Course Structure FOR Choice Based Credit System of B.Sc. (Chemistry)[UGCHE] Program with effect from 2020-21 School of Science, UPRTOU, Prayagraj

Semester	Course Code	Title of Paper	Credits	Max. Marks
I	UGCHE -101	INORGANIC CHEMISTRY I (BASIC INORGANIC CHEMISTRY)	2	100
	UGCHE -101P	Practical Work	2	100
II	UGCHE -102	ORGANIC CHEMISTRY I (BASIC ORGANIC CHEMISTRY)	2	100
	UGCHE -102P	Practical Work	2	100
ш	UGCHE -103	PHYSICAL CHEMISTRY I (BASIC PHYSICAL CHEMISTRY)	2	100
	UGCHE -103P	Practical Work	2	100
	Skill Enhancement Course			
	SBSCHE-01	ORGANIC CHEMISTRY II (ADVANCE ORGANIC CHEMISTRY)	4	100
IV	UGCHE -104	INORGANIC CHEMISTRY II (ADVANCE INORGANIC CHEMISTRY)	2	100
	UGCHE -104P	Practical Work	2	100
V	Discipline Centric Elective Course			
	DCECHE -105	PHYSICAL CHEMISTRY II (ADVANCE PHYSICAL CHEMISTRY)	2	100
	DCECHE -106	INORGANIC CHEMISTRY III (SELECTED TOPICS IN INORGANIC CHEMISTRY)	2	100
	DCECHE -107P	Practical Work	2	100
VI	Discipline Centric Elective Course			
	DCECHE -108	ORGANIC CHEMISTRY III (SELECTED TOPICS IN ORGANIC CHEMISTRY)	2	100
	DCECHE -109	PHYSICAL CHEMISTRY III (SELECTED TOPICS IN PHYSICAL CHEMISTRY)	2	100
	DCECHE -110P	Practical Work	2	100
Total Credit/Max. Marks			32	1500

B.Sc. (CHEMISTRY-UGCHE) UGCHE -101: INORGANIC CHEMISTRY I (BASIC INORGANIC CHEMISTRY)

BLOCK-1

Unit 1: Atomic Structure

Historical concepts of atomic structure. Idea of de-Broglie's matter waves, Heisenberg's uncertainly principle, significant of ψ and ψ^2 , Schrodinger's wave equation for H atom; Radial and angular wave functions: quantum numbers and shapes of s, p, d and f orbitals; Aufbau and Pauli Exclusion Principle. Variation of orbital energies with atomic number and energy level diagram; Long form of periodic table based on electronic configuration.

Unit 2: Periodic properties of elements

Types of radii (Covalent, Crystal and Van der Waal); Electron affinity and its variation; Ionisation potential, Factors affecting the magnitude of I.P., Concept of effective nuclear charge and shielding effect (Calculation of Screening constant with Slater's rules.); Electronegativity (Pauling, Mulliken and Allred Rochow scale) and its variation.

Unit 3: Chemical Bonding

(i) **Ionic Bonding:** Conditions favouring the ionic bond, radius ratio and structure of ionic solids.

Concept of lattice energy and Born-Haber cycle, Polarisation of ions and Fajan's rules.

(ii) Covalent and brief idea of other bonds:

Concept of directed valence bond theory (VBT) and hybrid orbital description (sp, sp², sp³, sp³d and sp³d²) using simple illustrations, determination of the shapes of molecules and ions viz. NH₃, H₂O, H₃O⁺, SF₄, ClF₃, ICl²⁻ and I³⁻ by VSEPR concept, Concept of maximum covalency. Odd electron bond, three centre bond. MO Theory, homonuclear (H₂,H²⁺, B₂, N₂, O₂, Cl₂) and heteronuclear (CN, CO and NO) diatomic molecules, bond strength, and bond energy, percent ionic character from dipole moment and electronegativity. Multicenter bonding in electron deficient molecules.

(iii) Weak Interactions: Hydrogen bonding (Inter and Intra Molecular), Vander Waals forces.(iv) Metallic Bond: Theories of bonding in metals; Free electron, VB and Band theories.

BLOCK-2

Unit 4: General Studies of s block elements

Comparative study, diagonal relationships, salient features of hydrides, solvation and complexation tendencies including their function in biosystems, an introduction to alkyls and aryls; Chemical reactivity of alkali and earth alkaline metals; Uses of s-block elements and their compounds (Li, Na and K only), Organometallic compounds of Li, Na, K, Be and Mg. Polyether complexes (Crown ether complexes) of alkali metals; Extraction and isolation of Li, Be and Ra from their minerals.

Unit 5: General Studies of p- block elements

Group wise discussion with respect to electronic configuration, ionisation potential, electron affinity, electronegativity, atomic and ionic radii, oxidation states, catenation and inert pair effect (wherever applicable). Preparation, properties and structures of diborane, borazine, hydrazine,

interhalogens and polyhalides and fluorides of xenon. Structure and basicities of oxyacids of B, P and S. Structural features of hydrides, halides, oxides and oxyacids.

Unit 6: Oxidation and Reduction

Electrode potential, electrochemical series and its applications. EMF diagrams and their utility. Principle involved in the extraction of the elements.

