

PROFORMA

DETAILS OF ENTRANCE TEST – 2014-2015

Name of the Faculty: *Faculty of Natural Sciences*

Department/Centre: *Department of Chemistry*

Name of the Program: *M.Sc. (Chemistry)*

About Program's Prospects:

Summary of Entrance Test

S.No.	Test-Component (Strike off, if not applicable)	Test Duration (in minutes)	Max. Marks	Passing Marks	Negative Marking (Yes/No)
✓	Part-A (Objective/Multiple Choice Questions/ Practical)	<i>1 hr. 45 min.</i>	<i>100</i>	<i>15</i>	<i>Yes</i>
	Part-B/Subjective/Descriptive/Theory				
	Interview				
	Group Discussion				
	Portfolio				

Any other information about the Entrance Test:

Important Instructions for Test (Pl. add/modify as required)

Permissible Material/equipment for Entrance Test (as required):

- Black/Blue Ball Pen,
- ~~Calculator,~~
- Pencil

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Detailed Syllabus for the Entrance Test

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HEAD
DEPARTMENT OF CHEMISTRY
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Correct date of Completion of Admission Formalities is 2 July 2014 (Wednesday)

Syllabus for M.Sc. (Chemistry) Entrance Test

INORGANIC CHEMISTRY:

Atomic Structure

Idea of de Broglie matter waves, Heisenberg uncertainty principle, atomic orbitals, Schrodinger wave equation, significance of ψ and ψ^2 , quantum numbers, radial and angular wave functions and probability distribution curves, shapes of s, p, d orbitals, Aufbau and Pauli exclusion principles, Hund's multiplicity rule. Electronic configurations of the elements, effective nuclear charge.

Periodic Properties

Atomic and ionic radii, ionization energy, electron affinity and electronegativity – definition, methods of determination or evaluation, trends in periodic table and applications in predicting and explaining the chemical behaviour.

Chemical Bonding

- A. Covalent Bond – Valence bond theory and its limitations, directional characteristics of covalent bond, various types of hybridization and shapes of simple inorganic molecules and ions. Valence shell electron pair repulsion (VSEPR) theory to NH_3 , H_3O^+ , ClF_3 , SF_4 , ICl_2 and H_2O . MO theory, homonuclear and heteronuclear (CO and NO) diatomic molecules, multicenter bonding in electron deficient molecules, bond strength and bond energy, percentage ionic character from dipole moment and electronegativity difference.
- B. Ionic Solids – Ionic structures, radius ratio effect and coordination number, limitation of radius ratio rule, lattice defects, semiconductors, lattice energy and Born-Haber cycle, solvation energy and solubility of ionic solids, polarizing power and polarisability of ions, Fajan's rule. Metallic bond-free electron, valence bond and band theories.

Weak Interactions-Hydrogen bonding, van der Waals forces

Oxidation and Reduction

Oxidation-reduction reactions, oxidation state, rules for the determination of oxidation states, electrode potential, standard electrode potential and their determination, electrochemical series, applications of electrochemical series.

Acids and Bases

Arrhenius, Bronsted – Lowry, the Lux -Flood, solvent system and Lewis concepts of acid and bases.

S – Block Elements

Comparative study of these elements with special reference to their D-hydrides, oxides, hydroxides and halides. Diagonal relationship, solvation and complexation tendencies including their function in biosystems, and introductions to alkyls and aryls.

Groups III (13) Elements

Comparative study of physical and chemical properties of these elements with special reference to their oxides, hydrides, halides and nitrides. Preparation and properties of boric acids (ortho & metaboric acids) and borax, borax bead test. Study of hydrides formed by boron, structure and bonding in diborane, an idea of three center-two electron bond in the light of molecular orbital theory, borazine, borohydrides.

Group IV (14) Elements

Comparative study of physical and chemical properties of these elements with special reference to their oxides, hydrides, halides, nitrides, sulphides and carbides, fluorocarbons, study of silicates (structural aspect only) organosilicon compound and silicones.

Group V (15) Elements

Comparative study of the physical and chemical properties of these elements with special reference to their hydrides, oxides, halides, oxyhalides and sulphides, study of oxyacids of nitrogen and phosphorus.

