

MASTER OF SCIENCE IN CHEMISTRY (MSc CHEMISTRY)

DURATION:2 YEARS

4th Year

Subject Code	Subject Title	IA Max. Marks	University Examinations		Total Marks	Min. Pass	Credits
			Max. Marks	Min. Pass			
MC401	LIFE SKILLS	20	80	35	100	35	4
MCH402	ORGANIC CHEMISTRY I	20	80	35	100	35	4
MCH403	INORGANIC CHEMISTRY I	20	80	35	100	35	4
MCH404	PHYSICAL CHEMISTRY I	20	80	35	100	35	4
MCH405	POLYMER CHEMISTRY	20	80	35	100	35	4
MCH406	SPECTROSCOPY-I	20	80	35	100	35	4
MCH407	ORGANIC CHEMISTRY PRACTICAL I	20	80	35	100	35	4
MCH408	INORGANIC CHEMISTRY PRACTICAL I	20	80	35	100	35	4
MCH409	PHYSICAL CHEMISTRY PRACTICAL I	20	80	35	100	35	4
Total Credits							36

5th Year

Subject Code	Subject Title	IA Max. Marks	University Examinations		Total Marks	Min. Pass	Credits
			Max. Marks	Min. Pass			
MC501	LIFE SKILLS	20	80	35	100	35	4
MCH502	ORGANIC CHEMISTRY II	20	80	35	100	35	4
MCH503	INORGANIC CHEMISTRY II	20	80	35	100	35	4
MCH504	PHYSICAL CHEMISTRY II	20	80	35	100	35	4
MCH505	PHOTOCHEMISTRY	20	80	35	100	35	4
MCH505	SPECTROSCOPY-II	20	80	35	100	35	4
MCH506	ENVIRONMENTAL CHEMISTRY	20	80	35	100	35	4
MCH507	ORGANIC CHEMISTRY PRACTICAL II	20	80	35	100	35	4

MCH508	INORGANIC CHEMISTRY PRACTICAL II	20	80	35	100	35	4
MCH509	PHYSICAL CHEMISTRY PRACTICAL II	20	80	35	100	35	4
Total Credits							40

1st YEAR

ORGANIC CHEMISTRY – I

UNIT – I Types of Reactions, Mechanisms and Reaction intermediates

Types of reactions : **Substitutions, Additions, Eliminations, Rearrangements, Oxidations and Reductions reactions – a general study.**

Reaction mechanisms: **Types of mechanisms : Heterolytic, Homolytic and Pericyclic mechanisms – a general study.**

Reaction intermediates: **Formation, stability and structure of carbonium ions, carbanions, carbenes, nitrenes and free radicals.**

Long lived and short lived free radicals, methods of generation and detection of free radicals, free radical reactions: Sandmeyer reaction, Gomberg-Bachmann reaction, Pschorr reaction and Ullmann reaction, mechanism of Hunsdiecker reaction.

UNIT – II Stereochemistry

Concept of chirality, recognition of symmetry elements and chiral structures, R – S nomenclature, Fischer, Newman and Sawhase projections of erythro and threo forms of organic molecules and their interconversion. Optical activity in the absence of chiral carbon – biphenyls, allenes and spiranes – R and S notations. Chirality due to helical shape, trans cyclooctene, cyclononene. E – Z isomerism of olefins containing one double bond . Stereochemistry and Conformational Analysis : Stereospecific and stereoselective synthesis with one suitable example, asymmetric synthesis – Cram's rule, Conformational analysis and stereochemical features of disubstituted cyclohexanes (1,2 ; 1,3 ; 1,4 dialkyl cyclo hexanes), conformation and stereochemistry of cis and trans decalins,

UNIT – III Aliphatic Nucleophilic Substitution Reactions

The S_N^2 , S_N^1 , mixed S_N^1 and S_N^2 , S_N^i and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon.

Reactivity effects of substrates structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity.

Substitution at carbon doubly bonded to oxygen and nitrogen, Williamson

reaction, Von-braun reaction, hydrolysis of esters, Claisen and Dieckmann condensation.

UNIT IV Heterocyclic Compounds

Synthesis and properties of imidazole, oxazole, thiazole and indole.

General methods of Synthesising Anthocyanidins, Synthesis and Structural elucidation of Cyanidin Chloride, Synthesis and Structural elucidation of flavones and isoflavones (Daidzein), Synthesis of pyrimidine and its derivativess, Synthesis of purine, uric acid and caffeine).

UNIT V Aromatic electrophilic, nucleophilic substitution reactions and Aromaticity

The arenium ion mechanism, typical reactions like nitration, sulphonation, halogenation, Friedal-Crafts alkylation, acylation and diazonium coupling, electrophilic substitution on monosubstituted benzene, orientation and reactivity-ortho, meta and para directing groups, Gatterman, Gatterman-koch, Vilsmeier, Reimer-Tiemann reaction.

