COURSES OF STUDIES FOR M.Sc.

IN

CHEMISTRY

SESSION: - 2021-2024

UNDER
CHOICE BASED CREDIT SYSTEM

D.A.V. AUTONOMOUS COLLEGE, TITILAGARH

Syllabus of M. Sc. in Chemistry

FIRST SEMESTER

Course No	Course Title	Credit	Mark
PAPER-I	GROUP THEORY AND SOLID STATE CHEMISTRY AND TRANSITION METAL CHEMISTRY	06	100
PAPER-II	STRUCTURE AND REACTIVITY AND STEREOCHEMISTRY	06	100
PAPER-III	THERMODYNAMICS AND DYNAMICS	06	100
PAPER-IV	INORGANIC PRACTICAL-I & ORGANIC PRACTICAL-I	06	100
	Total	**24**	**400/16**

SECOND SEMESTER

Course No	Course Title	Credit	Mark
PAPER-V	METAL $\bar{\pi}$-COMPLEXES AND CLUSTERS AND BIOINORGANIC CHEMISTRY	06	100
PAPER-VI	ORGANIC REACTION MECHANISM - I AND ORGANIC REACTION MECHANISM - II	06	100
PAPER-VII	STATISTICAL THERMODYNAMICS & HMO THEORY AND SURFACE CHEMISTRY	06	100
PAPER-VIII	INORGANIC PRACTICAL-II AND ORGANIC PRACTICAL-II	06	100
	Total	**24**	**400/16**

THIRD SEMESTER

Course No	Course Title	Credit	Mark
PAPER-IX	INSTRUMENTAL METHODS OF ANALYSIS AND INORGANIC REACTION DYNAMICS & NUCLEAR CHEMISTRY	06	100
PAPER-X	ORGANIC REDOX REACTION & SPECTROSCOPY AND PERICYCLIC REACTION, PHOTOCHEMISTRY & RETROSYNTHESIS	06	100
PAPER-XI	QUANTUM CHEMISTRY AND ATOMIC & MOLECULAR SPECTROSCOPY	06	100
PAPER-XII	PHYSICAL PRACTICAL	06	100
PAPER-XIII	PROJECT	06	100
	Total	**30**	**500/20**

FOURTH SEMESTER

Course No	Course Title	Credit	Mark
PAPER-XIV	ADVANCED ORGANOMETALLIC CHEMISTRY	06	100
PAPER-XV	ADVANCED SPECTROSCOPY	06	100
PAPER-XVI	CHEMISTRY OF NANOMATERIALS	06	100
PAPER-XVII	INDUSTRIAL PROCESSES	06	100
PAPER-XVIII	PRACTICAL ANALYTICAL CHEMISTRY	06	100
	Total	**30**	**500/20**

SEM-I Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-I :

GROUP THEORY & SOLID STATE CHEMISTRY 6 credits

UNIT-I: Symmetry and Group Theory

Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, platonic solids, group multiplication table, group generators, conjugacy relation and classes, matrix representation of symmetry elements, character of a representation, reducible and irreducible representation, the great orthogonality theorem (without proof) and its explanation, properties of irreducible representation.

UNIT-II: Symmetry and Spectroscopy

Character table (explanation and significance), construction of character tables for C_{2v}, C_{3v}, C_{4v} and D_4 point groups, direct product, the standard reduction formula, Applications of group theoretical methods for selection rules in Infrared, Raman and electronic spectroscopy.

UNIT-III: Solid State Chemistry

General idea of crystal lattice, unit cell, classification of crystals, crystal planes, Miller indices, Bragg's law and applications, determination of cubic crystal structure from systematic absences in diffraction pattern, perfect and imperfect crystals, point defects, Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defects, bonding in ionic solids, colour centers, non-stoichiometry defects, general idea of band theory of solids.

TRANSTION METAL CHEMISTRY

UNIT-I Theories of Metal-Ligand Bonding

a. Crystal field theory (CFT): Splitting of d-orbital under the influence of octahedral, tetrahedral, tetragonal, square planar, trigonal bipyramidal and square pyramidal fields, Streochemical and thermodynamic effect of CF splitting, CFSE and Jahn- Teller effect.
b. Molecular orbital theory (MOT): Sigma bonding in octahedral complexes:
   Classification of metal valence orbitals into sigma symmetry, formation of ligand group orbitals (LGOs) of sigma symmetry, Formation of molecular orbitals of sigma symmetry, construction of molecular orbital energy level diagram involving only sigma bond contribution from ligands, pi bonding in octahedral complexes, Classification of metal valence orbital into pi symmetry, Formation of LGOs of pi symmetry. Formation of pi MOs and construction of molecular orbital energy level diagram involving sigma and pi contribution from pi donor ligands, Sigma and pi bonding in tetrahedral complexes.
c. Ligand field theory (LFT) and adjusted crystal field theory (ACFT).