Group VI (16) Elements

Comparative study of physical and chemical properties of these elements with special reference to their hydrides, oxides, halides and oxyhalides. Detailed study of oxyacids, peroxyacids and thio-oxyacids of sulphur (with special emphasis on their structure)

Group VII (17) Elements

Comparative study of physical and chemical properties of these elements with special reference to their electron affinity, electronegativity, bond dissociation energy, oxidation number, oxidizing power, reactivity of the elements, hydrides, oxides and oxyacids. Detailed study of oxyacids, peroxyacids, interhalogens, polyhalide ions (with special emphasis on their structures). Basic properties of halogens. Pseudohalogens.

Zero Group-Noble Gases

Position of zero group in the periodic table. History of discovery of noble gases. Detailed study of the compounds of xenon with fluorine (with special emphasis on their structures and bonding). Clathrates.

Chemistry of Elements of First Transition Series

Characteristic properties of d-block elements. Properties of the elements of the first transition series, their binary compounds and complexes illustrating relative stability of their oxidation states, coordination number and geometry.

Chemistry of Elements of Second and Third Transition Series

General characteristics, comparative treatment with their 3d analogues in respect of ionic radii, oxidation states, magnetic behaviour, spectral properties and stereochemistry.

Coordination compounds

Werner's coordination theory and its experimental verification, effective atomic number concept, chelates, nomenclature of coordination compounds, isomerism in coordination compounds.

Metal – Ligand Bonding in Transition Metal Complexes.

Valence bond theory of transition metal complexes, limitations of valence bond theory, an elementary idea of crystal field theory, crystal field splitting in octahedral, tetrahedral and square planar complexes. Structural, magnetic and thermodynamic properties from crystal field splitting. Jahn-Teller effect.

Silicones and Phosphazenes

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

Bio – inorganic Chemistry

Essential and trace elements in biological processes, metalloporphyrins with special reference to haemoglobin and myoglobin. Biological role of alkali and alkaline earth metal ions with special reference to Ca^{2+} .

Chemistry of Lanthanide Elements

Electronic structure, oxidation states and ionic radii and lanthanide contraction, magnetic properties, complex formation, occurrence and isolation, lanthanide compounds.

Chemistry of Actinides

Electronic structure, oxidation states and ionic radii, complex formation, chemistry of separation of Np, Pu and Am from U, similarities between later actinides and the later lanthanides.

Thermodynamic and Kinetic Aspects of Metal Complexes

A brief outline of thermodynamic stability of metal complexes and factors affecting the stability.

Hard and Soft Acids and Bases (HSAB)

Classification of acids and bases as hard and soft, Pearsons' HSAB concept, acid base strength and hardness and softness. Symbiosis, theoretical basis of hardness and softness, electronegativity hardness and softness.

Magnetic Properties of Transition Metal Complexes

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

Electron 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 to d^9 states, discussion of the electronic spectrum of $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ complex ion.

ORGANIC CHEMISTRY:

Structure and Bonding

Hybridisation (sp^3 , sp^2 , sp), bond length, bond angle and bond energy, sigma & pi bonds. Localised and delocalised bonds, vander Waals interactions, Inductive & field effects, Charge transfer complexes, Resonance, Hyper conjugation, Hydrogen bonding Aromaticity.

Mechanism of Organic Reactions

Curved arrow notation, drawing electron movements with arrows, half headed and double headed arrows, homolytic and heterolytic bond breaking. Types of reagents (electrophiles & nucleophiles). Types of org. reactions, Energy considerations. Reactive intermediates (carbocations, carbanions, free radicals, carbenes, arennes and nitrenes with examples). Methods of determination of reaction mechanism (Product analysis, Intermediates, isotopes effects, kinetic & stereochemical studies).

Stereochemistry of Organic Compounds

Concept of isomerism, Types of isomerism.

Optical isomers, elements of symmetry, molecular chirality, enantiomers, stereogenic center, optical activity, properties of enantiomers, chiral & achiral molecules with two stereogenic centers, diastereomers, threo & erythro diastereomers meso compounds, resolution of enantiomers, inversion, retention and racemization.