Aromatic nucleophilic substitution reactions, the S_NAr mechanism, aromatic nucleophilic substitution of activated halides-Ziegler alkylation, Chichibabin reaction.

Aromaticity of benzenoid, heterocyclic and non-benzenoid compounds, Huckel rule, aromatic systems with pi electron compounds other than six pi electrons, non-aromatic (cyclooctatetraene, etc.,) and anti aromatic systems (cyclobutadiene, etc.,), systems with more than 10 pi electrons.

INORGANIC CHEMISTRY - I

UNIT I Structure and Bonding

van der Waals bonding, Hydrogen bonding and applications, Hard and Soft acids and bases-classification, Acid-Base strength, hardness, Symbiosis, Theoretical basis of Hardness and Softness, applications of HSAB.

Polyacids - Isopolyacids of V, Cr, Mo and W; Heteropolyacids of Mo and W (only structural aspects).

Inorganic polymers – Silicates – structure, Pauling's rule, properties, correlation and application; Molecular sieves.

Rings – Phosphazenes – Structure, Craig and Peddock model, Dewar model, polyorganophosphazenes, Polysulphur-nitrogen compounds.

UNIT – II Nuclear Chemistry

Nuclear properties - Nuclear spin and moments, origin of nuclear forces, features of the liquid drop and the shell models of the nucleus; Modes of radioactive decay - orbital electron capture, nuclear isomerism, internal conversion; Detection and determination of activity - Cloud chamber,

nuclear emulsion, Bubble chamber, GM, Scintillation and Cherenkov counters.

Nuclear reactions - Types, reaction cross section, Q-value, threshold energy, compound nuclear theory, high energy nuclear reactions, nuclear fission and fusion reactions as energy sources, direct reactions, photonuclear and thermo nuclear reactions, Stellar energy, synthesis of elements.

Applications relating to Nuclear Chemistry - Neutron activation analysis, Radio pharmacology, Radiation protection and safety precautions, Isotope dilution analysis.

Radiation Chemistry - Range of alpha and beta radiations, radiation dosimetry, radiolysis of water, the hydrated electron.

UNIT III Stability and bonding in complexes Stability of complexes - Factors affecting stability of complexes, thermodynamic aspects of complex formation, Stepwise and overall formation constants, stability correlations, statistical and chelate effects; Determination of stability constant - polarographic, photometric and potentiometric methods.

Stereochemical aspects - Stereoisomerism in inorganic complexes, isomerism arising out of ligand distribution and ligand conformation, chirality and nomenclature of chiral complexes; application of ORD and CD in the identification of chirality of complexes.

Macrocyclic ligands - types - porphyrins, corrins, Schiff's bases, crown ethers and cryptates. (simple complexes)

Metal-Ligand Bonding

Crystal field theory - Splitting of d- orbitals under various geometries, factors affecting splitting, CFSE, evidences for CFSE (Structural and thermodynamic effects), Spectrochemical series, Jorgensen relation, site preferences; Jahn-Teller distortion - Splitting pattern in trigonal pyramid, square pyramidal and cubic symmetries, Dynamic and Static J.T. effect, Jahn-Teller effect and Chelation; Limitations of CFT; Evidences for metal-ligand overlap; M.O. theory and energy level diagrams, concept of weak and strong fields, sigma and pi bonding in complexes, nephelauxetic eff

UNIT IV Electronic Spectra of Complexes

Spectroscopic Term symbols for d^n ions - derivation of term symbols and ground state term symbol, Hund's rule; Selection rules – break down of selection rules, spin- orbit coupling, band intensities, weak and strong field limits- correlation diagram; Energy level diagrams; Orgel and Tanabe-Sugano diagrams; effect of distortion and spin orbit coupling on spectra; Evaluation of Dq and B values for octahedral complexes of Nickel; Charge transfer spectra; , magnetic properties of complexes.

UNIT V Analytical Chemistry

Polarography - Theory, apparatus, DME, diffusion, kinetic catalytic currents, current voltage curves for reversible and irreversible systems; qualitative and quantitative applications to Inorganic systems.

Amperometric titrations - Theory, apparatus, types of titration curves, successive titrations and two indicator electrodes; applications; Complexometric titrations - Chelating agents; types of EDTA titration - direct and back titrations; replacement titrations - masking and demasking reagents.

Chromatography - Gas liquid chromatography – principle; retention volumes; instrumentation; carrier gas; columns preparations; stationary phase; detectors - thermal conductivity, flame ionization, electron capture; applications of GLC.

High performance liquid chromatography – scope; column efficiency; instrumentation; pumping systems; columns; column packing; detectors; applications.