UGCHE -102: ORGANIC CHEMISTRY I (BASIC ORGANIC CHEMISTRY)

BLOCK-1

Unit 1: Structure and Bonding

Atomic orbitals, hybridization, orbital representation of methane, ethane, ethyne and benzene. Polarity of bonds: Inductive, resonance and steric effects hyperconjugation, and their influence on acidity and basicity of organic compounds. Homolysis and Heterolysis; Concept of Carbocation, Carbanion and Free radicals.

Unit 2: Mechanism of Organic Reactions and Reaction Intermediates

Curved arrow notation, drawing electron movements with allows, half-headed and doubleheaded arrows, hemolytic and heterolytic bond breaking. Types of reagents – electrophiles and nucleophiles, Types of organic reactions, Energy considerations. Reactive intermediates – Carbocations, carbanions, free radicals, carbenes, arynes and nitrenes (with examples). Assigning format charges on intermediates and other ionic species. Methods of determination of reaction mechanism (product analysis, intermediates, isotope effects, kinetic and stereochemical studies).

Unit 3: Alkanes and Cycloalkanes

IUPAC nomenclature of branched and unbranched alkanes, the alkyl group, classification of carbon atom in alkanes, Isomerism in alkanes, sources methods of formation (with special reference to Wurtz reaction, Kolbe reaction, Corey-House reaction and decarboxylation of carboxylic acids), physical properties and chemical reactions of alkanes. Mechanism of free radical halogenation of alkanes: orientation, reactivity and selectivity.

BLOCK-2

Unit 4: Stereochemistry of Organic Compounds

Concept of isomerism. Types of isomerism. Optical isomerism – elements of symmetry, molecular chirality, enantionmers, stereogenic center, optical activity, properties of enantiomers, chiral and achiral molecules with two stereogenic centers, diastereomers, threo and erythro diastereomers, meso compounds, resolution of enantiomers, inversion, retention and recemization. Relative and absolute configuration, sequence rules, D & L and R & S systems of nomenclaute. Geometric isomerism – determination of configuration of geometric isomers. E & Z system of nomenclature, geometric isomerism in oximes and alicyclic compounds. Conformational isomerism -- conformational analysis of ethane and n-butane; conformations of cyclohexane, axial and equatorial bonds, conformation of mono substituted cyclohexane derivatives. Newman projection and Sawhorse formulae, Fischer and flying wedge formulae. Difference between configuration and conformation.

Unit 5: Alkenes, Cycloalkenes, Dienes and Alkynes

Nomenclature of alkenes, methods of formation, mechanisms of dehydration of alcohols and dehydrohalogenation of alkyl halides, regioselectivity in alcohol dehydration. The Saytzeff rule, Hofmann elimination, physical properties and relative stabilities of alkenes. Chemical reactions of alkenes - mechanism involved in hydrogenation, electrophilic and free radical hydroborationoxidation, additions. Markownikoff's rule. oxymercuration-reduction. Epoxidation. ozonolysis, hydration, hydroxylation and oxidation with KMnO4. Polymerization of alkenes. Substitution at the allylic and vinylic positions of alkenes. Industrial applications of ethylene and propene. Methods of formation, conformation and chemical reactions of cycloalkenes. Nomenclature and classification of dienes: isolated, conjugated and cumulated dienes. Structure of allenes and butadiene, methods of formation, polymerization, Chemical reaction - 1,2 and 1,4 additions, Diets-Alder reaction. Nomenclature, structure and bonding in alkynes. Methods of formation. Chemical reactions of alkynes, acidity of alkynes. Mechanism of electrophilic and nucleophilic addition reactions, hydroboration-oxidation, metal-ammonia reductions, oxidation and polymerization.

Unit 6: Arenes and Aromaticity

Nomenclature of benzene derivatives. The aryl group. Aromatic nucleus and side chain. Structure of benzene: molecular formula and kekule structure. Stability and carbon-carbon bond lengths of benzene, resonance structure, MO picture. Aromaticity: the Huckel rule, aromatic ions. Aromatic electrophilic substitution – general pattern of the mechanism, role of σ and π complexes. Mechanism of nitration, halogenation, sulphonation, mercuration and Friedel-Crafts reaction. Energy profile diagrams. Activating and deactivating substituents, orientation and ortho/para ratio. Side chain reactions of benzene derivatives. Birch reduction. Methods of formation and chemical reactions of alhylbenzenes, alkynylbenzenes and biphenyl.

Unit 7: Alkyl and Aryl Halides

Nomenclature and classes of alkyl halides, methods of formation, chemical reactions. Mechanisms of nucleophilic substitution reactions of alkyl halides, SN2 and SN1 reactions with energy profile diagrams. Polyhalogen compounds: chloroform, carbon tetrachloride. Methods of formation of aryl halides, nuclear and side chain reactions. The addition-elimination and the elimination-addition mechanisms of nucleophilic aromatic substitution reactions. Relative reactivities of alkyl halides vs allyl, vinyl and aryl halides. Synthesis and uses of DDT and BHC.

UGCHE 103: PHYSICAL CHEMISTRY I (BASIC PHYSICAL CHEMISTRY)

BLOCK-1

Unit 1: Mathematical Concepts and Computers

(A) Mathematical Concepts

Logarithmic relations, curve sketching, linear graphs and calculation of slopes, differentiation of functions like $f_{(x)}$, e_x , x_n , sin x, log x; maxima and minima, partial differentiation and eciprocity relations. Integration of some useful/relevant functions; permutations and combinations, Factorials, Probability and Regrations.

