

DEPARTMENT OF CHEMISTRY
Netaji Subhas University
Jamshedpur

Syllabus for M. Sc. Chemistry

The examination for M. Sc. (Chemistry) course shall consist of four semesters. Each semester carrying four papers of 100 (hundred marks) marks 30% marks in each paper shall be awarded through internal assessment based on discipline, attendance and performance at written tests and seminar presentation 70% marks will be awarded through external evaluation.

A theory paper shall be of 4 credits (i.e. 15x4=60 hours) but practical paper shall be 8 credits (i.e. 15x8=120 hours) each semester shall be 20 credits and entire course shall be of 80 credits.

Students failing to qualify 40% marks in each paper and 50 % aggregate in the 1st Semester in any paper shall have to clear that paper in the second semester along with paper of the same semester. Similar condition shall be applicable while clearing the second and third semester at the time of examination for the 4th semester.

Semester – I

Theory	Course	Full Marks in Written Exam	Duration of Exam (Hours)	Internal Assessment Marks	Credits
Paper-I	Physical Chemistry – I	75	03	25 (5-attendance 10-test exam 5-discipline 5-Seminar Presentation)	4 (15x4=60 hours)
Paper-II	Inorganic Chemistry – I	75	03	25	4
Paper-III	Organic Chemistry – I	75	03	25	4
Practical					
Paper-IV	(A) Physical Lab. Course	40	06	10	4
	(B) Inorganic Lab. Course	40	06	10	4

Semester – II

Theory	Course	Full Marks in Written Exam	Duration of Exam (Hours)	Internal Assessment Marks	Credits
Paper-V	Physical Chemistry – II	75	03	25 (5-attendance 10-test exam 5-discipline 5-Seminar Presentation)	4 (15x4=60 hours)
Paper-VI	Inorganic Chemistry – II	75	03	25	4
Paper-VII	Organic Chemistry – II	75	03	25	4
Practical					
Paper-VIII	Internship related to Project Work	75		25	

Semester – III

Theory	Course	Full Marks in Written Exam	Duration of Exam (Hours)	Internal Assessment Marks	Credits
Paper-IX	Spectroscopy	75	03	25 (5-attendance 10-test exam 5-discipline 5-Seminar Presentation)	4 (15x4=60 hours)
Paper-X	Environmental Chemistry and Analytical Chemistry	75	03	25	4
Paper-XI	Bio-inorganic and Bio-organic	75	03	25	4
Practical					
Paper-XII	(A) Organic Lab. Course	40	06	10	4
	(B) Environmental Lab. Course	40	06	10	4

Semester – IV

Candidates have to select one of the following groups

Group A Theory	(Elective Papers)				
Paper-XIII A	Quantum Chemistry	75	03	25 (5-attendance 10-test exam 5-discipline 5-Seminar Presentation)	4 (15x4=60 hours)
Paper-XIV A	Statistical Mechanics and thermodynamics	75	03	25	4
Paper-XV A	Advance chemical kinetics	75	03	25	4
Practical					
Paper-XVI A	Physical Lab. Course	75	12	25	8

Group B Theory

Paper-XIII B	Magneto chemistry and Spectroscopy	75	03	25 (5-attendance 10-test exam 5-discipline 5-Seminar Presentation)	4 (15x4=60 hours)
Paper-XIV B	Reaction mechanism and supra molecular chemistry	75	03	25	4
Paper-XV B		75	03	25	4
Practical					
Paper-XVI B	Inorganic Lab. Course	75	12	25	8

Group C Theory

Paper-XIII C	Medicinal Chemistry	75	03	25 (5-attendance 10-test exam 5-discipline 5-Seminar Presentation)	4 (15x4=60 hours)
Paper-XIV C	Natural Products	75	03	25	4
Paper-XV C	Polymers and Heterocyclic	75	03	25	4
Practical					
Paper-XVI C	Organic Lab. Course	75	12	25	8

SEMESTER – I
Paper – I
Physical Chemistry – I

Unit-1: Chemical Thermodynamics

- (a) Partial molar properties in ideal gas mixture, Chemical Potential, its determination and variation with temperature and pressure, Gibb's Duhem equation.
- (b) Fugacity and activity its variation with 'T' and 'P', its determination. Fugacity of a gas mixture, Duhem, Margules equation and its application.