Relation absolute configuration, sequence rules, D & L, R & S Systems of nomenclature. Geometrical isomerism – determination of geometric isomers, E & Z systems of nomenclature, geometric in oximes & alicyclic compounds.

Conformational isomerism – conformational analysis of ethane and n-butane, conformation of cyclohexane, axial & equatorial bonds, conformation of monosubstitued cyclohexane derivatives. Newman projection & saw horse formulae, Fischer & flying wedge formula.

Difference between configuration & conformation.

Synthetic reagents

Compounds of active methylene group-synthesis of malonic ester and acetoacetic ester. Properties and application of malonic ester and acetoacetic ester.

Organomagnesium compound – Grignard reagent, preparation, properties and applications.

Alkenes, cycloalkenes, Dienes and Alkynes

- A. Nomenclature of alkenes, Methods of formation – Mechanism of dehydration of alcohols & dehydrogenation of alkyl halides, regioselectivity in alcohol dehydration. Saytzeff rule, Hofmann elimination, Physical properties & relative stabilities of alkenes. Chemical reactions of alkenes-mechanism involved in hydrogenation, electrophilic & free radical additions. Markownikoff's rule, hydroboration-oxidation, Oxymercuration-reduction, Epoxidation, Ozonolysis, hydration, hydroxylation & oxidation with KMnO_4 , Polymerisation of alkenes. Substitution at the allylic & vinylic position of alkenes. Industrial application of ethane & propene.
- B. Methods of formation, conformation & chemical reactions of cycloalkenes.
- C. Nomenclature and classification of dienes: Isolated, conjugated and cumulated dienes. Structure of allenes and butadiene, methods of formation, polymerization. Chemical reactions- 1,2 and 1,4 addition, Diels-Alder reaction.
- D. Nomenclature, structure and bonding in alkynes. Methods of formations, chemical reactions, acidity of alkynes. Mechanism of electrophilic and nucleophilic addition reactions, hydroboration oxidation, metal-ammonia reductions, oxidation and polymerization.

Arenes and Aromaticity Data

Nomenclature of zene derivatives, Aromatic nuclear and side chain reactions of benzene: Molecular formula and kekule structure. Stability and C-C bond lengths of benzene, resonance structure, MO picture

Aromaticity: The Huckles rule, aromatic ions.

Aromatic electrophilic substitution – general pattern of the mechanism, role of σ and π complexes.

Mechanism of nitration, halogenation, sulphonation, mercuration and Friedal craft reaction. Energy profile diagrams. Activating and deactivating substituents, orientation and ortho/para ratio. Side chain reaction of benzene derivatives. Birch reduction.

Alcohols

Classification and nomenclature

Dihydric alcohols- Nomenclature, methods of formation, chemical reactions of vicinal glycols, oxidative cleavage [$\text{Pb}(\text{OAc})_4 + \text{HIO}_4$] and pinacol-pinacolone rearrangement.

Trihydric alcohols- Nomenclature and methods of formation, chemical reactions of glycol.

Phenols.

Nomenclature, structure and bonding of phenols, physical properties and acidic character. Comparative acidic strengths of alcohols and phenols, resonance stabilization of phenoxide ion. Reactions of phenol- Electrophilic aromatic substitution, acylation and carboxylation, mechanism of Fries rearrangement, claisen rearrangement, Gatterman synthesis, Hauben-Hoesch reaction, Reimer Tiemann reaction.

Ethers and Epoxides

- A. Nomenclature of ethers and methods of their formation, physical properties. Chemical reactions- Cleavage and autoxidation, Ziesel's method.
- B. Synthesis of epoxides. Acid and base catalysed ring opening of epoxides, orientation of epoxide ring opening, reaction of Grignards and organolithium reagents with epoxides.

Aldehydes and Ketones

Nomenclature and structure of the carbonyl group. Synthesis of aldehydes from acid chlorides, synthesis of aldehydes and ketones using 1,3-dithiones.

synthesis of ketones from nitriles and from carboxylic acids. Physical properties, Mechanism of nucleophilic addition to carbonyl group with special emphasis on Benzoin, Aldol, Perkin and Knoevenagel condensations. Condensation with ammonia and its derivatives. Wittig reaction, Mannich reaction.