UNIT-II Complex Equilibria and Term Diagram

a. Complex Equilibria: Types of complex equilibria in solution and types of complex equilibrium constant (stability constant), The complex formation functions, Determination of stability constant by spectrophotometric method and pH titration method, Stabilization of unusual oxidation state.
b. Term Diagram: Russell-Saunders or L-S coupling scheme, Term symbols and their derivation by Pigeon-Hole diagram especially for p_n and d_n configuration, Interelectron repulsion parameters and spin-orbit coupling parameters, The effect of weak crystal field on S, P, D, F, G, H and I terms, Orgel diagram for d_1 to d_9 configuration, Term interaction and the energies of the levels.
c. Correlation diagram: Strong field configuration of O_h symmetry, the method of descending symmetry, correlation diagram for d_2 and $d_3$confuguration, Tanabe- Sugano diagram (qualitative explanation and significance).

Unit-III Electronic Spectral and Magnetic Properties of Metal Complexes

a. Electronic spectral properties of metal complexes: Introduction, types of experimental recording of the spectra, selection rules (mechanism of electronic transition, orbital selection rule, Laporte rule or purity selection rules, spin selection rule), Relaxation of selection rules (departure from cubic symmetry d-p mixing vibronic coupling), Nature of electronic spectral bands with respect to band intensity and bandwidth, Classification of electronic spectra. Ligand field spectra of octahedral and tetrahedral complexes and evaluation of Dq, B' and beta(β) parameters for the complex with T_1 ground state and A_2 ground state, Spectrochemical and nephlelauxetic series, charge transfer spectra.
b. Magnetic properties of metal complexes: Origin of magnetic behavior, concept of magnetic susceptibility, dia, para, ferro and antiferro magnetism, magnetic moments from multiple width cases, quenching of orbital magnetic moment by crystal field, spin-orbit coupling and anomalies magnetic moments, Spin-crossover in coordination compounds.

Group A consists of 10questions covering all units out of which 8 questions shall be answer each carrying 5 marks

Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

SEM-I Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-II :

STRUCTURE AND REACTIVITY 6credits

UNIT-I: Nature of Bonding in Organic Molecules

Delocalized chemical bonding, Conjugation, Cross conjugation, Resonance, Hyperconjugation, Bonding in fullerenes, Tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, energy levels of pi-molecular orbitals of simple systems, Annulenes, Anti-aromaticity, Homo-aromaticity, Bonds weaker than covalent-addition compounds.

UNIT-II: Reaction Mechanism: Structure and Reactivity

Types of mechanisms, Types of reactions, Thermodynamic and kinetic requirements, Kinetic and thermodynamic control, Hammond's postulate, Potential energy diagrams, Transition states and intermediates, Methods of determining mechanisms, Hard and soft acids and bases, Effect of structure on reactivity: Resonance and field effects, Steric effect, Quantitative treatment, The Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation.

UNIT-III: Reagents in Organic Synthesis

Gilman's reagent, Lithium dimethyl cuprate, Lithium diisopropyl amide, DCC, 1,3- Dithiane, Trimethyl sillyl iodide, Tri-n-butyl tin hydride, Osmium tetroxide, Selenium dioxide, Phase transfer catalysis (Crown ether, Merrifield resin, Wilkinson's catalyst), Dichloro dicyano benzoquinone (DDQ).

STEREOCHEMISTRY

UNIT-I: Chirality, Fischer projection and R and S notations, Threo and erythro nomenclature, E and Z nomenclature, Optical isomerism in biphenyls and allenes, Concept of Prostereoisomerism and Assymetric synthesis (including enzymatic and catalyticnexus), Conformation of a few acyclic molecules (alkanes, haloalkanes), Conformation of cyclic systems having one and two sp2 carbon atoms.

UNIT-II: Dynamic stereochemistry: Conformation and reactivity, Selection of substrates, Quantitative correlation between conformation and reactivity, (Weinstein-Eliel equations and Curtin-Hammett principles), Conformational effects on stability and reactivity in acyclic compounds (ionic elimination, intramolecular rearrangements, NGP) and in cyclic systems, (Nucleophilic substitution reaction at ring carbon, Formation and Cleavage of epoxide rings, Addition reactions to double bonds, Elimination reactions).

UNIT-III: Molecular dissymmetry and chiroptical properties, Linearly and circularly polarized lights, Circular birefringence and circular dicroism, ORD, Plane curves, Cotton effect, Rotatory Dispersion of ketones, Axial haloketone rule, the Octane rule. Helicity rule.