Unit-2: Statistical Thermodynamics

Partition function and its significance, Relationship with thermodynamic functions, Translational, Rotational, Vibrational and Electronic partition function. Its application in the case of monoatomic and diatomic molecules.

Unit-3: Surface Chemistry

Surface tension and Surface Free energy on liquids. Pressure difference across curved Surface (Laplace equation), Vapour pressure of droplets (Kelvin equation). Gibbs absorption isotherm, Estimation of surface area. (B.E.T equation), Unimolecular and bimolecular surface reactions.

Unit-4: Chemical Kinetics

- (i) Mechanism and Kinetics of consecutive and opposing reactions.
- (ii) Activated complex theory of Uni-molecular reaction.
- (iii) Mechanism and Kinetics of Photolysis of acetaldehyde and Photo dimerisation of Anthracene, Polymerization and Auto oxidation reaction.
- (iv) Homogeneous catalysis, Kinetic Enzyme catalysis, study of fast reactions by flow method and relaxation methods.

Unit-5 Electro Chemistry

- (i) Electrode potential in terms of Chemical Potential and activity.
- (ii) Debye Huckle theory of conductance of electrolytic solution, its applications and limitations.
- (iii) Quantitative treatment of Debye Huckle Limiting law and its modification for finite size ions, effect of ion solvent interaction on activity coefficients.
- (iv) Butler-Volmer equation under equilibrium and non-equilibrium condition. Exchange current density Tafel Plot.

Unit-6: Macro Molecules

Types of Polymers, Kinetics and mechanism of Polymerization Molecular mass-number and mass average molecular mass, determinations of molecular mass by osmometry, viscosity and light scattering method.

Books Suggested:

1. Physical Chemistry: P.W. Atkins (ELBS)
2. Comprehensive Physical Chemistry : Hemant Snehi
3. Theoretical Physical Chemistry : Glasstone
4. Physical Chemistry : G. M. Barrow
5. Modern Electrochemistry: JOM Bockris and A.K.N.
6. Text Books of Polymer Science: F. W. Billmayer Jr.
7. Advanced Physical Chemistry : Gurdeep Raj

SEMESTER 1
Paper – II
Inorganic Chemistry – I

Unit-1: Stereochemistry and Binding

- (a) M. O. Diagram for hetero-nuclear di- and triatomic molecules.
- (b) Walsh diagram (tri-atomic molecules), $d\pi - P\pi$ bonds, Bent rule.

Unit-2: Magnetochemistry

interaction Term symbol, spin orbit coupling, Quenching of orbital contribution in metal complexes, Derivation of expression with small and large multiple width. Anomalous magnetic moments, magnetic properties of inner transition element.

Unit-3: Metal-Ligand Equilibrium in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin. Determination of formation constants by pH metry and spectrometer.

Unit-4: Metal Ligand Bonding

Limitation of crystal field theory (CFT), MOT with σ - & π -bonding.

Unit-5 Reaction Mechanism of Transition metal complexes

Inert and labile complexes, kinetic application of VBT and CFT, kinetics of octahedral substitution, acid hydrolysis, CB mechanism, Evidences of CB mechanism, Anation reaction, reaction without M-L bond cleavage, substitution reaction in square planar complexes, The trans-effect, Theories of trans-effect, Electron transfer reaction-inner and outer sphere mechanism, Marcus –Hush theory.

SEMESTER – I
Paper – III
Organic Chemistry – I

Unit-1: Nature of Bonding in Organic molecules

Delocalized Chemical Bonding – Conjugation, cross conjugation, resonance, hyper-conjugation and automatism.

Unit-2: Aromaticity in Benzenoid and non-Benzenoid compounds

Alternant and non alternant hydrocarbons, antiaromaticity, Homo-aromaticity, Huckle Rule, Energy level of p molecular orbital, PMO approach.

Unit-3: Stereo Chemistry

Elements of symmetry, chirality-molecules with more than one chiral center, methods of resolution of di mixture, enantiotropic and dia-stereotopic synthesis, Optical activity in the absence of chiral carbon atom such as biphenyls, allenes, spiranes and helical phenathrene.

Conformational analysis of cycloalkanes, decalins. Effect conformation on reactivity.

Stereochemistry of compounds contain N, S & P

Unit-4: Reaction Mechanism

Types of reactions, Hammond's postulate, Curtin Hammett principle, Potential energy diagram, transition state and intermediates. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbene & nitrene.