(B) Computers

General introduction to computers, different components of a computer, hardware and software, input-output devices; binary numbers and arithmetic; introduction to computer

languages. Programming, operating systems. Use and application of different software in the Chemistry.

Unit 2: Gaseous and Liquid States

(A) Gaseous States

Postulates of kinetic theory of gases, deviation from ideal behaviour, van der Waals equation of state.

Critical Phenomena : PV isotherms of real gases, continuity of states, the isotherms of van der Waals equation, relationship between critical constants and van der Waals constants, the law of corresponding states, reduced equation of state.

Molecular Velocities : Root mean square, average and most probable velocities. Qualitative discussion of the Maxwell's distribution of molecular velocities, collision number, mean free path and collision diameter. Liquefaction of gases.

(B) Liquid State

Intermolecular forces, structure of liquids (a qualitative description). Structural differences between solids, liquids and gases.

Liquid crystals: Difference between liquid crystal, solid and liquid. Classification, structure of nematic, smectic and cholesteric phases and applications.

Unit 3: Solid State

Definition of space lattice and unit cell.

Laws of crystallography:

(i) Law of constancy of interfacial angles

(ii) Law of rationality of indices

(iii) Law of symmetry - Symmetry elements in crystals.

X-ray diffraction: Derivation of Bragg's equation. Determination of crystal structure of NaCl, CsCl and KCl.

A brief introduction to point defects in crystals, semiconductors, superconductors and nanomaterials (only qualitative idea).

BLOCK-2

Unit 4: Thermodynamics – I

Definition of terms: system, surroundings, open system, isolated system, intensive and extensive properties, State and path functions and their differentials, reversible and irreversible processes, Concept of heat and work.

First Law of Thermodynamics: Concepts of internal energy and enthalpy, heat capacities at constant volume and constant pressure and their relationship. Calculation of w, q, dU & dH for the expansion of ideal gases under isothermal and adiabatic conditions for a reversible process.

Thermochemistry : standard state, standard enthalpy of formation- Hess's Law of constant heat summation and its applications, heat of reaction at constant pressure and at constant volume,

Bond dissociation energy and its calculation from thermo-chemical data, Kirchhoff's equation.

Unit 5: Electrochemistry – I and Solution

Electrical transport - conduction in metals and in electrolyte solutions, specific conductance and equivalent conductance, measurement of equivalent conductance, variation of equivalent and specific conductance with dilution.

Migration of ions and Kohlrausch law, Arrhenius theory of electrolyte dissociation and its limitations, weak and strong electrolytes, Ostwald's dilution law, its uses and limitations.

Debye-Huckel-Onsager's equation for strong electrolytes (elementary treatment only). Activity and activity coefficient. Transport number, definition and determination by Hittorf method and moving boundary method.

Solution

Thermodynamic derivation of relation between molecular weight and elevation in boiling point and depression in freezing point. Experimental methods for determining various colligative properties. Abnormal molar mass, degree of dissociation and association of solutes.

Unit 6: Chemical Kinetics and Catalysis

Rate of a reaction- factors influencing the rate of a reaction such as concentration, temperature, pressure, solvent, light and catalyst. Concentration dependence of rates, mathematical characteristics of simple chemical reactions - zero order, first order, second order, pseudo order, half life and mean life. Determination of the order of reaction - differential method, method of integration, method of half life period and isolation method. Radioactive decay as a first order phenomenon. Experimental methods for the studies of chemical kinetics.

Theories of chemical kinetics: Effect of temperature on rate of reaction, Arrhenius equation, concept of activation energy, Simple collision theory based on hard sphere model, transition state theory (equilibrium hypothesis). Expression for the rate constant based on equilibrium constant and thermodynamic aspects.

Catalysis: Characteristics of catalyzed reactions, classification of catalysis, Industrial catalysts and enzyme kinetics.

UGCHE 104: INORGANIC CHEMISTRY II (ADVANCE INORGANIC CHEMISTRY)

BLOCK-1

Unit 1: Molecular Symmetry

Symmetry Elements, Symmetry Operations and Point groups of different compounds. Character Tables of H₂O and NH₃.

Unit 2: Chemistry of Transition Elements

Position in periodic table, electronic configuration, General Characteristics, viz., atomic and ionic radii, variable oxidation states, ability to form complexes, formation of coloured ions and catalytic behaviour. General comparative treatment of 4d and 5d (Zr/Hf, Nb/Ta, Mo/W) elements with their 3d analogues with respect to ionic radii, oxidation states and magnetic properties.

Unit 3: Coordination Compounds

(i) Definition of ligand: Classification with respect to denticity. (Examples of mono-to hexadentate ligands).

(ii) IUPAC-Nomenclature of Transition Metal complexes.

(iii) Werner's postulates, Sidgwick's effective atomic number concept and limitations, Valence Bond Theory of coordination compounds, Stereochemistry of coordination numbers two, four, five and six with examples of hybrid orbital participation in the following :

 $[Ag(NH_3)_2]+, [Ag(CN)_2]^{-}, [Ni(CN)_4]^{n-}$ (n=2 and 4), $[Cu(NH3)4]^{2+}, [Zn(NH_3)_4]^{2+}, [MnO_4]^{-}, [Fe(CN)_6]^{n-}$ (n=3 and 4), $[FeF_6]^{3-}, [Fe(H_2O)_6]^{3+}, [Fe(C_2O_4)_3]^{3-}, [Co(NH_3)_6]^{3+}, [Co(en)_3]^{3+}, [Ni(NH_3)_6]^{2+}, [PbCl_6]^{2-}$

(iv) Stability Constant of Transition Metal complexes and Chelate effect

(v) Various types of isomerism, viz., hydrate, ionisation, linkage, polymerization and coordination position. Stereoisomerism in C.N.-4 and C.N.-6 (only ML_4L_2 and ML_3L_3 complexes).