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Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

PAPER-III: THERMODYNAMICS 6 credits

UNIT-I: Classical Thermodynamics

Brief resume of the concepts of laws of thermodynamics, Free energy, chemical potential and entropy, Third law of thermodynamics and determination of entropy, Entropy and probability, Boltzmann-Planck equation, Partial molar properties (partial free energy, molar volume and molar heat content), Their significance and determination. Concept of fugacity and its determination.

UNIT-II Thermodynamics of Living Systems

Bioenergetics and thermodynamics, Phosphate group transfer and ATP, Biological oxidation-reduction reactions.

UNIT-III Non-Equilibrium Thermodynamics

Microscopic reversibility, Entropy productions and irreversible process, Different types of forces and fluxes, Steady states & Cross phenomena, Phenomenological equations, Onsager reciprocity theorem, Chemical Reactions.

DYNAMICS

UNIT-I: Chemical Kinetics

Theories of reaction rates, Collision theory, Transition state theory, Arrehenius equation and the activated complex theory, Reaction between ions, Salt effect, Steady-State Kinetics, Kinetic and Thermodynamic concept of Reactions, Treatment of unimolecular reaction (Lindemann-Hinshelwood and Rice-Ramspeger-Kassel-Marcus (RRKM) theories), Dynamic chain (H_2 + Br_2 reaction, pyrolysis of CH_3CHO, Decomposition of ethane).

UNIT-II: Catalytic & Fast Reaction

Kinetics of Catalytic Reactions: Acid-base Catalysis, Enzyme Catalysis, Homogeneous & Heterogeneous Catalysis. Fast reactions: General feature, Study of Fast reactions by relaxation, Stopped flow and Flash photolysis.

UNIT-III: Electrochemistry

Interionic attraction theory and Debye-Huckel treatment, Derivation of Onsager limiting law and its verification and modification, Activities, activity coefficients, Debye-Huckel treatment, Debye-Huckel-Bronsted equation, Salt effect, Determination of activity coefficients from solubility method, Ion association, Determination of thermodynamic dissociation constant of weak electrolytes by Shedlovsky method and by EMF method, Nernst equation, redox systems, electrochemical cells.

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PAPER-IV:

INORGANIC PRACTICAL-I 3 credits

Analysis of an inorganic mixture containing not more than 6 radicals. The mixture will include rare earth like Tungstate, Vanadate, Molybdate and Cerium (IV). Insoluble matters and other interfering radicals will also be included. Organic radicals are excluded.

ORGANIC PRACTICAL-I 3 credits

Isolation and identification of multi-functional compounds in a mixture of two organic compounds.

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SEM-II Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-V:

METAL π-COMPLEXES AND CLUSTERS 6 credits

UNIT-I Carbon Monooxide Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reaction of metal carbonyls, carbonylate anions and carbonylate hydride, carbonyl halides and related compounds. Nature of M-C bond in carbonyls.

UNIT-II Complex of Carbon Monoxide Analogs

(a) Preparation, bonding and important reaction of transition metal complexes with isocyanide, cyanide, dinitrogen, carbon disulphide and nitrogen monoxides.

(b) Transition metal to carbon multiple bonded: compounds chemistry of carbenes, carbynes.

UNIT-III Metal Cluster and Polyacids

Metal cluster: Occurrence of metal-metal bonds in metal complexes, Bonding in metal cluster. Metal carbonyl type clusters. Anionic and hydride cluster. Method of synthesis, super large cluster, electron counting in medium size cluster (Wade's rule, Capping rule), Isolable relationship, cluster of Fe, Ru, Os groups. Cluster of Co, Rh, Ir groups. Cluster of Ni, Pd, Pt groups. Catalysis by cluster. Isopoly and heteroply acids and salts.

BIOINORGANIC CHEMISTRY

UNIT-I Biomolecules and their Roles in Metal Ions Storage and Transportation

Amino acids, peptides and proteins, structures of proteins, Ramachandran's plot, lipids, lipid bilayer, biological membranes, chemistry of biologically relevant molecules like ADP, ATP, FAD, NADP, nucleotides. Biologically important metal ions (Na, K, Mg, Ca, Cu, Fe, Zn, Co and Mo) and their functions, mechanism of transport of metal ions through biological fluids and membranes, different types of passive and active transport processes and their mechanism, Na^+/K^+ pump, calcium pump, and ionophores. Storage and transport of iron, copper and zinc, siderophores, structure and function of ferritin, transferrin in regard to Fe-storage and transportation,

UNIT-II Role of Proteins as Oxygen and Electron Carriers

Chemistry of porphyrin, Iron porphyrins (Heme proteins): Hemoglobin (Hb), Myoglobin (Mb) and their behavior as oxygen carrier, O_2 affinity, cooperativity and Bohr's effect, Heme protein as electron carrier with particular reference to cytochrome-c and cytochrome-450, and cytochrome oxidase. Catalases and peroxidases. Non-heme oxygen uptake protein (hemerythrin and hemocyanin). Magnesium porphyrins
(Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle). Non-heme iron-sulphur protein as electron carrier, rubredoxins and ferredoxins.