Use of acetals as protective group. Oxidation of aldehydes, Baeyer-Villiger oxidation of ketones, Cannizzaro reaction, Clemmensen, Wolff Kishner, LiAlH_4 and NaBH_4 reduction. Halogenation of enolizable ketones. An introduction of α,β unsaturated aldehydes and ketones.

Carboxylic acids.

Nomenclature, structure and bonding, physical properties, acidity of carboxylic acids, effects of substituents on acid strength. Preparation and reactions of carboxylic acids. Hell-Volhard-Zelinsky reaction. Synthesis of acid chlorides, esters and amides. Reduction of carboxylic acids. Mechanism of decarboxylation. Preparation and reactions of halocarboxylic acids, Malic, Tartaric and Citric acids.

Organic Compounds of Nitrogen.

Preparation of nitroalkanes and nitroarenes. Chemical reactions of nitro alkanes. Mechanism of nucleophilic substitution in nitro arenes and their reduction in acidic, neutral and alkaline media. Picric acid.

Structure and nomenclature of amines, stereochemistry of amines, separation of a mixture of primary, secondary and tertiary amines structural features effecting basicity of amines preparation of alkyl and arylamines by reduction of nitro compounds and nitriles, reductive amination of aldehydes and ketones compounds, Gabriel phthalimide reaction Hofmann bromamide reaction.

Reaction of amines, electrophilic aromatic substitution in aryl amines. Reactions of amines with nitrous acid, synthetic transformations of aryl diazonium salts, azocoupling.

Amino acids, Peptides, Proteins and Nucleic acids.

Classification, structure and stereochemistry of amino acids. Acid-base behaviour, isoelectric point and electrophoresis. Preparation and reaction 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. Structures of peptides and proteins. Levels of protein structure. Protein denaturation/ renaturation. Nucleic acids: introduction. Constituents of nucleic acids. Ribonucleoside and ribonucleotides. The double helix structure of DNA.

Fats, Oils and Detergents

Natural fats, edible and industrial oils of vegetable origin, common fatty acids, glycerides, hydrogenation of unsaturated oils, Saponification value, iodine value, acid value, soaps, synthetic detergents, alkyl and aryl sulphonates.

Synthetic Polymers

Addition or chain growth polymerization. Free radical polymerization, ionic vinyl polymerization, Ziegler Natta Polymerization and vinyl polymers.

Condensation or step growth polymerization. Polyesters, polyamides, phenol formaldehyde resins, urea formaldehyde resins, epoxy resins and polyurethanes. Natural and synthetic rubbers.

Synthetic Dyes

Colour and constitution (electronic concept). Classification of dyes. Chemistry and synthesis of methyl orange, Congo red, Malachite

green Crystal violet, Phenolphthalein, Fluorescein, Alizarin and Indigo.

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.

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 catalysis. Preparation of alkyl and aryl amines (reduction of nitro compounds, nitriles), 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 transformation of aryl diazonium salt, azo coupling.

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.

Electromagnetic Spectrum

Absorption spectra, Ultraviolet (UV) absorption spectroscopy – absorption laws (Beer Lambert Law) molar absorptivity, presentation and analysis of UV spectra, types of electronic transitions, effect of conjugation. Concept of chromophores and auxochrome. Bathochromic hypsochromic and hyperchromic shifts UV spectra of conjugated enes and enones.

Infrared (IR) absorption spectroscopy- Molecular vibrations, Hooke's law, selection rules, intensity and position of IR bands, measurement of IR spectrum, fingerprint region, characteristic absorptions of various functional groups and interpretation of IR spectra of simple organic compounds.

Spectroscopy

Nuclear magnetic Resonance (NMR) 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 PMR spectra of simple organic molecules such as ethyl bromide, ethanol, acetaldehyde, 1,2 tribromoethane, ethyl acetate, toluene and acetophenone, Problems pertaining to the structure elucidation of simple organic compounds using UV, IR and PMR spectroscopic techniques.

ORGANOSULPHUR COMPOUNDS

Nomenclature, structural features, methods of formation and chemical reactions of thiols, thioethers, sulphonic acids, sulphonamides and sulphaguanidine.