BLOCK-2

Unit 4: Chemistry of Lanthanides and Actinides

i. Electronic Configuration,

ii. Atomic, Ionic radii and Lanthanide Contraction.

iii. Ionisation energy,

iv. Calculation of magnetic moments and correlation with experimental data (specially for lanthanides),

v. Colour and spectral behaviour,

vi. Oxidation states and their stability,

vii. Ability to form complexes and examples of complexes of different coordination numbers.

viii. Occurrence and principle of separation of lanthanides.

ix. Chemistry of separation of Np, Pu and Am from U and

x. One synthesis each of Np to Lr.

Unit 5: Chemistry of Nobel Gases

Properties, Occurrence, Isolations and Applications. Chemistry of Noble Gases, Compounds of Xenon & Krypton and their reactions. Clathrates.

Unit 6: Acid - Base and Non-aqueous solvents

Acid - Base concept -Lewis concept, Concept and classification of hard and soft acids and bases. Applications of HSAB principle.

Non-aqueous solvents-Classification and characteristic properties of solvents. Types of chemical reactions occurring in liquid ammonia (NH₃) and liquid sulphur dioxide (SO₂).

SBSCHE- 01- ORGANIC CHEMISTRY II (ADVANCE ORGANIC CHEMISTRY) BLOCK-1

Unit 1: Electromagnetic Absorption Spectra

Electromagnetic Radiations, Electromagnetic spectrum and absorption of radiations. The Absorption Laws. UV-Visible spectrophotometer, formation of Absorption Band. Chromatophore Concept, Calculation of Absorption Maximum. Infra Red Spectroscopy Fundamental and Applications.

Unit 2: Alcohols and Phenols

Classification and nomenclature. Monohydric alcohols – nomenclature, methods of formation by reduction of aldehydes, Ketones, Carboxylic acids and Esters, Hydrogen bonding, Acidic nature, Reactions of alcohols. Dihydric alcohols – nomenclature, methods of formation, chemical reactions of vicinal glycols, oxidative cleavage [Pb(OAc)₄ and HIO₄] and pinacolo-

pinacolone rearrangement. Trihydric alcohols – nomenclature and methods of formation, chemical reactions of glycerol.

Phenols

Nomenclature, structure and bonding, Preparation of phenols, physical properties and acidic character. Comparative acidic strengths of alcohols and phenols, resonance stabilization of phenoxide ion. Reactions of phenols – electrophilic aromatic substitution, acylation and carboxylation. Mechanisms of Fries rearrangement, Claisen rearrangement, Gatterman synthesis, Hauben-Hoesch reaction, Lederer-Manasse reaction and Reimer- Tiemann reaction.

Unit 3: Ethers and Epoxide

Ethers

Nomenclature of ethers and methods of their formation, physical properties, Chemical reactions – cleavage and autoxidation, Ziesel's method. Williamson's synthesis, formation and cleavage of oxonium salts, elementary idea about crown ethers.

Epoxides

Synthesis of epoxides, Acid and base-catalyzed ring opening of epoxides, orientation of epoxide ring opening, reactions of Grignard and organolithium reagents with epoxides.

BLOCK-2

Unit 4: Aldehydes and Ketones

Nomenclature and structure of the carbonyl groups, synthesis of aldehydes and ketones with particular reference to the synthesis of aldehydes from acid chlorides, synthesis of alkedydes and ketones using 1,3-dithianes, synthesis of ketones from nitrites and from carboxylic acids. Physical properties. Mechnism of nucleophillic additions to carbonyl group with particular emphasis on benzoin, aldol, Perkin and Knoevenagel condensations, Condensation with ammonia and its derivatives. Wittig reaction, Mannich reaction. Use of acetals as protecting group, Oxidation of aldehydes, Baeyer-Villiger oxidation of Ketones, Cannizzaro reaction, MPV, Clemmensen, Wolff-Kishner, LiAlH4 and NaBH4 reductions. Halogenation of enolizable ketones. An introduction to α,β unsaturated alkehydes and ketones.

Unit 5: Carboxylic Acids and Derivatives

Nomenclature, structure and bonding, physical properties, acidity of carboxylic acids, effects of substituents on acid strength. Preparation of carboxylic acids, Reactions of carboxylic acids, Hell-Volhard-Zelinsky reaction, Synthesis of acid chlorides, esters and amides. Reduction of carboxylic acids, Mechanism of decarboxylation. Methods of formation and chemical reactions of halo acids, Hydroxy acids: malic, tartaric and citric acids. Methods of formation and chemical reactions of unsaturated monocarboxylic acids. Dicarboxylic acids: methods of formation and effect of heat and dehydrating agents.

Carboxylic Acid Derivatives

Structure and nomenclature of acid chlorides, esters, amides(urea) and acid anhydrides.

Relative stability of acyl derivatives. Physical properties, interconversion of acid derivatives by nucleophilic acyl substitution Preparation of carboxylic acid derivatives, chemical reactions. Mechanisms of esterification and hydrolysis (acidic and basic).