UNIT-III Biomolecular Catalysis

Preliminary idea about enzyme, cofactor, co-enzyme, apoenzyme, prosthetic group, metal-activated enzyme and metalloenzyme. Enzyme-substrate binding problem, carboxypeptidase, carbonic anhydrase and their biological significance, Interchangeability of zinc and cobalt enzyme. Blue-oxidases (ascorbate oxidase,
cerulloplasmin, laccase) and non-blue Oxidases (amine oxidase, galactose oxidase, lysyl oxidase, cytochrome c oxidase), structure and biological functions of molybdenum nitrogenase, superoxide dismutase.

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SEM-II Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-VI: ORGANIC REACTION MECHANISM – I 6 credits

UNIT-I The S_N2, S_N1, mixed S_N1 and S_N2 and SET mechanisms. The neighbouring group mechanism, Neighboring group participations by sigma and pi bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carbocations. The S_NI mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile, regioselectivity.

UNIT-II Alipahatic Electrophilic Substitution mechanism: S_E1, S_E2 and $S_{E\,I}$ mechanisms, Effect of substrate, leaving group and solvent, Reactions (hydrogen exchange, migration of double bonds, keto-enol tautomerism, halogenation, aliphatic diazonium coupling, Stork-enamine reaction). Aromatic electrophilic substitution mechanism: Structure reactivity relationship in mono-substituted benzene, ring isomer proportions, orientation in benzene ring with one or more than one substituent, Orientation in other ring systems, Vilsmeir – Haack reaction, Pechmann reaction.

UNIT-III Aromatic Nucleophilic Substitution mechanism: Introduction to different mechanisms, Aromatic nucleophilic substitutions (S_NAr, S_N1 aryne), Effect of substrates, leaving groups, and nucleophile, Reactions: Nucleophilic displacement in areno-diazonium salts by different nucleophiles, Chichibabin reaction. Free radical Substitution: Intermediates, Reaction at sp^2 carbon, Reactivity in aliphatic substrates, Reactivity at bridge head position, Reactivity in aromatic substrates.

ORGANIC REACTION MECHANISM – II

UNIT-I Addition to carbon-carbon multiple bonds, Electrophilic, Nucleophilic and Free radical addition, Orientation and Reactivity, Addition to cyclopropanes, Reactions: Hydroboration, Michael reaction, Sharpless Asymmetric epoxidation. Addition to carbon-heteroatom multiple bonds: Mechanism and reactivity, Reactions: Mannich reaction, $LiAlH_4$ reduction of carbonyl compounds, acids, esters, nitriles, addition of Grignard reagents - Reformatsky reaction, Aldol condensation, Knoevenagel condensation, Perkin reaction, Tollens reaction, Wittig reaction, Prins reaction, Benzoin condensation.

UNIT-II Elimination mechanism: E_1, E_2, E_1CB and E_2CB mechanisms, Orientation, Effect of substrate, base, leaving group and medium, Orientation of double bond, Sayetzeff and Hoffman rules, Pyrolytic elimination reaction, Oxidative elimination (oxidaton of alcohol by chromium, Moffatt oxidation). Reactions: Cleavage of quaternary ammonium hydroxides, Chugaev reaction, Shapiro reaction.

UNIT-III General mechanistic considerations – nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements, Wagner-Meerwein, Favorskii, Carbene intermediate, Arndt-Eistert synthesis, Neber, Nitrene intermediates (Beckmann, Hofmann, Schmidt, Lossen, Curtius), Baeyer-Villiger, Shapiro reaction, Von-Richter, Sommelet-Hauser rearrangement.

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SEM-II Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-VII : STATISTICAL THERMODYNAMICS & HMO THEORY 6 credits

UNIT-I Classical and Quantum Statistical Mechanics

Concept of probability, Starling approximations, Most probable distribution, System, Phase Space, Space, Space, Liouville's Theorem, Statistical Equilibrium, Brief Concepts on Ensembles, Canonical, Grand Canonical and Micro-canonical ensembles. Bose-Einstien statistics, Fermi-Dirac statistics and Maxwell-Boltzmann statistics

UNIT-II Partition Functions & Statistical Thermodynamic Properties of Solids

Significance of partition function, Calculation of thermodynamic properties and equilibrium constant in terms of partition functions, Evaluation of transnational, vibrational and rotational partition function for monoatomic and polyatomic ideal gases, electronic partition function. Some thermal characteristics of crystalline solids, Classical treatment of solids, Einstein Model, Debye Modification, Limitation and modification of Debye theory.