Heterocyclic Compounds

Introduction : Molecular orbital picture and aromatic characteristics of pyrrole, furan, thiophene and pyridine. Methods of synthesis and chemical reactions with particular emphasis on the mechanism of electrophilic substitution reactions in pyridine derivatives. Comparison of basicity of pyridine, Piperidine and pyrrole.

Organic Synthesis via enolates

Acidity of α hydrogens, alkylation of diethyl malonate and ethyl acetate. Synthesis of ethyl acetoacetate : the Claisen condensation. Keto-enol tautomerism of ethyl acetoacetate. Alkylation of 1,3 – dithianes. Alkylation and acylation of enamines.

Carbohydrates

Classification and nomenclature. Monosaccharides, mechanism of osazones 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, ethyl and esters. Determination of ring size of monosaccharides. Cyclic structure of D (+) glucose. Mechanism of mutarotation. Structures of ribose and deoxyribose. An introduction to disaccharides (maltose, sucrose and lactose) and polysaccharides (starch and cellulose) without involving structure determination.

PHYSICAL CHEMISTRY:

Mathematical Concepts and Computers

A. Mathematical Concepts

Logarithmic relations, curve sketching, linear graphs and calculation of slopes, differentiation of functions like K_x , e^{x^n} , $\sin x$, $\log x$, maxima and minima, partial differentiation and reciprocity relations. Integration of some useful/relevant functions; permutations and combinations. Factorials Probability.

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.

Gaseous States

Postulates of kinetic theory of gases, deviation from ideal behavior, 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. Liquifaction of gases (based on Joule – Thomson effect).

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 and cholestric phases. Thermography and seven segment cell.

Solid State

Definition of space lattice, 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 of crystals. Derivation of Bragg's equation. Determination of crystal structure of NaCl, KCl (Laua's method and powder method).

Colloidal State.

Definition of colloids, classification of colloids.

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.

Chemical Kinetics

Chemical kinetics and its scope, rate of a reaction, factors influencing the rate of a reaction – concentration, temperature, pressure, solvent, light, catalyst. Concentration and temperature 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 methods, method of integration, method of half life period and isolation method. Theories of reaction rates – collision theory and theory of absolute reaction rates, Lindemann theory of unimolecular reactions.

Radioactive decay as a first order phenomenon.

Thermodynamics – I

Definition of thermodynamic terms: system, surroundings etc. Types of systems, intensive and extensive properties. State and path functions and their differentials. Thermodynamic process. Concepts of heat and work.

First Law of Thermodynamics: Statement, definition of internal energy and enthalpy. Heat capacity, heat capacities at constant volume and pressure and their relationship. Joule's law, Joule-Thomson coefficient and inversion temperature. Calculation of w , q , dU & dH for the expansion of ideal gases under isothermal and adiabatic conditions for reversible process.

Thermochemistry: standard state, standard enthalpy of formation, Hess law of heat summation and its applications Heat of reaction at constant pressure and at constant volume. Enthalpy of neutralization. Bond dissociation energy and its calculation from thermo-chemical data, temperature dependence of enthalpy, kirchoff's equation.

Thermodynamics – II

Second law of thermodynamics, need for the law, different statement of the law. Carnot cycle and its efficiency, Carnot theorem, Thermodynamic scale of temperature.

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 change. Clausius inequality, entropy as a criteria of spontaneity and equilibrium. Entropy change in ideal gases and mixing of gases.

Third law of thermodynamics: Nernst heat theorem, statement and concept of residual entropy, evaluation of absolute entropy from heat capacity data. Gibbs and Helmholtz function: Gibbs function (G) and Helmholtz function (A) as thermodynamic quantities, A & G as criteria for thermodynamic

equilibrium and spontaneity, their advantage over entropy change. Variation of G and A with P , V and T .

Electrochemistry – I

Electrical transport-conduction in metals and in electrolyte solution, 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). Transport number, definition and determination by Hittorf method and moving boundary method.

Applications of conductivity measurements: determination of degree of dissociation, determination of K_a of acids, determination of solubility product of a sparingly soluble salt, conductometric titrations.

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) , polarization, over potential and hydrogen over voltage.

Concentration cell with and Without transport, liquid junction potential application of concentration cells, valency of ions, solubility product and activity coefficient, potentiometer titration's.