PHYSICAL CHEMISTRY – I

UNIT- I Classical Thermodynamics –I

Maxwell's relations and thermodynamic equations of state – applications in the evaluation of $C_p - C_v$ for solids and for vanderwaals gases, $C_p - C_v$ in terms of coefficient of expansion and coefficient of compressibility – Relation between C_p and C_v – Partial molar properties- Gibbs – Duhem equation- Partial molar free energy (Chemical Potential) – Determination of chemical potential [Direct method and Method of Intercepts] and partial molar volume – variation of chemical potential with Temperature and Pressure – Thermodynamic derivation of phase rule – application to three component systems involving solids and liquids

($\text{CH}_3\text{COOH} - \text{CHCl}_3 - \text{H}_2\text{O}$, $\text{NaCl} - \text{Na}_2\text{SO}_4 - \text{H}_2\text{O}$ and $\text{NH}_4\text{NO}_3 - (\text{NH}_4)_2\text{SO}_4 - \text{H}_2\text{O}$).

UNIT –II Statistical Thermodynamics

Objectives of Statistical Thermodynamics – concept of thermodynamical and mathematical probabilities – Distribution of distinguishable and non- distinguishable particles.

Maxwell – Boltzmann, Bose – Einstein and Fermi – Dirac statistics – comparison and application.

Partition Functions – evaluation of Translational, Vibrational, Rotational and Electronic partition Function – Thermodynamic Functions in terms of partition Function – Application of Partition Function to monatomic and diatomic gases – Statistical expression for equilibrium Constant – Calculation of Equilibrium Constant from Partition Function – (isotope exchange equilibrium and dissociation of diatomic molecules) – Heat capacities of Monatomic crystals – Einstein and Debye theory of heat capacities.

UNIT –III Group Theory –I

Symmetry elements and symmetry operations – Point groups – identification and representation of groups – comparison of Molecular symmetry with Crystallographic symmetry – Reducible and irreducible representation – Direct product representation – Great orthogonality theorem and its consequences – Character Table and their uses.

UNIT –IV Group Theory – II

Symmetry selection rules for vibrational, Electronic and Raman Spectra – determination of representation of vibrational modes in non- linear molecules such as H₂O, CH₄, XeF₄, SF₆ and NH₃ – symmetry of Hybrid

orbitals in non-linear molecule (BF_3 , CH_4 , XeF_4 , PCl_5 , and SF_6 ,) –
Electronic spectra of formaldehyde – application of group theory.

UNIT –V Chemical Kinetics

Theories of Reaction rates – Arrhenius theory – effect of temperature on reaction rate – Hard – Sphere collision theory of reaction rates – molecular beams – collision cross section – effectiveness of collisions – Probability factor.

Transition state theory of reaction rates - Potential energy surface – Partition functions and activated complex – Eyring equation - Comparison of results with Eyring and Arrhenius equations – Estimation of free energy, enthalpy and entropy of activation and their significance.

POLYMER CHEMISTRY

UNIT I Basic Concepts

Monomers, repeat units, degree of Polymerization, Linear , branched and network Polymers. Condensation Polymerization :Mechanism of stepwise polymerisation .Kinetics and statistics of linear stepwise polymerization. Addition polymerization :Free radical , cationic and anionic polymerization. Polymerization conditions. Polymerization in homogeneous and heterogeneous systems.

UNIT II Co-ordination Polymerization

Kinetics, mono and bimetallic mechanism of co-ordination polymers..
Co-Polymerization : Block and graft co-polymers, Kinetics of copolymerization. Types of co-polymerization. Evaluation of monomer. Reactivity ratio. Rate of Co-Polymerization.

UNIT III Molecular Weight and Properties

Polydispersion – average molecular weight concept, number ,weight and viscosity average molecular weights. Measurement of molecular weights. Gel permeation chromatography, viscosity, light scattering, osmotic and ultracentrifugation methods. Polymer structure and physical properties – crystalline melting point T_m . The glass transition temperature. Determination of T_g . Relationship between T_m and T_g .

UNIT IV Polymer Processing

Plastics, elastomers and fibres. Compounding processing techniques : calendering, die casting , rotational casting, film casting , injection moulding, blow moulding extrusion moulding, thermoforming, foaming , reinforcing and fibre spinning.

UNIT V Properties of Commercial Polymers

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

SPECTROSCOPY – I

UNIT I Microwave Spectroscopy

Interaction of matter with radiation – Einstein's theory of transition probability – Rotation spectroscopy – Rigid Rotor – Intensity of spectral lines – Molecular parameters from Rotation spectra – Effect of isotopic substitution on the rotation spectra.

UNIT II IR and Raman Spectra

Theory, principle, instrumentation of IR and Raman Spectra.

Characteristic group frequencies of organic molecule, Factors influencing vibrational frequencies, interpretation of IR spectra of organic molecules.

Raman spectroscopy – Raman effect – Rotational and vibrational Raman Spectra. Applications of Raman Spectra.

UNIT III UV-VIS and Emission Spectra

Theory, principle, instrumentation of UV – VIS and Emission spectra.