Effect of structure on reactivity, resonance and field effect and steric effect.

Unit-5 Aromatic Electrophilic Substitution

The arenium ion mechanism. Orientation and reactivity in mono substituted benzene ring, o/p ratio, orientation in other ring systems. Ipso substitution. Sommerlet –Hauser and Smile rearrangement.

Unit-6: Addition of C=O

Mechanism of metal hydride reduction of saturated carbonyl compounds, acid & esters. Witting reaction. Aldol condensation, Perkin reaction and Benzoin condensation.

Unit-7: Elimination Reactions

E₁, E₂ and E₁CB mechanism, Orientation of the double bond. Reactivity effect of substrate structure, attacking base, leaving group & the medium.

Unit-8: Free radical reactions

Free radical substitution mechanism at an aromatic substrate, Allylic halogenations. Oxidation of aldehyde to carboxylic acid, Sandmeyer reaction, Hinsinger reaction.

Unit-9: Conservation of Orbital symmetry in Pericyclic reactions

Woodward-Hoffman rules, Cycloaddition [2+2], [4+2] and electrocyclic reactions, Prototropic and Sigmatropic rearrangements, Ene reaction and cheletropic reactions and 1, 3 Dipolar reactions.

SEMESTER – I
Paper IV
(A) Physical lab course

1. Water equivalent of calorimeter and determination of
 - (i) Heat of solution of potassium nitrate
 - (ii) Heat of neutralization of strong acid and strong base.
 - (iii) Basicity of Polybasic acids.
2. Determination of rate constant of hydrolysis of methyl acetate in acid medium.
3. To study saponification of ethyl acetate by sodium hydroxide and determination of rate constant.
4. To determine the distribution coefficient of
 - (i) Acetic acid
 - (ii) Benzoic acid
5. Determination of specific and molar rotation of sucrose in different concentrations and to determine the concentration of given solution.
6. Determination of rate constant by INVERSION OF CANE SUGAR BY Polarimetrically.
7. Conductrometric Experiments.
Determination of
 - (i) Dissociation constant of acetic acid.
 - (ii) Acid-base titration.
 - (iii) Solubility product of sparingly soluble salt.
8. Potentiometric Experiments.
Determination of
 - (i) E.M.F of Concentration cell.
 - (ii) pH of a given solution using electrode and quinhydrone electrode.
 - (iii) Acid-base titration.

Distribution

- (i) One Experiment – 40 Marks
- (ii) Note Book – 05 Marks
- (iii) VivaVoce – 05 Marks

Paper IV
(B) Inorganic Lab course

1. Quantitative analysis of inorganic mixture containing six radicals including interfering radicals.
2. Quantitative analysis of two constituent ions of the following.
(a) Cu, Zn (b) Fe, Ni, (c) Ca, Mg (d) Al, Mg
The cations Mg^{2+} , Ca^{2+} and Al^{3+} can be estimated using EDTA.
3. Inorganic Preparation
 - (a) Pot trioxalato ferrate (II)
 - (b) Pot trioxalato chromate (III)
 - (c) Hexa ammine Ni (II) chloride
 - (d) Diaquo dioxalato chromate (III)

Viva-voce **05**

Record **05**

SEMESTER – II
Paper – V
Physical Chemistry – II

Unit-1: Solid state chemistry

Perfect and imperfect crystals, intrinsic and extrinsic defects, line defects, plane defects, Vacancies-schottky and Frenkel defect. Non-stoichiometric defects.

Unit-2: Non-Equilibrium Thermodynamics

Entropy production in irreversible process Fluxes and forces, linear phenomenological relation, reverse osmosis and electrokinetic phenomena.

Unit-3: Introduction of Quantum mechanics

- (i) Particle in three dimensional box.
- (ii) Hermitian operators, properties of operators.
- (iii) Angular momentum operator, their Eigen function and Eigen values, Theorem of operators.

Unit-4: Exactly Soluble System

- (i) Linear Harmonic oscillator, Harmonic Vibration Hermit differential equation and its solution through recursion relation, Hermit polynomial.
- (ii) H-like atoms, separation of r , θ , ϕ equation. Laguerre and associated Laguerre polynomial. Legendre polynomial equation and their solution.