UNIT-III Huckels Molecular Orbital Theory

Huckel theory of conjugated systems (Ethylene, Allyl systems, butadiene, cyclopropenyl, cyclobutadiene, bicyclobutadiene, H_3^+, H_3 and H_3^-), Calculation of bond order, charge density, free valence index, Application of group theory for the simplification of MO determinants of 1,4- butadiene and naphthalene.

SURFACE CHEMISTRY

UNIT-I Phase Rule

Concept of Equilibrium between phases, Derivation of phase rule, Ideal Solution, Liver Rule, Brief concept on one and two component system, Application of phase rule to three component systems of both solids and liquids.

UNIT-II Adsorption

Surface tension, Capillary action, Adsorption, types of adsorption, Gibbs adsorption isotherm, Freundlich's adsorption isotherm, Langmuir's adsorption isotherm and its limitations, BET adsorption isotherm and its applications, Heat of adsorption, estimation of surface areas of solids from solution adsorption studies.

UNIT-III Macromolecules

Polymer-definition, Classification of polymer, Polymer structure, Number average and molecular weight average, Step growth & chain growth polymerization, Kinetics of polymerization, Stereochemistry of polymerization.

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SEM-II Full Marks-100 PRACTICAL

PAPER-VIII:

INORGANIC PRACTICAL-II 3 credits

1. Principle of estimation of the main constituents of Brass and Portland Cement.
(a) Estimation of Ca and Mg in a given solution prepared from a sample of cement by EDTA method.
(b) Estimation of Cu and Zn in a given solution prepared from a sample of Brass.
2. Determination of MnO_2 in pyrolusite.
3. Preparation and characterisation of the following inorganic compounds:
(i) Tetramminecupric sulphate $[Cu(NH_3)_4]SO_4 .H_2O$
(ii) Sodium cobaltinitrite , $Na_3[Co(NO_2)_6]$
(iii) Potassium chromioxalate , $K_3[Cr(C_2O_4)_3]$.

ORGANIC PRACTICAL-II 3 credits

1. Preparation of benzoin, benzil and benzillic acid from benzaldehyde.
2. Preparation from p-idotoluene from p-toluidene.
3. Preparation of ethyl acetoacetate from ethyl acetate.
4. Estimation of nitrogen by Kjeldahl method.
5. Estimation of keto group by gravimetric method.
6. Dibenzalacetone from benzaldehyde.
7. Cannizaro reaction – 4-chloro benzaldehyde as substrate.
8. Grignard reaction – synthesis of triphenyl methanol from benzoic acid.

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Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

SEM-III Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-IX:

INSTRUMENTAL METHOD OF ANALYSIS 3 credits

UNIT-I Spectroscopical Method

Flame Emission Spectroscopy (FES): Basic Principle, instrumentation-Atomizers, Burners, optical system, Detectors, interference in FES and ways to overcome it, Application of FES – Qualitative and Quantitative Analysis, standard addition method and Internal standard method, Error in FES, Limitation of FES. Atomic Absorption Spectroscopy (AAS): Basic Principle, difference between FES and AAS, Standard instruments used, Experimental Procedure, Application of AAS, interferences and remedial measures, comparative study between AAS and FES, sensitivity of Instruments.

UNIT-II Electroanalyctical Method

Polarography: Basic principle, instrumentation, theory of current-voltage curve, Theory of diffusion current, Ilkovic equation, polarography wave and half wave potential. Application of polarography. Principle, Application, advantage and disadvantage of Cyclic voltammetry anodic stripping voltammetry, amperometry, conductrometry and ion selective electrodes.

UNIT-III Thermo Analytical Methods

Thermogravimetric analysis (TGA): Principle, instrumentation, factors affecting TGA curve, derivative thermogravimetric analysis (DTGA) and application of thermogravimetric analysis, Differential thermal Analysis (DTA), instrumentation of DTA and application of DTA, Simultaneous study of TGA, DTA with examples. Differential scanning calorimetry (DSC) and thermometric titration.

INORGANIC REACTION DYNAMICS AND NUCLEAR CHEMISTRY 3 credits

UNIT-I: Substitution Reactions of Octahedral Co(III) Compounds

The nature of substitution reactions, Kinetic Application of Crystal Field Theory, Acid hydrolysis of octahedral Co(III) complexes with reference to effect of charge, chelation, steric crowding & effects of leaving group, Base hydrolysis of octahedral Co(III) complexes: Conjugate base mechanism, Test of conjugate base mechanism, Anation reaction, Substitution reaction without cleavage of metal-ligand bond.