UV-VIS : Woodward – Fieser rules for dienes, enones. Calculation of λ_{max} for organic molecules. Chromophores and effect of conjugation, substituents with unshared electrons and their capability of π - conjugation . Colour in compounds.

Applications of UV – VIS and Emission spectra.

UNIT IV ^1H and ^{13}C NMR Spectra

NMR spectroscopy : Theory, principle, instrumentation, Chemical shift, factors influencing chemical shift, spin-spin coupling, NMR of simple AX and AMX type organic molecules, calculation of coupling constants, identification of H in various chemical environments to assign structure to the organic molecules using chemical shift values, resonance coupled and decoupled spectra ^{13}C NMR, applications of ^{13}C NMR to find the different carbon functional groups.

UNIT V Mass spectra

Mass spectra – theory, principle, instrumentation and applications. McLafferty rearrangement, fragmentation pattern, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

ORGANIC CHEMISTRY PRACTICAL – I

I. Identification of components in a two component mixture and preparation of their derivatives. Determination of boiling point/melting point for components and melting point for their derivatives.

II. Preparation

1. Beta naphthyl methyl ether from beta naphthol
2. s-Benzyl isothiuronium chloride from benzylchloride
3. Beta glucose penta acetate from glucose
4. ortho- Benzoyl benzoic acid from phthalic anhydride
5. Resacetophenone from resorcinol
6. para- Nitrobenzoic acid from para nitrotoluene
7. meta-Nitroaniline from meta dinitrobenzene
8. Methyl orange from sulphanilic acid
9. Anthraquinone from anthracene
10. Benzhydrol from benophenone

CHEMISTRY PRACTICAL - I

Part – I

Semimicro qualitative analysis of mixtures containing two common and two rare cations. The following are the cations to be included: W, Tl, Mo, Te, Se, Ce, Th, Be, Zr, V, U and Li.

Part – II

- a) Colorimetric analysis: visual and photometric; determination of iron, nickel, manganese and copper.
- b) Preparation of the following:
 - i. Potassium trioxalatoaluminate (III) trihydrate
 - ii. Trithiourea copper (I) chloride
 - iii. Potassium trioxalatochromate (III) trihydrate
 - iv. Sodium bis (thiosulphato) cuprate (I)
 - v. Tetramminecopper (II) sulphate
 - vi. Potassium Tetrachlorocuprate (II)
- c) Separation of mixture of two metal ions by paper chromatography.
- d)

PHYSICAL CHEMISTRY PRACTICAL – I

Experiments in chemical kinetics, phase rule, Chemical equilibrium and

Conductivity measurements:

DETAILED LIST OF EXPERIMENTS

Typical list of possible experiments are given. Experiments of similar nature and other experiments may also be given. The list given is only a guideline. A minimum of 15 experiments have to be performed in a year.

1. Study the kinetics of acid hydrolysis of an ester, determination of the temperature coefficient of the reaction and determination of the activation energy of the hydrolysis of ethylacetate.

2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half life method and determine the order with respect to iodine and acetone.
3. Study of the saponification of ethylacetate by sodium hydroxide conductometrically and determine the order of the reaction.
4. Determination of association of ethylacetate by sodium hydroxide conductometrically and determine the order of the reaction.
5. Study the phase diagram for m-toluidine and glycerine system.
6. Construction of phase diagram for a simple binary system (naphthalene-phenanthrene and benzophenone-diphenylamine).
7. Construction of the phase diagram of the three component of partially immiscible liquid systems (DMSO-Water-Benzene; Water-Benzene-Acetic acid; Ethyl alcohol-Benzene-Water; Acetone-Chloroform-Water; Chloroform-Acetic acid-Water).
8. Determination of the equilibrium constant of the reaction between Iodine and KI by partition method.

9. Determination of equivalent conductance of a weak acid at different concentrations and verify Ostwald's dilution law and calculation of the dissociation constant of the acid.
10. Determination of equivalent conductivity of a strong electrolyte at different concentrations and examine the validity of the Onsager's theory as limiting law at high dilutions.
11. Conductometric titrations of a mixture of HCL and CH_3COOH against Sodium hydroxide
12. Compare the relative strength of acetic acid and monochloroacetic acid by conductivity method.

2nd YEAR

ORGANIC CHEMISTRY – II

UNIT I Molecular Rearrangements

A detailed study of the mechanism of the following rearrangements: Nucleophilic, Electrophilic and Freeradical rearrangements- memory effects, migratory aptitudes, Pinacol-Pinacolone, Wagner-Meerwin, Demyanov, Dienone-Phenol, Favorski, Baeyer-Villiger, Wolff, Stevens, Von-Richter, Claisen, Hofmann, Schmidt, Lossen, Curtius, Beckmann and Fries rearrangements (a few examples in each rearrangement are to be studied).