Unit 6: Organic Compounds of Nitrogen

Preparation of nitroalkanes and nitroarenes. Chemical reactions of nitroalkanes. Mechanisms of nucleophilic substitution in nitroarenes and their reductions in acidic, neutral and alkaline

media. Picric acid. Halonitroarenes: reactivity, Structure and nomenclature of amines, physical properties. Stereochemistry of amines. Separation of a mixture of primary, secondary and tertiary amines. Structural features effecting basicity of amines. Amine salts as phase-transfer catalysts. Preparation of alkyl and aryl amines (reduction of nitro compounds, nitrites), reductive amination of aldehydic and ketonic compounds. Gabriel-phthalimide reaction, Hofmann bromamide reaction. Reactions of amines, electrophilic aromatic substitution in aryl amines, reactions of amines with nitrous acid. Synthetic transformations of aryl diazonium salts, azo coupling.

DCECHE -105- PHYSICAL CHEMISTRY II (ADVANCE PHYSICAL CHEMISTRY) BLOCK-1

Unit 1: Chemical Equilibrium and Phase Equibrium

Equilibrium constant and free energy. Thermodynamic derivation of law of mass action. Le Chattelier's principle.

Phase Equilibrium

Statement and meaning of the terms - phase, component and degree of freedom, derivation of Gibbs phase rule, phase equilibria of one component system - water, Sulpher and Hellium. First and second order phase transitions. Phase equilibria of two component systems - solid-liquid equilibria, simple eutectic - Pb-Ag system, desilverisation of lead, Systems involving compound formation with a congruent melting point (Mg-Zn) and an incongruent melting point (CuSO4-H2O). Nernst distribution law and its thermodynamic derivation

Unit 2: Thermodynamics –II

Second law of thermodynamics: concept of entropy, entropy as a state function, entropy as a function of V & T, entropy as a function of P & T, entropy change in physical process.

Gibbs and Helmholtz functions; Criteria for thermodynamic equilibrium and spontaneity in term of changes in entropy, Gibbs and Helmholtz functions. Concept of chemical potential.

Unit 2: Electrochemistry – II

Types of reversible electrodes - gas-metal ion, metal-metal ion, metal-insoluble salt-anion and redox electrodes. Electrode reactions, Nernst equation, derivation of cell E.M.F. and single electrode potential, standard hydrogen electrode-reference electrodes-standard electrode potential, sign conventions, electrochemical series and its significance.

Electrolytic and Galvanic cells - reversible and irreversible cells, conventional representation of electrochemical cells.

EMF of a cell and its measurements. Computation of cell EMF. Calculation of thermodynamic quantities of cell reactions (ΔG , ΔH and K).

Concentration cell with and without transport, liquid junction potential, application of concentration cells, valency of ions, solubility product and activity coefficient, potentiometric titrations.

Definition of pH and pKa determination of pH using hydrogen, quinhydrone and glass electrodes, by potentiometric methods.

Buffers - mechanism of buffer action, Henderson-Hazel equation. Hydrolysis of salts.

Electrochemical corrosion and its prevention.

BLOCK-2

Unit 4: Colloidal State and Macromolecules

Definition of colloids and classification of colloids. Donnan membrane theory and its application. Electrokinetic Potential (Zeta potential).

Solids in liquids (sols): properties - kinetic, optical and electrical; stability of colloids, protective action, Hardy-Schulze law, gold number.

Liquids in liquids (emulsions): types of emulsions, preparation, Emulsifier.

Liquids in solids (gels): classification, preparation and properties, inhibition, general applications of colloids.

Macromolecules : Determination of molecular weight of macromolecules by osmotic pressure and viscosity methods. Concepts of micelles and critical micelle concentrations.

A brief introduction to conducting and light emitting polymers.

Unit 5: Surface Phenomenon Surface Chemistry

Adsorption, difference between Physical adsorption and chemisorption, Adsorption isotherms - Langmuir adsorption isotherm and Freundlich adsorption isotherm, Gibbs adsorption equation, BET equation, Determination of surface area.

Unit 6: Physical Properties and Chemical Constitution

Molar volume, Parachor Molar refraction and Polarisation, Dipolemoment, Debey equation (derivation not required) and Clausius-Mosotti equation.

DCECHE -106- INORGANIC CHEMISTRY III (SELECTED TOPICS IN INORGANIC CHEMISTRY)

BLOCK-1

Unit 1: Metal-ligand Bonding in Transition Metal Complexes

Limitations of valance bond theory, an elementary idea of crystal field theory, Crystal Field Stabilization Energy (CFSE), crystal field splitting in octahedral, tetrahedral and square planner complexes, factors affecting the crystal-field parameters.

Thermodynamic and Kinetic Aspects of Metal Complexes

A brief outline of thermodynamic stability of metal complexes and factors affecting the stability, substitution reactions of square planar complexes and trans effect.

Unit 2: Magnetic and Electronic spectra of Transition Metal Complexes

(a) Electronic spectra of Transition Metal Complexes

Types of electronic transitions, selection rules for d-d transitions, spectroscopic ground states, spectrochemical series. Orgel-energy level diagram for d^1 and d^9 states, discussion of the electronic spectrum of $[Ti(H_2O)_6]^{3+}$ complex ion.