UNIT-II Substitution Reactions of Square Planar Pt (II) Complex and Redox Reactions

Thermodynamic and kinetic stability, Trans effect and its synthetic applications, theories of trans effect (polarization & π-bonding theories), Factors affecting the rate law and reaction profile (leaving group, steric group, charge, electrophillic catalysis, nucleophile and temperature). Redox reactions: electron tunneling hypothesis, concept of Marcus-Hush theory, atom transfer reactions, one and two electron transfer, complementary and non complementary reactions, inner sphere and outer sphere reactions, electron transfer through extended bridges, concept of hydrated electron.

UNIT-III Nuclear Chemistry

Atomic nucleus, nuclear stability, magic numbers, Radioactivity, General characteristics of radioactive decay, nature of α- and β-particles, and γ-rays, decay kinetics, nuclear reaction, Bethe's notation, types of nuclear reaction, conservations in nuclear reactions, nuclear cross section, compound nuclear theory, the Brett-Wigner Formula, nuclear fission, Process of nuclear fission, liquid drop model, shell model, hard core preformation theory, Fission fragments and their mass distribution, charge distribution, Ionic charge of fission fragments, fission energy, fission cross-sections, Fission neutrons, concept of nuclear reactor and working principle, concept of nuclear fusion.

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SEM-III Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-X:

ORGANIC REDOX REACTION AND SPECTROSCOPY 3 credits

UNIT-I Oxidation: Oxidation of hydrocarbons, oxidation of alcohols by various reagents, and methods, oxidation of carbon-carbon double bonds to diols and epoxides, Chromium (VI), Manganese (VII) oxidants, Oxidation with peracids, oxidation with hydrogen peroxide, with singlet oxygen. Oxidation with ruthenium tetroxide, iodobenzene diacetate, and thallium (III) nitrate, DMSO. Reduction: Catalytic hydrogenation, selectivity of reduction,

UNIT-II Reduction by hydride transfer reagents: Aluminium alkoxid, Lithium aluminium hydride (LAH) and Sodium borohydride ($NaBH_4$), di-isobutylaluminium hydride, Sodium cyanoborodydride, Lithium trialkylborohydride, reduction with hydrazine and diimide, reduction with trialkyltinhydride, the Birch reduction, the Wolff-Kischner reduction, the Cannizarro reduction, the Resenmund reduction.

UNIT-III NMR: Magnetic properties of nuclei, Theory of magnetic nuclear resonance with special reference to proton, Instrumentation, Chemical shift, Simple spin-spin interaction, Shielding effects, Diamagnetic anisotropy, NOE, $_{13}C$, $_{15}N$, $_{19}F$, $_{31}P$ NMR (preliminary idea).

PERICYCLIC REACTION, PHOTOCHEMISTRY AND RETROSYNTHESIS 3 credits

UNIT-I Pericyclic reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann rules, Correlation diagrams and FMO approaches. Electrocyclic reactions - Conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddition reactions - suprafacial and antarafacial additions, 4n and 4n+2 systems,
[2+2] and [4+2] reactions (thermal and photochemical), 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements - [i,j] shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements. Ene reaction.

UNIT-II First order Photochemical processes Light absorption, Fluorescence and Phosphorescence.
Introduction to photochemical reactions: Cis-Trans Isomerization, Dissociation, Reduction of ketones, Paterno-Buchi reaction, Norrish type I and II reactions, Di-pimethane rearrangement, Photochemistry of arenes, Barton reaction.

UNIT-III Synthetic design: Introduction, Retrosynthetic approach, Terminology in Retro synthetic analysis, One group disconnection, (alcohol, carbonyl compound, olefins and acids), Two group disconnections (α-hydroxy compounds, α,β-unsubstituted carbonyl compounds, 1,3-dicarbonyl compounds, 1,5 dicarbonyl compounds), Synthesis of some organic molecules by disconnection approach.

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Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

SEM-III Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-XI:

QUANTUM CHEMISTRY 6 credits

UNIT-I Exact Quantum Mechanical Results

The Schrodinger equation and the postulates of quantum mechanics, Elementary application of the Schrodinger equation, Particle in a box, Harmonic oscillators, Rigid rotator and hydrogen atom.

UNIT-II Approximate Methods & Angular Momentum

The variation theorem, Time independent perturbation of non-degenerate systems, Application of Variation Method and Perturbation Theory to the He atom. Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Addition of angular momentum.

UNIT-III Chemical Bonding in Diatomics

Born-Oppenheimer Approximation, Molecular Orbital Theory and its Applications, Valence Bond Theory and its Applications, LCAO-MO Theory.