UNIT II Reagents in Organic Synthesis

Synthesis of simple organic molecules using standard reactions like acylation and alkylation of enamines and active methylene compounds. Sulphur ylides, Robinson annulation, protection and deprotection of functional groups (R-OH, R-CHO, RCOR, R-NH₂ and R-COOH) Reagents and their uses: DCC, trimethyl silyl iodide, trimethyl silyl chloride, 1,3-dithiane (umpolung), diisobutylaluminium hydride (DIBAL), 9BBN.

UNIT III Oxidation and Reduction Reactions

Study of the following oxidation reactions with mechanism: Oxidation of alcohols by CrO₃, DMSO alone, DMSO in combination with DCC; acetic anhydride and oxalyl chloride, oxidation of arylmethane, oxidation of methylene alpha to carbonyl, allylic oxidation of olefins, oxidative cleavage of glycols, oxidative cleavage of double bonds by ozonolysis.

Study of the following reduction reactions with mechanism: Reduction of carbonyl compounds by hydrides, selectivity in reduction of 4-ter-butyl cyclohexanone using selectrides, Clemmensen and Wolff Kishner reductions, Birch reduction, MPV reduction.

UNIT IV Elimination and Addition Reactions \

Elimination Reactions : E1, E2, E1cB mechanisms, Orientation of the double bond - Hofmann and Saytzeff rule, dehydration and dehydrohalogenation reactions, stereochemistry of E2 eliminations in cyclohexane ring systems, mechanism of pyrolytic eliminations, Chugaev reaction and Cope elimination.

Addition Reactions : Addition of halogen and nitrosyl chloride to olefins, hydration of olefins and acetylenes, hydroboration, Michael addition, 1,3 dipolar addition, Diels-Alder reaction. Mechanism and reactivity. Mannich, Stobbe, Darzen Glycidic ester condensation, Peterson olefination(Silyl Wittig reaction), Strecker synthesis, Perkin , Thorpe , Ritter , Prins reactions.

UNIT V BioOrganic Chemistry

Proteins, polypeptides and their synthesis (upto a tripeptide), solid phase synthesis (Merrifield synthesis), determination of primary structure of proteins (end group assay), discussion on secondary and tertiary structure of proteins.

Structure and role of (genetic code) DNA and RNA.(Determination of structure is not required) Biosynthesis of amino acids (phenylalanine, tyrosin, 3,4-dopa, praline only) and cholesterol.

INORGANIC CHEMISTRY-II

UNIT I Boron compounds and Clusters

Boron hydrides - polyhedral boranes, hydroborate ions-a general study of preparation, properties and structure, styx numbers , Wade's rules.

Carboranes - types such as closo and nido-preparation, properties and structure. Metallo carboranes - a general study.

Metal clusters - Chemistry of low molecularity metal clusters only-structure of Re_2Cl_8 ; multiple metal-metal bonds.

UNIT II Solid - State Chemistry

Structure of Solids; comparison of X-ray, neutron and electron diffractions; Structure of NiAs, CdI_2 , Pervoskite, spinels and inverse spinels; defects in solids - point defects, line defects and surface defects; Non-stoichiometric compounds; Use of X-ray powder data in identifying inorganic crystalline solids; details for cubic systems.

Electrical properties of solids - Band Theory, semiconductors, superconductors, solid state electrolytes; Magnetic properties - dia, para, ferro, antiferro and ferrimagnetism; hysteresis; ferrites; garnets; Optical properties – solid - state lasers and Inorganic phosphors.

Reactions in solid state and phase transitions - diffusion coefficient, diffusion mechanism, vacancy and interstitial diffusions, formation of spinels; solid solutions, order-disorder transformations and super structure.

UNIT III Reaction mechanisms in Complexes

Electron transfer reactions - Outer and inner sphere processes; atom transfer reaction, formation and rearrangement of precursor complexes, the bridging ligand, successor complexes; Cross reactions and Marcus-Hush theory; Application of electron transfer reactions in synthesis.

Reaction mechanism of coordination compounds - Substitution reactions, Labile and inert complexes; Kinetic application of V.B and C.F.Theories.

Substitution in square planar complexes - General mechanism; reactivity of Platinum complexes; influences of entering and leaving groups; the trans effect - theories, trans influence.

Substitution in octahedral complexes - general mechanism, discussion of A , D , I_A , I_D and DC_B mechanism; replacement of coordinated water; mechanism of acid hydrolysis and base hydrolysis - Conjugate base mechanism; direct and indirect evidences in favour of the mechanism; application of substitution reaction in the synthesis of Platinum and Cobalt complexes.

UNIT – IV Organometallic Chemistry & Catalysis

Carbon donors - Alkyls and Aryls-preparation and properties; Carbonyls - 18 electron rule, isolobal concept - application to structure of carbonyls (simple and polynuclear); Nitrosyls - bridging and terminal nitrosyls, bent and linear nitrosyls; dinitrogen complexes; Chain Carbon donors - Olefins, acetylene and allyl complexes - synthesis, structure and bonding; Cyclic Carbon donors - Metallocene - synthesis, structure and bonding (Ferrocene only).