Unit-5 Approximate Method

- (i) Variation method, Linear application to Harmonic oscillator, perturbation method, first order perturbation, Application to He-atom.
- (ii) Huckle theory of conjugated systems, bond order and charge density-its calculation. Application to ethylene and butadiene.

Books Suggested:

1. Quantum Chemistry: I.R. Lavine Prentice Hall.
2. Quantum Chemistry: Pillar
3. Quantum Chemistry: R. K. Prasad
4. Quantum Chemistry: Satya Prakash Swati Saluja
5. Solid State Chemistry: D. K. Chakraborty, New Age International
6. New Direction in Solid state Chemistry: C. N. R. Rao & J. Gopal Krishnan
7. Introduction to quantum: A. K. Chandra, Tata

SEMESTER – II
Paper – VI
Inorganic Chemistry – II

Unit-1: Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operations, definition of groups, sub-group, conjugate and class. Point symmetry group. Requirements of a mathematical group, multiplication table for C_{2v} , C_{3v} . Representation of group by matrices. Working out representation of C_{2v} , C_{3v} point groups. Character of a representation. The great orthogonality theorem (without proof) and its importance in derivation of character table of point group- C_{2v} .

Unit-2: Electronic spectra and magnetic properties of transition metal complexes.

Derivation of spectroscopic ground states, Orgel diagram, basic idea & calculation of Dq , B and β parameters, spectroscopic method for assignment of absolute configuration in optically active metal chelates and their stereo-chemical information.

Unit-3: Metal π -complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation. Preparation, bonding, structure and important reactions of transition metal nitrosyls. Dinitrogen, tertiary phosphines as ligands.

Unit-4: Metal clusters

Structural aspects of Boranes and Corboranes.

SEMESTER – II
Paper – VII
Organic Chemistry – II

Unit-1: Carbohydrate

Conformation of monosaccharide's and important derivatives of monosaccharide – glycosides, deoxysugar, aminosugar.

Disaccharides – Structure determination and chemical synthesis of sucrose, maltose & lactose.

Unit-2: Lipids

Lipid metabolism, β -oxidation of fatty acids. Detergents, Soaps.

Unit-3: Amino acids, peptides and proteins

Chemical and enzymatic hydrolysis of proteins, amino acid sequencing. Secondary structure of protein, forces responsible for secondary structure of protein. α -helix, β -sheet. Super secondary structure, tertiary structure of proteins folding.

Unit-4: Nucleotides and nucleic acids.

Chemical properties of pyrimidine and Purine derivatives, Synthesis of purines & pyrimidine derivatives. Structure of RNA and DNA. Chemical and enzymatic hydrolysis of nucleic acids.

Unit-5 Terpenoids

Introduction, classification, isoprene rule and special isoprene rule. Structural determination of citral, α -Terpeniol and camphor. .

Unit-6: Alkaloids

Introduction, classification general method of structure determination. Structure and synthesis of the following compounds-papavarine, Nicotine, Atropine.

SEMESTER – II
Paper – VII

INTERNSHIP RELATED TO PROJECT WORK----- 75 Marks

SEMESTER – III
Paper – IX
Spectroscopy – II

Unit-1: Rotational Spectra

Classification of molecules, Rigid rotator model, Non-rigid rotator, Quantization of rotational energy level, Fine structure of rotational spectra, Bond Length calculation.

Unit-2: Vibrational rotational spectra

Quantization of vibrational energy level, vibration energy of diatomic molecule, zero point energy, Force constant, Anharmonicity, Group frequency, Fingerprint region, factors influencing vibrational frequency.

Unit-3: NMR Spectroscopy

Nuclear spin, nuclear resonance, shielding of magnetic nuclei, chemical shift and its measurement, Factor influencing chemical disheilding and coupling constant.

Unit-4: Mass Spectroscopy

Ion production, ion analysis, factors affecting fragmentation, Mass spectral fragmentation of organic compounds.