ATOMIC & MOLECULAR SPECTROSCOPY

UNIT-I: Atomic Spectroscopy

The electromagnetic spectrum, A general discussion on various molecular excitation processes, Spectra of hydrogen and hydrogen like atoms, alkali metals spectra, L-S coupling, Term symbols, Space quantisation, Zeeman effect, Stark effect, Paschen- Back effect.

UNIT-II Vibrational and Rotational Spectroscopy

Molecular Spectra of Diatomic Gases, Classification of molecules, Rotational Spectra, Vibrational Spectra, Vibrational-Rotational Spectra, P, Q and R Branches.

UNIT-III Raman Spectroscopy

Theory of Raman spectra, Rotational Raman spectra, Vibrational Raman spectra, Rotational-Vibrational Raman spectra, comparison with IR spectra.

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SEM-III Full Marks-100

PAPER-XII :

PHYSICAL PRACTICAL 6 credits

1. Determination of ionization constants of weak acids and verification of Oswald's Dilution law.
2. Verification of Onsager's limiting law.
3. Conductometric titration of a mixture of HCl+CH_3COOH with NaOH
4. Determination of solubility product of $BaSO_4$.
5. Potentiometric titration of strong acid with strong base.
6. Verification of Beer's Lambert Law and unknown concentration determination.
7. Verification of additivity rule spectrophotometrically.
8. Determination of temperature coefficient and energy of activation of hydrolysis of ethyl acetate.
9. To determine the rate constant of base hydrolysis of ester titrometrically.
10. To study the complex formation between ammonia and Cu^{+2}.
11. To study of an equilibrium $KI + I_2 = KI_3$.
12. To study the simultaneous equilibria in benzoic acid - benzene water system.
13. Determination of unknown dextrose solution by polarimetry
14. Study of inversion of cane sugar in acid medium by polarimetry.

PAPER-XIII: PROJECT 6 credits

SEM-IV Full Marks-100 Mid Sem-20 Marks Term End Exam-80 Marks

PAPER-XIV:

ADVANCED ORGANOMETALLIC CHEMISTRY 6 credits

UNIT-I: σ- and π-Bonded Organometallic Compounds

History and perspective, definition of organometallic compound, classifications, nature of metal-carbon bond, nomenclature, the 18-electron rule, general methods of preparation and properties of σ-bonded alkyl and aryl compounds, synthesis, properties and bonding of organometallic complexes of olefinic, acetylenic, allylic, acyclic- and cyclic butadiene ligands. Transition metal π-complexes of η^5-cyclopentadienyl, acyclic pentadienyl, η^5-cyclohexadienyl and η^5-cycloheptadienylligands: synthesis and reactions. Davis-Green-Mingos (DGM) rules.

UNIT-II: Organometallic Compounds and Unique Reactions

Transition metal π-complexes of η^6-arene, η^6-cycloheptatriene and η^6-cyclooctatriene ligands: synthesis and reactions. Coordinative unsaturation, oxidative addition reaction, reductive elimination reaction, insertion reaction, mechanism of insertion of CO into $CH_3Mn(CO)_5$, deinsertion reaction, intramolecular hydrogen transfer reaction, Agostic interaction, fluxionality in organometallic compounds, Transition metal compounds with bonds to hydrogen.

UNIT-III: Organometallic Compounds in Catalysis

General idea of catalysis, classification catalysis, hydrogenation of alkenes, Tolman catalytic loop, droformylation of alkenes (using cobalt and rhodium catalyst), enantioselective hydrofomylation, Zeigler-Natta polymerization of olefins, reduction of carbon monoxide by hydrogen (Fischer-Tropsch reaction), wacker process, mosanto acetic acid synthesis, hydrosilylation reactions, activation of C-H bond, alkene metathesis reactions, metathesis catalysts, classification of metathesis reactions, Importance of metathesis reactions.

UNIT-IV:Organometallic chemistry of Transition Elementsand Applicatons in Organic Synthesis:

Preparatory structural and characteristic aspect; oxidative insertion, reductive elimination, ligand migration from metal to carbon. Organo lithium, organo copper compounds, organo boranes, organometallic compounds of Zinc, Cadmium, Nickel, palladium, mercury and their utilization in chemical reactions. Reactions involving triple bond (Sonogashira reaction), C-C (Kumada, Negishi, Heck, Suzuki and Stille reactions) and C-N (Buchwald-Hartwig reaction) cross-coupling reaction

Group A consists of 10questions covering all units out of which 8 questions shall be answer each carrying 5 marks

Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

PAPER-XV:
ADVANCED SPECTROSCOPY

UNIT-I: Electron Spin Resonance Spectroscopy

Theory, instrumentation, g-values, hyperfine splitting, ESR spectra of systems with more than one unpaired electrons, double resonance, ENDOR and ELDORtechniques.

