, 36-PA, 36-PB (Each 25 marks : Total 100 marks)

CEMAT 36-OA

UNIT I

13 marks

Organic synthesis : Disconnection approach towards synthesis of bifunctional molecules (both cyclic and acyclic) : Concept of synthons, synthetic equivalents (ethyl acetoacetate, ethyl cyanoacetate and diethyl malonate as examples), functional group interconversion (FGI), protection and deprotection of common functional groups (-OH, -carbonyl, -NH₂, -COOH) in synthetic route, activation of synthetic equivalents, umpulong, illogical electrophiles and nucleophiles, disconnection and synthesis of 1,3-, 1,4, 1,5 and 1,6-dioxygenated compounds, Robinson ring annulation, Favorskii rearrangement, large ring compound synthesis (High dilution principle), stereoselective synthesis (Cram's rule, Prelog's rule).

Pericyclic reactions : Definition and classification, Electrocyclic reactions : FMO approach, examples of electrocyclic reactions (thermal and photochemical) involving 4- and 6π -electrons and corresponding cycloreversion reactions, Cycloaddition reactions : FMO approach, Diels-Alder Reaction, photochemical [2+2] reactions, Sigmatropic shifts and their order, [1,3] and [1,5] H shifts, [3,3] shifts with references to Claisen and Cope rearrangements, ene reaction (simple treatment)

Polynuclear hydrocarbons: Nomenclature, synthesis and important reactions of naphthalene, anthracene and phenanthrene.

<u>UNIT II</u>

12 marks

Heterocyclic compounds : Synthesis (including retrosynthetic approach), reactivity, orientation and important reactions of furan, pyrrole, thiophene, pyridine, indole, quinoline and isoquinoline, Knorr pyrrole synthesis, Hantzsch pyridine synthesis, Fischer indole synthesis and Bischler-Napieralsky synthesis.

Pharmaceuticals : Preparation and uses of sulphadiazine, chloroquine, metronidazole, chlorpromazine, indomethacin, ranitidine.

CEMAT 36-OB

<u>UNIT I</u>

13 marks

Streochemistry of cyclohexanes, mono- and disubstituted, Baeyer strain theory, Concept of I-strain, conformational analysis of cyclohexanes, energy profile of ring inversion of cyclohexane, symmetry properties of chair, boat and skew boat conformations, conformational analysis of mono and di-substituted cyclohexanes, Dynamic stereochemistry: E_2 , SN_2 and NGP, lactonisation reactions of cyclohexane systems, oxidation of cyclohexanols with chromic acid, pinacol-pinacolone rearrangements, esterification, saponification of ester, steric assistance and steric hindrance there in, cyclohexene and cylohexanone: stereochemistry, bromine addition and epoxydation of cyclohexene, nucleophilic addition to cyclohexanone.

Carbohydrates: monosaccharides: classification of monosaccharides, osazone formation, stepping up and stepping down of aldoses, interconversion of aldose and ketose, epimerization, constitution and configuration of D- glucose and D- fructose, ring structure and conformational aspects of D- glucose and its derivatives, anomeric effect, mutarotation of D- glucose, Disaccharides : Structure of sucrose only.

<u>UNIT II</u>

Amino acids, peptides and proteins: synthesis of α - amino acids [Gabriel, Strecker, azlactone, hydantoin, acetamidomalonic ester methodologies], isoelectric point, ninhydrin reaction, peptides: geometry of peptide linkage, peptide synthesis including Merrifield ptotocol, C - terminal and N- terminal determination, determination of amino acid sequence, proteins: classification, structure (primary only).

Natural products: Terpenoids : Classification, isoprene rule, structure and synthesis of citral, geraniol and nerol.

Alkaloids: Structure and synthesis of ephedrine and nicotine.

CEMAT 36-PA

Unit-I: Statistical Thermodynamics and Third Law

13 marks

Macrostates and microstates, thermodynamic probability, entropy and probability, Boltzmann distribution formula (with derivation). Applications to barometric distribution. Partition function. Derivation of expression of thermodynamic functions using partition function.

Dulong-Petit's law and Einstein's theory of heat capacity of solids. Limitation of Einstein's theory and Debye's modification (qualitative). Nernst heat theorem. Approach towards zero kelvin, adiabatic demagnetisation. Planck's formulation of third law and absolute entropies.

Unit-II : Molecular Spectroscopy

Rotational spectroscopy of diatomic molecules: rigid rotor model, selection rules, spectrum, characteristic features of spectral lines (spacing and intensity). Determination of bond length, effect of isotopic substitution.

Vibrational spectroscopy of diatomic molecules: SHO model, selection rules, spectra; anharmonicity and its consequences on energy levels, overtones, hot bands. Raman Effect. Characteristic features and conditions of Raman activity with suitable illustrations. Rotational and vibrational Raman spectra. Rule of mutual exclusion with examples.