Unit-5 Approximate Method

- (i) Various electronic transitions, Beer Lambert Law, effect of solvent on electronic transition Fieser Woodward rules for calculating λ_{max} in conjugated dienes & α , β -unsaturated carbonyl compounds.
- (ii) H_2 molecule, Ground & excited state terms derivation of H_2 molecule. Selection rule, Vibrational progression.
- (iii) ^{13}C nmr, spin decoupling, Shift reagent, ^{19}F and ^{31}P nmr

Books Suggested:

1. Molecular Spectroscopy: P. S. Sindhu
2. Modern Spectroscopy: J. Michael Halls
3. Molecular Spectroscopy: Jeanne L McHale
4. Elements of Spectroscopy: Gupta+Kumar+Sharma

SEMESTER – III

Paper – X

Environmental and Analytical Chemistry

Section – A: Environmental Chemistry

Unit-1: Environment & hydrosphere

Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, Biogeochemical cycles of C, N, P, S and O. Chemical composition of waterbodies, Hydrological cycle, Aquatic pollution: inorganic, organic, pesticide. Water quality parameters-dissolved oxygen, BOD, solids, metals, contents of chloride, sulfate, phosphate, nitrate and micro organisms. Analytical methods for measuring BOD, DO, COD, F, chloride and chlorine demand.

Unit-2: Solids and Industrial pollution

Composition of soils, micro and macro nutrients. Soil pollution-fertilizers, pesticides. Industrial pollution – cement and sugar

Unit-3: Atmosphere

Particles, ions and radicals in atmosphere, their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect. Green house effect. Acid rains.

Section – B Analytical Chemistry

Unit-4: Analytical methods for measuring air and water pollutants. Instrumental techniques for analysis of heavy metals in aqueous systems. Analysis of soil (pH, total N, P, Silica, lime, magnesia, Mn and S only).

Unit-5 Thermal Analysis and Calorimetry

Basic principles of thermal analysis, TG, DTA, DSC, TMA and microcalorimetry. Components of instruments (schematic only), Calibration, General features in curves, significance of local factors, Glass transition point, Onset temperature. Applications in polymer chemistry and solid state reactions.

Unit-6: Chromatography and colorimetry

Chromatography-Classification, chromatography terminology. Development of chromatography. Colorimetry:- Beer Lambert law, Photoelectric colorimetry, Estimation of carbohydrates and proteins.

SEMESTER – III

Paper – XI

Bioinorganic and Bioorganic Chemistry

Section-A: Bioinorganic

Unit-1: Metals in biological systems

- (a) Trace elements and their significance. Na⁺/K⁺ pump.
- (b) Transport and storage proteins, Structure and functioning of myoglobin & hemoglobin, idea of hemocyanine , Hemerythrin.
- (c) Metal complexes in transmission of energy, chlorophylls, photo system-I and photo system-II in cleavage of water.

Unit-2: Electron transfer and Redox systems

Cytochromes and iron-sulfur protein. Biological nitrogen fixation. Nitrogenase.

Unit-3: Cell membrane

Ion transport cell membrane.

Unit-4: Enzymes properties

Specify orientation and steric effects-coenzymes, cofactors as derived from vitamins, idea of prosthetic groups, thiamine, pyrophosphate, pyridoxal phosphate NADP, NAD, FMN & FAD.

Unit-5 Bioenergetics

Synthesis of ATP, Hydrolysis of ATP and entropy change in biological process.

Unit-6: Carbohydrate Metabolism

Calvin cycle, Krebs cycle, Glycolysis. Glucogenesis, glycogenesis, Biosynthesis of disaccharides, and polysaccharides, pentose phosphate pathway.

Unit-7: Protein synthesis

Chemical basis of heredity, Replication of DNA, Transcription and translation. The effect of x-ray and gamma-rays on nucleic acid, polypeptide and protein structure.

Books Suggested:

1. Elements of Bioinorganic Chemistry – G. N. Mukherji (Undhpur publishers)-Bertini Gray
2. Bioinorganic Chemistry – Lippard Valentine (Viva)

SEMESTER – III
Paper – XII
(A) Organic Practical

1. Identification of single organic compound
2. Estimation of Glucose, Acetyl/Methoxy group
3. N. B.
4. Viva-voce

SEMESTER – III
Paper – XII
(B) Environmental Lab Course

1. Sampling, preservation storage and processing of water and soil samples.
2. Estimation of hardness, Mg, Cs, alkalinity and chloride in water and soil.
3. Estimation of DO, BOD and COD.
4. Detection and estimation of phosphates, nitrates, nitrites and sulphates.
5. Estimation of nitrogen
6. Determination of pH of soil and water.
7. Determination of conductivity of water and soil.
8. Estimation of grease and oil in industrial effluents.
9. Estimation of heavy metals in water and soil e.g. Cr, Pb, Zn, Cu, Fe and Ni.