Reactions - Association reaction - Only ligand protonation; substitution - electrophilic and nucleophilic attack on ligands; addition and elimination; carbonylation and decarbonylation; oxidative addition to organometallics; fluxional isomerism.

Hydrogenation of olefins (Wilkinson's catalyst); hydroformylation of olefins using Cobalt or Rhodium catalysts (oxo process); Oxidation of olefins to aldehydes and ketones (Wacker process); polymerization (Ziegler-Natta catalyst); Cyclo oligomerization of acetylene using Nickel catalyst (Reppe's catalyst); polymer bound catalysts.

UNIT –V Bioinorganic Chemistry

Metal ions in biological systems - essential and trace metals, Na^+/K^+ Pump; Biologically important complexes of Iron (transport proteins) -

haemoglobin, myoglobin, iron-sulphur proteins, cytochrome-C, Magnesium (chlorophyll), Cobalt (vitamin B₁₂), Zinc (carbonic anhydrase, carboxy peptidase); macrocyclic effect; fixation of Nitrogen.

PHYSICAL CHEMISTRY – II

UNIT – I Quantum Chemistry –I

Photoelectric effect – De Broglie equation – Heisenberg uncertainty principle – Compton effect – operators and commutation relations – quantum mechanical postulates – Schrodinger equation and its solution to the problem of a particle in one , three dimensionel boxes and harmonic oscillator. Schrodinger equation for the rigid rotator and Hydrogen atom – arriving solution for energy and wave function – the orgin of quantum numbers and their physical significance – Probability distribution of electrons.

UNIT –II Quantum Chemistry –II

Born – Oppenheimer approximation, Approximation methods – Perturbation and Variation methods – application to Hydrogen and Helium atom – Spin- orbit interaction- LS coupling and JJ coupling- Term symbols and spectroscopic states. Concept of Hybridisation – sp, sp² and sp³ hybridisation , Huckel Molecular orbital (HMO) theory for conjugated π - system , application to simple systems such as Ethylene, butadiene and benzene, Self consistant field approximation – Hartree's and Hartree- Fock Self Consistent field theory, Slater type orbitals – Slater rules.

UNIT-III Electrochemistry –I

Ions in solutions – Debye – Huckel theory of strong electrolytes – Debye-Hückel- onsager equation – verification and limitation – Debye – Hückel limiting law and its extension. Electrode – Electrolyte interface adsorption at electrified interface – electrical double layers – Electro capillary phenomena – Lippmann capillary equation – structure of double layers – Helmholtz Perrin, Guoy Chappman and Stern models of electrical double layers-electro kinetic Phenomena - Tiselius method of separation of proteins – membrane potential.

UNIT –IV Electrochemistry –II

Mechanism of electrode reactions –the Butler Volmer equation for one step electron transfer reaction – significance of equilibrium exchange current density and symmetry factor – transfer coefficient and its significance – Cyclic voltametry – Principles and applications. Mechanism of Hydrogen and Oxygen evolution reactions. Corrosion and Passivation of metals – construction of Pourbaix and Evans diagrams – Prevention of Corrosion. Electrochemical energy systems – Primary and Secondary batteries – (dry cells, lead acid – storage batteries, silver - zinc cell, nickel - cadmium battery, mercury cell) – Fuel cells.

UNIT –V Surface Chemistry and Catalysis

Kinetics of surface reactions : Physical and chemical adsorption – adsorption isotherms – types of adsorption isotherms – Langmuir adsorption isotherm – B.E.T. theory for multilayer adsorption – application of transition state theory to adsorption – measurement of

surface area – Mechanism of heterogeneous catalytic reactions – the adsorption coefficient and its significance.

Acid – Base catalysis – mechanism – Bronsted catalysis Law – catalysis by enzymes – rate of enzyme catalysed reactions – effect of substrate concentration, pH and temperature on enzyme catalysed reactions – inhibition of enzyme catalyzed reactions.

PHOTOCHEMISTRY

UNIT - I Organic Photochemistry

Photochemical reactions: fate of excited molecules, Jablonski diagram, Norrish Type I and Norrish Type II reactions, photoreduction of ketone, photoaddition reactions, Paterno Buchi reaction, di-pi methane rearrangement, photochemistry of arenes, Photooxidation (Formation of peroxy compounds), Photoisomerization (Cis-trans isomerization), Photo addition of olefins and amines to aromatic compounds, Photo rearrangements: Photo-Fries rearrangement and Photo rearrangement of 2,5-Cyclohexadienones.