CEMAT 36PB

Unit-I : Properties of Solid, interface and dielectrics

Crystal, crystal planes, law of rational indices, Calculation of fraction occupied for simple cubic, bcc, and fcc. Miller indices. Bragg's law and its applications for the determination of crystal structure for cubic system single crystal. Crystal structures of NaCl and KCl. Brief idea about liquid crystals.

Special features of interfaces compared to bulk. Surface dynamics: Physical and chemical adsorption. Freundlich and Langmuir adsorption isotherms; multilayer adsorption and BET isotherm (no derivation required). Gibbs adsorption isotherm and surface excess. Heterogeneous catalysis (single reactant).

Electrical properties of molecules: Polarizability of atoms and molecules, dielectric constant and polarisation, molar polarisation for polar and non-polar molecules. Clausius-Mosotti equation and Debye equation (both without derivation) and their application. Determination of dipole moments.

Unit-II : Phase equilibria and colligative properties

Phase equilibrium and colligative properties. Definitions of phase, component and degrees of freedom. Phase rule and its derivations. Definition of phase diagram. Phase equilibria for one component system – water, CO2. First order phase transition and Clapeyron equation; Use of Clausius-Clapeyron equation.

Liquid vapour equilibrium for two component systems. Ideal solution at fixed temperature and pressure. Principle of fractional distillation. Duhem-Margules equation. Henry's law. Konowaloff's rule. Positive and negative deviations from ideal behaviour. Azeotropic

12 marks

13 marks

solution. Liquid-liquid phase diagram using phenol-water system. Solid- liquid phase diagram. Eutectic mixture. Nernst distribution law. Solvent extraction.

 ΔG , ΔS , ΔH and ΔV of mixing for binary solutions. Vapour pressure of solution. Ideal solutions, ideally diluted solutions and colligative properties. Raoult's law. Thermodynamic derivation of colligative properties of solution (using chemical potential) and their interrelationships. Abnormal colligative properties.

Paper VII Course : CEMAP 37-Pr (Total 100 marks)

Physical Chemistry

Experiments:

1. To study the kinetics of inversion of sucrose using polarimeter.

2. To study the phase diagram of a binary system (Phenol + water) and the effect of impurities (e.g. NaCl).

3. Determination of ionization constant of a weak acid by conductometric method.

4. To study the kinetics of saponification of ester by conductometric method.

5. Conductometric titration of HCl vs NaOH, AcOH vs NaOH.

6. Determination of formal potential of Fe^{+3}/Fe^{+2} couple in the hydrogen scale by potentiometric titration of ferrous ammonium sulfate solution using KMnO₄, or, K₂Cr₂O₇ as standard.

7. Determination of concentration of (i) AgNO₃ solution and (ii) solubility product of AgCl by potentiometic titration of standard KCl solution against AgNO₃ solution.

8. Determination of pK values of weak monobasic, dibasic and polybasic acid by pH-metric method (e.g. using, acetic acid, succinic acid, oxalic acid, phosphoric acid, etc.).

9. Study of the kinetics of the reaction $I + S_2O_8^{-2}$ by colorimetric method.

10. Determination of \land o of a strong electrolyte (KCl) conductometrically.

11. Determination of specific rotation of an optically active substance.

12. Determination of indicator constant by colourimetric method.

13. Verification of Lambert Beer's Law.

14. Conductometric titration of mixed acid.

Organic

25 marks

1. Identification of amino acids by TLC/paper.

2. Binary mixture separation (neutral + acid or base) and identification by TLC/Paper.

Laboratory Note Book & Viva

25 marks

Paper VIII Course : CEMAP 38-Pr (Total 100 marks)

Inorganic Chemistry

- $\begin{array}{l} Complexometric \ estimation: \\ i) \ (Ca^{2+} + Mg^{2+}) \ in \ solution. \\ ii) (Fe^{3+} + Al^{3+}) \ in \ solution. \end{array}$ 1)
- Dichromatometry and iodometry: 2)
 - i) $Fe^{3+} + Cr_2O_7^{2-}$ ii) $Fe^{3+} + Cu^{2+}$
 - iii) $Fe^{3+} + Mn^{2+}$.
- Permanganometry: $Fe^{3+} + Ca^{2+}$. 3)
- Analysis of Fe^{3+} in cement. 4)
- Gravimetry: 5)
 - i) Ni^{2+} as glyoximato complex. ii) Cu^{2+} as CuSCN.

Determination of temporary and permanent hardness in supplied water. 6)

Organic Preparation

25 marks

Preparation of an organic compound, purification and determination of its M.P., Nitration (cold, hot), Condensation, Hydrolysis, Oxidation, Halogenation (Green method), acetylation.

Laboratory Note Book & Viva

25 marks