SEMESTER – IV
Paper – XIII A

Physical Chemistry
Quantum Chemistry

Unit-1: Elementary Matrix Theory

Review of Matrix algebra and angular momentum, Matrix representation of Schrodinger wave equation, Matrix transformation of Linear equation.

Unit-2: Corrosion

Scope and economics of corrosion, causes and types of corrosion electrochemical theories of corrosion.

Unit-3: Hartree Fock Theory

Born-oppenheimer approximation. Salter-Condon rule, Hartree-Fock equation, Koopman theory.

Unit-4: Semi Empirical Theories

HMO theory of p systems. Bond order, Free valence and charge density, and its calculation.
Extended Theory

Unit-5 Density Functional Theory

Derivation of Hohenberg kohn theorem. Treatment of chemical concepts with density functional theory.

SEMESTER – IV
Paper – XIV A

Statistical mechanics and thermodynamics

Unit-1: Classical Statistical Mechanics

Foundation of molecular thermodynamics Liouville theorem, micro-canonical ensemble, canonical and grand canonical ensembles.

Unit-2: Molecular Statistics

- (a) Boltzmann distribution law of non degenerate case Determination of Boltzmann constant k_B and μ .
- (b) Bose-Einstein distribution, Fermi Dirac distribution, comparison of Bose Einstein and Fermi-Dirac statistics.

Unit-3: Molecular Partition function

Evaluation of translational partition function for mono atomic gas, Evaluation of rotational and vibrational partition function for ideal diatomic gases.

Unit-4: Thermodynamics of solids

Specific heat of solids, Einstein heat capacity equation, Debye theory of specific heat.

Unit-5 Irreversible thermodynamics

Microscopic reversibility, Entropy flow and entropy Production due to irreversible processes inside the system, Excess entropy production, Thermodynamic fluxes.

Books Suggested:

1. Physical Chemistry: P.W. Atkins
2. Introduction of thermodynamic of irreversible processes: I. Prigogine
3. Advance Physical Chemistry: Gurdeep Raj
4. An Introduction to chemical thermodynamics: R. R Mishra

SEMESTER – IV
Paper – XV A

Advanced Chemical Kinetics

Unit-1: Elementary Reaction in solution

Solvent effects on reaction rate, Factors determining rates in solutions. Reactions between ions, Ion Dipole and dipole reactions. Influence of hydrostatic pressure.

Unit-2: Kinetics of condensed phase Reaction

Factors determining reaction rate in solution, Transition state theory in solution , kinetics of ionic reaction. Dependence of rate constant on ionic strength and dielectric constant of the medium. Bronsted Bjerrum equation.

Unit-3: Catalysis and Oscillatory Behavior

Kinetics of catalytic reaction, Arrhenius intermediates, Vant-Haff intermediates, Theory of acid-base catalyst, Bronsted catalysis law, Hammett equation, Oscillatory reactions.

Unit-4: Study of Fast reactions

Flash Photolysis, relaxation techniques, Molecular beam and shock Tube kinetics, stop flow method.

Unit-5 Kinetic of Electrode reactions

Faradic and non-faradic current rate law in faradic process, current density , factors affecting electrode-reaction, Effect of double layer structure on electrode reaction rates.

Books Suggested:

1. Chemical Kinetics : Keith J. Laidler
2. Kinetics and Mechanism of chemical transformation: J. Rajaraman and J. Kuriacose, Mc Millan
3. Physical Chemistry : P. W. Atkins ELBS

SEMESTER – IV
Paper – XVI A

Physical Practical

1. Determine the distribution coefficient of I_2 between CCl_4 and water.
2. To determine the partition coefficient of benzoic acid(or acetic acid) between benzene and water.
3. To determine the equilibrium constant of the reaction $KI + I_2 \rightleftharpoons KI_3$.
4. To determine the velocity constant of hydrolysis (or saponification) of ethyl acetate with NaOH.
5. To determine the order of reaction between I_2 and acetone catalyzed by acids.
6. To determine the order of reaction and the energy of activation of the reaction between H_2O_2 and HI.
7. To determine the basicity of succinic acid conductometrically.
8. To determine the solubility and solubility product of sparingly soluble salt like $PbSO_4$.
9. To nitrate a mixture of HCl and acetic acid solution against NaOH solution, conductometrically.
10. To study concentration cells and hence to
 - (a) Ascertain the reversibility of Ag/Ag^+
 - (b) Determine the value of $2.303 \frac{cRT}{F} = k$.
 - (c) Determine the mean activity coefficient of $AgNO_3$ in N/10 solution.
11. To determine the E_o of quinhydrone electrode
12. To determine the ionic product of water (K_w).