(b) Magnetic Properties of Transition Metal Complexes

Types of magnetic behavior, methods of determining magnetic susceptibility, spin- only formula. L-S coupling, correlation of μ s and μ eff values, orbital contribution to magnetic moments, application of magnetic moment data for 3d-metal complexes.

Unit 3: Organometallic Chemistry

Definition, nomenclature and classification of organometallic compounds. Preparation, properties, bonding and catalytic applications of alkyls and aryls of Li, Al, Hg, Sn.

Unit 4: Metal Carbonyls and Nitrosyls

(a) Metal Carbonyls : Ligand behaviour of CO, General methods of preparation, 18 electron rule, nature of bonding (Synergic effect) in the mononuclear carbonyls, Representation of structures of the binary carbonyls of all nuclearities of V, Cr, Mn, Fe, Co and Ni.

(b) Metal Nitrosyls : Ligand behaviour of NO (NO⁺, NO⁻ and bridging NO), preparation and structures of nitrosyls of Cr, Fe and Ru; carbonyl nitrosyls and cyano nitrosyls

BLOCK-2

Unit 5: Inorganic Polymers

Silicones and Phosphazenes

Silicons and phosphazenes as examples of inorganic polymers, nature of bonding in triphosphazenes.

Unit 6: Inorganic Biochemistry

Essential and trace elements in biological processes, metalloporphyrins with special reference to oxygen carrieres hemoglobin chemistry and myoglobin. Vitamin B-12, Nitogenase and Chlorophyll structure and applications. Biological role of alkali and alkaline earth metal ions with special reference to Na⁺, K⁺ and Ca²⁺.

Unit 7: Environmental Chemistry and Green Chemistry

(a) **Environmental Chemistry** :The earth's atmosphere and its components, Lapse rate, Types of pollutants and their sources (in water, Air and Soil). Green house effect and global warming. Acid rains, Ozone layer (Importance and its protection).

(b) Green Chemistry

Principles and concept of green chemistry, atom economic and noneconomic reactions, reducing toxicity, a few examples of environmental friendly reactions and reaction media.

Unit 8: Metal and Metallurgy

General principles of extraction and purification of metals. Occurrence and isolation of elements, Extraction and isolation of Metals (Y, La, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Mn, Tc, Re, Fe, Co, Ni and platinum) from their minerals.

DCECHE -108- ORGANIC CHEMISTRY III (SELECTED TOPICS IN ORGANIC CHEMISTRY)

BLOCK-1

Unit 1: NMR (PMR) Spectroscopy

Proton magnetic resonance (1H NMR) spectroscopy, nuclear shielding and deshielding, chemical shift and molecular structure, spin-spin splitting and coupling constants, areas of signals, interpretation of 1H NMR spectra of simple organic molecules such as ethyl bromide, ethanol, acetaldehyde, 1,1,2-tribromoethane, ethyl acetate, toluene and acetophenone. Problems pertaining to the structures elucidation of simple organic compounds using UV, IR and 1H NMR spectroscopic techniques.

Unit 2: Organometallic Compounds

Organomagnesium compounds: the Grignard reagents, formation, structure and Chemical reactions. Organozinc compounds: formation and chemical reactions. Organolithium compounds: formation and chemical reactions.

Unit 3: Sulphur Containing Compounds

Nomenclature, structural formation, Methods of formation and chemical reactions of thiols, thioethers, sulphonic acids, sulphonamides & Sulphaguamidine.

Unit 4: Amino Acids, Peptides, Proteins and Nucleic Acids

Classification, structure and stereochemistry of amino acids. Acid-base behaviour, Isoelectric point and electrophoresis, Preparation and reactions of α -amino acids. Structure and nomenclature of peptides and proteins. Classification of proteins, Peptide structure determination, end group analysis, selective hydrolysis of peptides. Classical peptide synthesis, solid-phase peptide synthesis. Structures of peptides and proteins. Levels of protein structure, Protein denaturation/renaturation.

Nucleic acids: Introduction. Constituents of ncleic acids. Ribonucleosides and ribonucleotides. The double helical structure of DNA.

BLOCK-2

Unit 5: Active Methylene Group

Preparation and synthetic applications of ethyl acetoacetate and diethyl malonate, Tautomerism.

Unit 6: Carbohydrates

Classification and nomenclature, Monosaccharides, mechanism of osazone formation, interconversion of glucose and fructose, chain lengthening and chain shortening of aldoses. Configuration of monosaccharides. Erythro and threo diastereomers, Conversion of glucose into mannose. Formation of glycosides, ethers and esters. Determination of ring size of monosaccharides. Cyclic structure of D(+)-glucose. Mechanism of mutarotation. Structures of ribose and deoxyribose. An introduction to disaccarides (maltose, sucrose and lactose) and polysaccharides (starch and cellulose) without involving structure determination.

Unit 7: Problem based on Spectroscopy (UV-Vis., IR and PMR)

DCECHE -109- PHYSICAL CHEMISTRY III (SELECTED TOPICS IN PHYSICAL CHEMISTRY)

BLOCK-1

Unit 1: Elementary Quantum Mechanics

Black-body radiation, Planck's radiation law, photoelectric effect, heat capacity of solids, Bohr's model of hydrogen atom (no derivation) and its defects, Compton effect. de Broglie's hypothesis, the Heisenberg's uncertainty principle, Hamiltonian operator. Statement of the Born- Oppenheimer approximation, degrees of freedom.