UNIT –II Inorganic Photochemistry

Photosubstitution, Photoredox, photoisomerisation and photo rearrangement reactions in inorganic complexes. Photovoltaic and Photogalvanic cells – Photoelectrochemical cells – photoassisted electrolysis of water – aspects of solar energy conversion. Application of metal complexes in solar energy conversion

UNIT –III Physical Photochemistry

Absorption and emission of radiation – Franck – Condon principle – decay of electronically excited states , spin allowed and spin forbidden transition. – radiative and non –radiative processes - theory of radiationless transition – Internal conversion and intersystem crossing. Radiative processes - Fluorescence and Phosphorescence – Theory of Fluorescence and Phosphorescence. Factors affecting Fluorescence and Phosphorescence –Prompt and delayed Fluorescence- Fluorescence and structure. quenching of Fluorescence – static and dynamic quenching – Stern – volmer equation

UNIT IV Techniques and application of Photochemistry

Techniques and application of Photochemistry – Quantum yield – Experimental determination of quantum yield – Actinometry – chemical Actinometry - steady state treatment of quantum yield – Reasons for high and low quantum yield – life time measurements – radiative and non-radiative life time measurements – Kinetics of Photochemical reaction – Photosensitized reactions.

UNIT V Pericyclic Reactions

Pericyclic reactions, classification, orbital symmetry, Woodward Hofmann rules, selection rules and stereochemistry of electrocyclic reactions, cycloaddition and sigmatropic shifts, analysis by correlation diagram method and Frontier molecular orbital method, Sommelet, Hauser, Cope and Claisen rearrangements.

SPECTROSCOPY– II

UNIT I Atomic Absorption Spectroscopy

Atomic absorption spectroscopy – theory, principle, instrumentation. EMR sources – cells, furnaces, detectors; interferences and their corrections; applications of AAS.

UNIT –II ESR Spectroscopy

ESR Spectroscopy : Basic principles, Instrumentation, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants. Applications of ESR spectroscopy. Electronic Zeeman effect – hyperfine interactions – Spin densities – McConnell relationship – selection rules in ESR – bonding parameters from 'g' and coupling constants.

UNIT –III Mossbauer Spectroscopy

Mossbauer Spectroscopy - Doppler effect; isomer effect; electron-neutron hyperfine interactions; Quadrupole interactions and magnetic interactions; simple applications to Iron and Tin compounds.

UNIT –IV Photoelectron Spectroscopy

Photoelectron Spectroscopy - Principle, PES of diatomic molecules and polyatomic molecules (HCl, HBr, HI, CO, NH₃, H₂O and N₃⁻ ion); Core electron PES; X-ray photoelectron spectroscopy (ESCA) applications.

UNIT –V ORD-CD

ORD-CD : Definition, circular birefringence and circular dichroism, plain dispersion curves and their applications, single and multiple cotton effect

curves, structural and stereochemical applications – axial haloketone rule, octant rule for ketones, Comparison of ORD and CD.

UNIT I Atomic Absorption Spectroscopy

Atomic absorption spectroscopy – theory, principle, instrumentation. EMR sources – cells, furnaces, detectors; interferences and their corrections; applications of AAS.

UNIT –II ESR Spectroscopy

ESR Spectroscopy : Basic principles, Instrumentation, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants. Applications of ESR spectroscopy. Electronic Zeeman effect – hyperfine interactions – Spin densities – McConnell relationship – selection rules in ESR – bonding parameters from 'g' and coupling constants.

UNIT –III Mossbauer Spectroscopy

Mossbauer Spectroscopy - Doppler effect; isomer effect; electron-neutron hyperfine interactions; Quadrupole interactions and magnetic interactions; simple applications to Iron and Tin compounds.

UNIT –IV Photoelectron Spectroscopy

Photoelectron Spectroscopy - Principle, PES of diatomic molecules and polyatomic molecules (HCl, HBr, HI, CO, NH₃, H₂O and N₃⁻ ion); Core electron PES; X-ray photoelectron spectroscopy (ESCA) applications.

UNIT –V ORD-CD

ORD-CD : Definition, circular birefringence and circular dichroism, plain dispersion curves and their applications, single and multiple cotton effect curves, structural and stereochemical applications – axial haloketone rule, octant rule for ketones, Comparison of ORD and CD.

ENVIRONMENTAL CHEMISTRY

UNIT - I COMPOSITION

Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, biogeochemical cycles of C, N, P, S and O. Biodistribution of elements. Soil composition, micro and macro nutrients, pollution – fertilizers, , pesticides, plastics and metals. Waste treatment.

UNIT - II HYDROSPHERE

Aquatic pollution – inorganic, organic, pesticides, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro organisms, water quality standards.

UNIT - III ATMOSPHERE

Chemical composition of atmosphere – particles, ions and radicals and their formation, chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Air pollution control and their chemistry.

UNIT - IV INDUSTRIAL POLLUTION

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers and drugs. Radionuclide analysis, Disposal of wastes and their management.