SEMESTER – IV
Paper – XIII B
Inorganic Chemistry
Magnetochemistry and spectroscopy

Unit-1: Multiple and fine structure in atomic spectra

Free ion term, Hund's rule, LS and J-J coupling schemes, Racah parameters, Land's interval rules, Multiplet separation, spin orbital coupling constant.

Unit-2: Metal ions in chemical environment

Splitting of terms of O_h , T_d and D_{nh} symmetry, Transformation properties of s, p and d orbitals in a chemical environment by the use of character table. Sine formula and its derivatives, strong field configuration, strong field components. Non crossing rules. Correlation diagram for d^2 , d^3 , d^7 and d^8 systems in cubic symmetry, crossover points, T-S diagram.

Unit-3: M. O description for bonding in coordination compound

Classification of ligands as sigma and pi donor ligands, pi acceptor ligands, symmetry consideration of metal orbitals and ligand group orbitals in O_h point group for sigma and Pi bond formation, Use of character table for formation of M.O.s in O_h and T_d point group with and without pi bonding, MO energy level diagram.

Unit-4: Absorption Spectra and other spectroscopic evidences for ligand field effect.

Selection rule and their relaxation. Band assignment, determination of ligand field splitting parameters, nephelauxetic ratio, Jahn Teller distortion, Vibronic coupling, spin-orbit coupling, CT Bands and their assignment.

Unit-5 Magnetochemistry

Van Vleck susceptibility equation and its application, TIP effect of spin orbit coupling, magnetic properties of A, E and T ground term complexes, effect of electron delocalization on magnetic properties, anti ferromagnetic exchange interaction, super exchange interaction, low and high spin cross over.

Unit-6 Applications of spectra in coordination compounds

(a) IR – Metal carbonyls, nitrosyls, linkage isomerism, mode of metal-ligand bonding

NMR – Paramagnetic transition metal complexes

ESR – Hyperfine interaction, isotropic g and A values

Mossbauer – Spectra of Fe (57) and Sn (119) compounds

SEMESTER – IV

Paper – XIV B

Reaction Mechanism & Supramolecular Chemistry

Unit-1: Electron transfer reactions

Outer sphere and inner sphere mechanisms, Marcus Hush theory, Complementary and non-complementary reactions, mixed valence complexes and their electron transfer model.

Unit-2: Molecular rearrangement

D and A process, reactions of geometrical and optical isomers, optical inversions, isomerisations and racemisation of octahedral complexes, intermolecular rearrangement.

Unit-3: Photo chemistry of metal complexes

Basis of photochemistry, properties of excited states, excited states of metal complexes and their comparison with organic compounds. Photo-substitution, photo-oxidation and photo-reduction, Excited electron transfer, Reactions of 2, 2'-bipyridines and 1, 10-phenanthroline complexes, metal complex sensitizers, photochemistry of Co (II) and Cr (III) complexes, Application of photochemical reactions of co-ordination compound.

Unit-4: Supramolecular Chemistry

Introduction, some examples of self assembly in supramolecular chemistry, reactivity and catalysis designand synthesis.

Unit-5 Synthesis, structure, bonding and application of metal carboxylates, metal acetylacetonates, Schiff base metal complexes.

SEMESTER – IV
Paper – XV B

Organomettalic Chemistry

Unit-1: Alkyls and aryls of transition metals

Types, routes of synthesis, stability and decomposition pathways. Organocopper in organic synthesis.

Unit-2: Compounds of transition metal0carbon multiple bonds

Alkylidenes, alkylidynes, low valent carbenes and carbinos – synthesis, nature of bond, structural characteristics Nucleophilic and electrophilic reactions on the ligands, Roles in organic synthesis.

Unit-3: Transition metal π -complexes

Transition metal π -complexes with unsaturated organic molecule-alkenes, alkynes, allyl, diene, dienyl, arene, trienyl complexes, their structural features and important nucleophilic and electrophilic reactions.

Unit-4: Transition metal compounds with hydrogen

- (a) Transition metal compounds with bonds to hydrogen
- (b) Homogeneous Catalysis.