Unit 2: Molecular Statistics

The Boltzmann distribution. Maxwell distribution law for distribution of molecular speeds. The Maxwell-Boltzmann distribution law for the distribution of molecular energies. The partition functions. Thermodynamic quantities from partition functions. The Sackur-Tetrode equation for molar entropy of monatomic gases. Rotational and vibrational partition functions. The characteristic temperature. The calculation of Gibbs free energy changes and equilibrium constant in terms of partition functions.

Unit 3: Laws of Photochemistry

Interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry: Grothus – Drapper law, Stark – Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, nonradiative processes (internal conversion, intersystem crossing), quantum yield, photosensitized reactions – energy transfer processes (simple examples).

BLOCK-2

Unit 4: Vibrational, Rotational and Electronic Spectroscopy

Rotational Spectrum:

Diatomic molecules: Energy levels of a rigid rotor (semi-classical principles), selection rules, spectral intensity, distribution using population distribution (Maxwell-Boltzmann distribution) determination of bond length, qualitative description of non-rigid rotor, isotope effect.

Vibrational Spectrum:

Infrared spectrum: Energy levels of simple harmonic oscillator, selection rules, pure vibrational spectrum, intensity, determination of force constant and qualitative relation of force constant and bond energies, effect of of different functional groups.

Raman Spectrum: Concept of polarizability, pure rotational and pure vibrational Raman spectra of diatomic molecules, selection rules.

Electronic Spectrum: Concept of potential energy curves for bonding and antibonding molecular orbitals, qualitative description of selection rules and Franck-Condon principle.

Qualitative description of σ , π - and n M.O., their energy levels and the respective transitions.

Unit 5: Nuclear Chemistry

Nuclear reactions: Bethe notation, types of nuclear reactions (n, p, α , d and γ), conservation of quantities (mass-energy and linear momentum) in nuclear reactions, reaction cross-section, compound nucleus theory and nuclear reactions. Nuclear fission: the process, fragments, mass distribution, and fission energy. Nuclear reactor: the natural uranium reactor, classification of reactors, breeder reactor. Nuclear fusion and stellar energy.

Radiation chemistry: Elementary ideas of radiation chemistry, radiolysis of water and aqueous solutions, unit of radiation chemical yield (G-value), radiation dosimetry (Fricke's dosimeter), units of radiation energy (Rad, Gray, Rontgen, RBE, Rcm, Sievert).

Unit 6: Bioenergetics

Gibbs and Helmholtz energies with special emphasis on biological applications: study of energy transformations in living systems (bioenergetics): standard state in biochemistry, ATP-the currency of energy, Glycolysis, limitation of applicability of thermodynamics in biology.

UGCHE 101 (P): UGCHE-LAB-WORK-I

1. General – Principle and working of Chemical balance. Calibration of fractional weights and thermometer.

2 Inorganic Chemistry

Qualitative analysis of an inorganic mixture containing five radicals out of the following preferably by semi-micro technque (including insoluble substances):

 NH_4^+ , Na^+ , K^+ , Mg^{++} , Ca^{++} , Sr^{++} , Ba^{++} , Zn^{++} , Mn^{++} , Ni^{++} , Co^{++} , Al^{+++} , Fe^{+++} , Cr^{+++} , Cu^{++} , Bi^{++} , Hg^+ , Hg^+ , Cd^{++} , As^{+++} , Sb^{+++} , Sn^{++} , Pb^+ , Pb^{++} , Ag^+ , CO_3^{2-} , NO^{2-} , S^{2-} , SO_3^{2-} , SO_4^{2-} , F^- , Cl^- , Br^- , NO_3^- , CH_3COO^- , Borate, Oxalate, and Phosphate.

UGCHE 102 (P): UGCHE-LAB-WORK-II

Organic Chemistry

(a) Preparation of organic compounds:

- 1. Acetanilide
- 2. p-bromoacetanilide
- 3. picrates

(b) Crystallization and determination of melting point.

- 1. Phthalic acid from hot water (using fluted filter paper and stemless funnel)
- 2. Acetanilide from boiling water
- 3. Naphthalene from ethanol
- 4. Benzoic acid from water

UGCHE 103 (P): UGCHE-LAB-WORK-III

Physical Chemistry

1. To determine the specific reaction rate of the hydrolysis of methyl acetate/ethyl acetate catalysed by hydrogen ions at room temperature.

- 2. To study the effect of acid strength on the hydrolysis of an ester.
- 3. To compare the strength of HCl and H2SO4 by studying the kinetics of ethyl acetate.
- 4. To study kinetically the reaction rate of decomposition of iodide by H2O2.
- 5. Kinetics of precipitation of sulphur from sodium thiosulphate by mineral acid.
- 6. Kinetics of dissolution of Mg-ribbon in HCl.
- 7. To study the kinetics of reaction between acetone and iodine.

8. To determine the percentage composition of a given binary mixture (non-interacting systems) by viscosity methods.

9. To determine the percentage composition of a given binary mixture (non - interacting) by surface tension method.

10. To study the distribution of benzoic acid between water and CCl4.

UGCHE 104 (P): UGCHE-LAB-WORK-IV

Unit-1

1. General - Calibration of pipettes and burettes, preparation of standard solutions, strength and units of solution, dilution-0.1 M to 0.001 M solutions.

2. Inorganic Chemistry

Volumetric Exercises:

(i) Estimation of silver ions by volhard's and Mohr's method.