Definition of pH and pK_a , determination of pH using hydrogen, quinhydrone and glass electrodes by potentiometric method.

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

Corrosion – types, theories and methods of combating it.

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 hypothesis, the Heisenberg's uncertainty principle, Sinusoidal wave equation, Hamiltonian operator, Schrodinger wave equation and its importance physical interpretation of the wave function, postulates of quantum mechanics, particle in a one dimensional box.

Schrodinger wave equation for H-atom, separation into three equations (without derivation), quantum numbers and their importance, hydrogen like wave functions, radial wave functions, angular wave functions.

Molecular orbital theory, basic ideas – criteria for forming M.O. from A.O., construction of M.O's by LCAO- H_2^+ ion, calculation of energy levels from wave functions, physical picture of bonding and anti bonding wave functions, concept of σ , σ^* , π , π^* orbitals and their characteristics. Hybrid orbitals- sp , sp^2 , sp^3 , calculation of coefficients of A.O.'s used in these hybrid orbitals.

Spectroscopy

Introduction: electromagnetic radiation, regions of the spectrum basic features of different spectrometers, statement of the Born – Oppenheimer approximation, degrees of freedom.

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 anharmonic motion and isotope on the spectrum, idea of vibrational frequencies 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 III. 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, non-radiative processes (internal conversion, intersystem crossing) quantum yield, photosensitized reactions – energy transfer processes (simple examples)

Chemical Kinetics and Catalysis

Experimental methods of Chemical kinetics, conductometric, potentiometric, optical methods, polarimetry and spectrophotometer.

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, miscellaneous examples.

Physical Properties and Molecular Structure

Optical activity, polarization- (Clausius – Mossotti equation), orientation of dipoles in an electric field, dipole moment, induced dipole moment, measurement of dipole moment –temperature method and refractivity method, dipole moment and structure of molecules, magnetic properties paramagnetism, diamagnetism and ferromagnetism.

Solutions , Dilute Solutions and Colligative Properties

Ideal and non-ideal solutions, methods of expressing concentrations of solutions, activity and activity coefficient.

Dilute solution, colligative properties, Raoult's law, relative lowering of vapour pressure, molecular weight determination. Osmosis, Law of osmotic pressure and its measurement, determination of molecular weight from osmotic pressure. Elevation of boiling point and depression of freezing point, Thermodynamic derivation of

relation between molecular weight and elevation in boiling point and depression in freezing point, 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.

Phase Equilibrium – I

Statement and meaning of the terms- phase component and degree of freedom , derivation of Gibbs phase rule, phase equilibria of one component system – water , CO₂ and S systems.

Phase equilibria of two component system- solid liquid equilibria, simple eutectic Bi- Cd, Pb – Ag system, desilverisation of lead.

Solid solutions – compound formation with congruent melting point (Mg-Zn) and incongruent melting point, (NaCl-H₂O,) (FeCl₃-H₂O) and CuSO₄-H₂O) system, Freezing mixtures, acetone dry ice.

Liquid – liquid mixtures – ideal liquid mixtures , Raoult's and Henry's law. Non- ideal system azeotropes HCl-H₂O and ethanol - water systems.

Partially miscible liquids – Phenol - water, trimethylamine water,nicotine-water systems. Lower and upper consolute temperature. Effect of impurity on consolute temperature. Immiscible liquids, steam distillation.

Nernst distribution law-thermodynamic derivation, applications.

CHEMICAL EQUILIBRA

Formulation of equilibrium law, equilibrium law for ideal gases, interpretation of ΔG^0 , free energy change in a chemical reaction, chemical affinity and thermodynamic functions, equilibrium constants for ideal gases reactions, relation between K_p and K_c and K_x , change of K with the form of equation, thermodynamic validity of various statements, equilibrium constant and degree of dissociation, calculation of K from ΔG^0 , variation of equilibrium constant with temperature and pressure, effect of inert gas on reaction equilibrium, Le- Chatelier's principle (quantitative treatment in terms of ξ), free energy of mixing and spontaneity of reactions , equilibria between gases and solids, equilibrium constant for a system of real gases, equilibrium constant of reactions in solution, Clapeyron equation and Clausius – Clapeyron equation and applications.