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation. Ziegler Natta polymerization of olefins, catalytic reactions involving CP, [e.g. hydrocarbonylation of olefins, (oxo-reaction)], oxopalladation reactions, activation of C-H bond.

Unit-5 Fluxional organomettalic compounds

Fluxionality and dynamic equilibria in compounds such as η^2 -olefin, η^3 -allyl and dienyl complexes.

Transition metal clusters- bonding, Electron counting in clusters, Wade's rule, LNCC, HNCC

SEMESTER – IV
Paper – XVI B

Either of two from the following

1. Systematic qualitative analysis of inorganic mixture containing at least six radical including Mo, V, W, Ce
2. Analysis of at least two metal ion in alloys and minerals (Dolomite, Brass, Solder, Steel, Bauxite)
3. Preparation of complex compounds of Fe, Cr, Co and assignment of important peaks in given IR spectrum or reading of important features in given TG/DSC curve.

SEMESTER – IV
Paper – XIII C
Organic Chemistry
Medicinal Chemistry

1. **Drug Design**: Introduction, classification, SAR factors affecting bio activity. Theories of drugactivity, Assays of drugs.
2. **Antineoplastic agents** : Cancer chemotherapy, synthesis of Uracil, mustards, 6-mercaptopurine, Melphalan, Natural Products and Harmones.
3. **Cardiovascular Drugs** : Cardiovascular diseases, direct acting arteniolar, synthesis of amyl nitrate, sorbitrate, quinidine, Methyldopa, atenolol and oxyprenolol.
4. **Anti-tubercular Drugs** : PAS, Isoniazid, ethambutol, Thiosemicarbazone, Rifampein.
5. **Antiparkinson Drugs** : Introduction, levodopa, and some other dopaminergic agents – Anticholingeric, Antiparkinsonri agents Aminoalcohols, Ethers – A phenothiazine derivations.
6. **Lactum antibiotics** : Penicilin, cephalosporin, ciprofloxacin.
7. **Drug based on five mambered heterocycles fused to ix mambered rings**: Methotrexate, Acyclovir.

SEMESTER – IV
Paper – XIV C

Natural Products

1. **Terpenoids**: Isolation, Structure determination , stereochemistry synthesis and biosynthesis of the following compounds, longiloline, Santonin, Abietic acid and Taxol

2. **Alkaloids** : Occurrence, Isolation, structural determination, stereochemistry and synthesis, Ephedrine, Quinine, Morphine and Narcotine

3. **Steroids and Hormones** : Introduction, Diels hydrocarbon, structural determination and synthesis of cholesterol, oestrone, progesterone, Androsterone, Cartisone (only synthesis)

4. **Vitamins** : Occurrence, Classification, biological functions and structure determination and synthesis of Vit A, Vit B₁, Vit B₂, Vit B₁₂ and Vit C

5. **Plant Pigments** : Occurrence, structural determination and synthesis of flavones, Isoflavones, anthocyanins, anthocyanidines and coumarins.

6. Retrosynthesis analysis of morphine, reserpine and longitolene.

SEMESTER – IV
Paper – XV C

Polymer and Heterocyclic

1. **Biopolymers**: Polysaccharides, starch, amino acids and polypeptides, Proteins

2. **Synthetic polymers** : Polyester, polytetrafluoroethylene, polyureathanes, poly-amino acids, polycyanoacrylates.
Divinylether – maleic anhydride cyclopolymer (DIVEMA).

3. **Benzofused five membered heterocyclic compounds** : Classification, nomenclature of aromatic heterocycles, Synthesis and reaction of benzopyrrole, benzofuran, and benzothiophenes.

4. **Five and six membered Heterocycles with two or more heteroatoms** : Synthesis and reaction of oxazole, isooxazole, thiazole, diazine, and tetrazines.

5. **Seven and large membered Heterocycles with two or more heteroatoms** : Synthesis and reaction of azepines, oxepines, diazepines, azocines and thiapines.

SEMESTER – IV
Paper – XVI C

Organic Practical Paper

1. Identification of mixture of organic compounds
2. Two step synthesis of organic compounds.
3. Extraction of organic compounds from natural sources.
 - (a) Isolation of caffeine from tea leaves.
 - (b) Isolation of casein from milk.
 - (c) Isolation of nicotine dipicrate from tobacco.