UNIT-II: Photoelectron Spectroscopy

Basic principle, Instrumentation: the basic design of photoelectron spectrophotometer,X-ray photoelectron spectrophotometer, ultraviolet photoelectron spectrophotometer, chemical information from photoelectron spectroscopy, ultraviolet photoelectron spectra and their interpretation, application of X-ray photoelectron spectroscopy, auger lines.

UNIT-III: Mossbauer Spectroscopy

Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects,Quadrupole splitting, Magnetic hyperfine interaction.

UNIT-IV (a) Mass spectrometry: Introduction, Mass spectrum, Determination of molecular formulae, Parent peak, Base peak, Use of molecular fragmentation, Mass spectra of some classes of compounds (hydrocarbons, alcohols, phenols, ketones, aldehydes, acids and esters)

(b) Problems involving UV, IR, NMR and Mass spectroscopy.

Group A consists of 10questions covering all units out of which 8 questions shall be answer each carrying 5 marks

Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

PAPER-XVI :
CHEMISTRY OF NANOMATERIALS 6 credits

UNIT-I: Semiconductors and Devices

(a) Conducting and semiconducting organic materials. Synthesis and characterizations of organic semiconductors, band gap engineering. Doping of semiconductors.(b) Nanostructured Carbon based materials: Fullerene, Carbon nanotube, graphene.Artificial photosynthetic devices, storage-memory and sensors. Electronic devices and coating. High temperature resistant organic/inorganic polymers.

UNIT-II: Nanomaterials and Applications

(a) Nanomaterials for Solar Energy Conversion Systems. Principles of photovoltaic energy conversion (PV), Structural characteristics and concepts. Types of photovoltics Cells, Physical concept of photovoltaic cells, Organic solar cells, Dye-Sensitized Solar Cells, Organic-Inorganic Hybrid solar cells. Current status and future trends.

UNIT-III: Conducting and ferroelectric materials, structure and features of ferroelectric materials, ceramic materials, organic/inorganic hybrid materials and their applications.

UNIT-IV: Structure Properties of Polymers and Applications

(a) Structure-property relationship, stress-strain behavior, crystalline melting point, effect of chain flexibility and other steric factors, entropy and heat of fusion, glass transition temperature, relationship between Tm and Tg. Effect of molecular weight, property requirements and its utilization.

(b) Synthetic procedure commercial polymers (polycarbonate, polyurethane, polymethylmethacrylate, polyethyethyleneterpthalate, Nylon, polystyrene), Fire retarding and biomedical polymers

Group A consists of 10questions covering all units out of which 8 questions shall be answer each carrying 5 marks

Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

PAPER-XVII:
INDUSTRIAL PROCESSES 6 credits

UNIT-I: Petroleum and coal based chemicals: Composition of petroleum, cracking processes, Commercial production of ethylene, acetylene, polymerization mechanisms, Addition, condensation, step growth, chain growth, method of polymerization, Distillation of coal.

UNIT-II: (a) Oil based industries: Oils and fats: Solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes.

(b) Surface active agents: classification and manufacturing of detergents used for cleansing purpose.

(c) Fermentation industries. A general discussion on fermentation conditions, manufacturing of penicillin.

UNIT-III: Pesticides and Pharmaceutical industries: DDT manufacture, BHC manufacture, 2,4-D manufacture, parathion manufacture, Pharmaceutical industry

UNIT-IV: Cement (Types and their compositions, manufacture, setting and uses) Glass: Physical and chemical properties, manufacture and some optical glass.Chemical fertilizers: Classifications, Nitrogeneous fertilizers, Ammonium nitrate, Ammonium sulphate and urea.

Group A consists of 10questions covering all units out of which 8 questions shall be answer each carrying 5 marks

Group B consists of 4 Long questions in either or format covering all units each carrying 10 marks

PAPER-XVIII:

ANALYTICAL PRACTICAL 6 credits

1. Determine the pK value of an acid-base indicator.
2. To estimate metal ions by spectrophotometric titration.
3. To determine the pH of a given solution by spectrphotometrically.
4. Adsorption of CH_3COOH on activated charcoal and verification of Freundlich's &Langumir's adsorption isotherm.
5. Simultaneous estimation of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$.
6. Determination of hydrolysis constant of aniline hydrochloride.
7. Determination of ionisation constants of multibasic acid potentiometrically.
8. Determination of association constants of CH_3COOH by distribution method between water and toluene.
9. To study the rate of acid catalysed iodination of acetone in presence of excess acid and acetone.
10. To study the stability constant of a metal complex.
11. Estimation of Fe ion in a solution of Mhor's salt.