UNIT - V ENVIRONMENTAL TOXICOLOGY

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three miles island, Sewozo and Minamata disasters.

ORGANIC CHEMISTRY PRACTICAL – II

I. Organic Estimation

1. Phenol
2. Aniline
3. Methyl Ketone
4. Glucose
5. Iodine value of an oil
6. Saponification value of an oil.

II Organic Preparation, Involving Two Stages

1. Sym-tribromobenzene from aniline.
2. m-Nitrobenzoic acid from methyl benzoate
3. para -Nitroaniline from acetanilide.
4. Benzanilide from benzophenone.
5. para –Amino benzene sulphanamide from acetanilide
6. Anthraquinone from phthalic anhydride.

III. Extraction of Natural Products:

1. Caffeine from tea leaves.
2. Citric acid from lemon.

IV Chromatographic Separations

1. Column chromatography : separation of a mixture of ortho and para-Nitroanilines.
2. Thin layer Chromatography : separation of a mixture of ortho and para – Nitroanilines.
3. Paper chromatography – identification of natural alpha amino acids.

INORGANIC CHEMISTRY PRACTICAL II

Part I Quantitative analysis of complex materials

A) Quantitative analysis :

Quantitative analysis of mixture of iron and magnesium; iron and nickel, copper and nickel and copper and zinc.

B) Analysis of Ores

1. Determination of percentage of calcium and magnesium in dolomite.
2. Determination of percentage of MnO_2 in pyrolusite
3. Determination of percentage of lead in galena.

C) Analysis of Alloys

1. Determination of tin and lead in solder.
2. Determination of copper and zinc in brass.
3. Determination of Chromium and nickel in stainless steel.

Part II : Preparations of the following :

1. Sodium hexanitrocobaltate (III)
2. Tris (ethyleneamine) Cobalt (III) chloride
3. Chloropentammine Cobalt (III) chloride
4. Bis (acetylacetonato) Copper (II)
5. Hexamminecobalt (III) chloride
6. Hexamminenickel (II) chloride.

PHYSICAL CHEMISTRY PRACTICAL – II

Experiments in electro chemistry, Polarography and Chemical Kinetics.

EMF Measurements

Determination of standard potentials (Cu and Ag)

Determination in thermodynamic quantities from EMF measurements,

Potentiometric titrations

Determination of p_H and calculation of p^K_a .

Determination of stability constant of complex.

Determination of solubility product of a sparingly soluble salt,
Redox titrations.

Precipitation titration of mixture of halides by emf measurements.

DETAILED LIST OF EXPERIMENTS

Typical list of possible experiments are given. Experiments of similar nature

and other experiments may also be given. The list given is only a guideline.

A minimum of 15 experiments have to be performed.

1. Determination of the activity coefficient of an electrolyte at different molalities by emf measurements.
2. Determination of the dissociation constant of acetic acid by titrating it with sodium hydroxide using quinhydrone as an indicator electrode and calomel as a reference electrode.
3. Determination of the strength of a given solution of KCl using differential potentiometric titration technique.
4. Determination of the P^H of the given solutions with the help of the indicators using buffer solutions and by colorimetric method.

5. Determination of the P^H of a given solution by emf method using hydrogen electrode and quinhydrone electrode.
6. Determination of the composition and instability constant of a complex by mole ratio method.
7. Calculation of the thermodynamic parameters for the reaction

$$\text{Zn} + \text{H}_2\text{SO}_4 \longrightarrow \text{ZnSO}_4 + \text{H}_2$$
 by emf method.
8. Determination of the formation constant of silver ammonia complex and stoichiometry of the complex potentiometrically.
9. Solubility and Solubility products by emf method.
10. Determination of the activity coefficient of Zinc ions in the solution of 0.002 M Zinc sulphate using Debye – Huckel Limiting law.
11. Determination of solubility product of Silver bromide and calculate its solubility in water and 0.01 M and 0.01 M KBrO_3 using Debye – Huckel limiting law.
12. Determinations of the electrode potentials of Zn and Ag electrodes in 0.1 M and 0.001 M solutions at 298 K and find the standard potentials for these electrodes and test the validity of Nernst equations.
13. Study the inversion of cane sugar in presence of acid using polarimeter.
14. Determination of the rate constant and order of reaction between potassium persulphate and potassium iodide and determine the temperature coefficient and energy of activation of the reaction.

15. Study the primary salt effect on the kinetics of ionic reactions and test the Bronsted relationship (iodine ion is oxidized by persulphate ion).
16. Determination of the viscosities of mixtures of different compositions of liquids and find the composition of a given mixture.
17. Determination of the partial molar volume of the glycine/methanol/formic acid/sulphuric acid by graphical method and by determining the densities of the solutions of different comparisons.
18. Study the surface tension – concentration relationship for solutions (Gibb's equation)