(ii) Redox titrations e.g. titration of ferrous ion with permanganate and dichromate using internal and external indicators.

(iii) Iodometric Estimation of Copper Sulphate and Potassium dichromate.

(iv) Estimation of Ca^{2+} ions using KMnO₄ solutions.

(v) Determination of acetic acid in commercial vinegar using NaOH.

Unit-2

Unit-3

4. Organic Practical

Identification of organic compounds containing any one of the following groups:

aldehyde, carbohydrate, acid, phenol, ketone, alcohol, amine, amide, nitro, hydrocarbon unsaturation.

This would include - determination of melting or boiling point, element detection, test for solubility and unsaturation test for functional groups, specific test if any and preparation of suitable derivatives wherever possible.

DCECHE --107(P) UGCHE-LAB-WORK-V

Quantitative Inorganic Analysis –

Gravimetric Estimation-Estimate the following ions gravimetrically

1. Ba/Pb as Barium sulphate/ lead sulphate.

2. Zn/Fe/Cr as Zinc Oxide / Iron Oxide/ Chromium Oxide

6. Nickel as bis (dimethylglyoximato) nickel (II)

Hardness of water

Temporary and permanent hardness.

Physical Chemistry

- (i) Determination of heat of neutralization of
- (a) Strong acid-strong base
- (b) Strong acid-weak base
- (c) Weak acid strong base

(ii) Determination of enthalpy of solution of solid calcium chloride and calculation of lattice energy of CaCl₂ by using BORN-HABER cycle.

(iii) Determination of the transition temperature of the given substance by thermometric method (e.g. $MnCl_2.4H_2O/SrBr_2.2H_2O$).

(iv) To construct the phase diagram of two component system (diphenyl amine + benzophenone) by Thaw-melt method/cooling curve method.

(v) To prepare arsenious sulphide sol and compare the precipitating powder of mono-, bi-and trivalent anions.

(vi) To titrate potentiometrically the given ferrous ammonium solution using $KMnO_4/K_2Cr_2O_7$ as titrant and calculate the redox potential of Fe⁺⁺/Fe⁺⁺⁺ system on the hydrogen scale.

(vii) To determine the solubility of simple salt by evaporation method and draw the solubility curve.

(viii) To determine the solubility of benzoic acid by titration method.

(ix) To determine the solubility product of calcium hydroxide.

DCECHE --110(P) UGCHE-LAB-WORK-VI

Organic Chemistry

1. Identification of an Organic Compound.

2. Systematic analysis of each component leading to their final identification laying emphasis on solubility, element detection, melting point, boiling point determination, ignition test, unsaturation test, functional group test and preparation of a suitable derivative.

3. Preparation of the following compounds:

- a. Soap from either one of the following line seed oil, mahua oil, neem oil or coconut oil.
- b. Phenyl benzoate from phenol
- c. Aspirin from salicylic acid
- d. Picric acid from phenol.
- e. Oxalic acid from cane sugar.

f. Benzoic acid from ethyl or methyl benzene.

Physical Chemistry

1. Determination of pH value by pH-Meter.

2. Determination of rate of reaction.

3. To verify Beer-Labert law for KMnO4/K2Cr2O7 and determine the concentration of the give solution of the substrate.

4. To verify law of refraction of mixture (e.g. of glycerol and water) using Abbe's refractometer.

5. To determine the specific rotation of a given optically active compound.

6. Determine the molecular weight of a non volatile solute by Rast method/ Backmann freezing point method.

7. Determination of the apparent degree of dissociation of an electrolyte (NaCl) in aqueous solution at different concentration by ebullioscopy.

UGCHE 113- ADVANCED ANALYTICAL TECHNIQUES BLOCK-1

Unit 1: Statistical Analysis

Definition of terms mean and median, precision, standard deviation, relative standard deviation, accuracy, absolute error, types of error in experimental data, determinate (systematic), indeterminate (or random) and gross, sources of errors and effects upon the

analytical results, methods for reporting analytical data, statistical evaluation of data, indeterminate errors, uses of statistics.

Unit 2: Volumetric analysis

General principles of acid – base titration, precipitation titration, oxidation-reduction titration, iodimetry and iodometry, complexometric titrations, use of EDTA for the determination of Ca^{2+} and Mg^{2+} and hardness of water, types of EDTA titrations, metal ion indicators.

Unit 3: Gravimetric analysis

Precipitation from homogeneous medium, purity of precipitates, co-precipitation, post-precipitation, washing and ignition of precipitates, contamination and their removal.

BLOCK-2

Unit 4: Separation techniques

Principle, technique and analytical applications of the following:

(a) Solvent extraction

(b) Chromatography (Paper, Thin Layer, Column and HPLC)

(c) Ion exchange

Unit 5: Nano Chemistry

Nanomaterials – An Introduction, Size Effects, Defining Nanodimensional Materials, Potential Uses for Nanodimensional Materials, The General Methods Available for the Synthesis of Nanodimensional Materials, Precipitative Methods, Reactive Methods in High Boiling Point Solvents, Hydrothermal and Solvothermal Methods, Gas-Phase Synthesis of Semiconductor Nanoparticles, Synthesis in a Structured Medium, The Suitability of Such Methods for Scaling, Conclusions and Perspectives on the Future, Oxide Nanoparticles, Nanotubes and Nanowires.

Study of different characterization tools (XRD, TEM, SEM, AFM, etc.) for Nanomaterials.