

RADHA GOVIND UNIVERSITY

RAMGARH, JHARKHAND



Department of Chemistry
Under Faculty of Science

Choice Based Credit System Curriculum for
M.Sc. Chemistry

(Effective from Academic Session 2025-2026)

Semester – I			Course Credits	Hours /Week	Full Marks	End Sem + Mid Sem
S.	Course	Course-Name				
1.	CHE F-01 (Paper 1)	Fundamental of chemistry	5	5	100	70+30
2.	CHE C-02	Inorganic chemistry	5	5	100	70+30
3.	CHE C-03	Organic chemistry	5	5	100	70+30
4.	CHE C/P-04	practical	5	5	100	70+30
Semester – II			Course Credits	Hours /Week	Full Marks	End Sem + Mid Sem
S.	Course	Course-Name				
1.	CHE S-05	Skill development	5	5	100	70+30
2.	CHE C-06	Physical chemistry	5	5	100	70+30
3.	CHE C-07	Theoretical chemistry	5	5	100	70+30
4.	CHE C/P-08	practical	5	5	100	70+30
Semester – III			Course Credits	Hours /Week	Full Marks	End Sem + Mid Sem
S.	Course	Course-Name				
1.	CHE A-09(A/B/C)	Choice based elective	5	5	100	70+30
2.	CHE C-10	Inorganic chemistry	5	5	100	70+30
3.	CHE C-11	Organic chemistry	5	5	100	70+30
4.	CHE C/P-12	practical	5	5	100	70+30
Semester – IV			Course Credits	Hours /Week	Full Marks	End Sem + Mid Sem
S.	Course	Course-Name				
1.	CHE E-13(A/B/C)	Elective I	5	5	100	70+30
2.	CHE E-14(A/B/C)	Elective II	5	5	100	70+30

3.	CHE E/P-15(A/B/C)	Laboratory course	5	5	100	70+30
4.	CHE D-16	Project/Dissertation	5	5	100	50+50

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Regulation:

Each Paper (Theory & Practical) carries full marks of 100, out of which Sessional exam (Internals) will carry 30 marks and End Semester Exam (External) will carry 70 marks.

Sessional (Internals) Exam: 20 marks and General awareness, Attendance 05 and assignment 05.

End Semester Exam: 70 marks. The end semester exam will consist total nine questions. Candidates will be required to answer any five questions from long answer type questions. All questions will carry equal marks. Duration of paper will be of 3 hours.

M.Sc. Chemistry
Semester-I
Fundamentals of Chemistry

Paper-I
Full Marks:70

CHEF-01
Time:3 hrs.

UNIT-1 Mathematics for Chemists

A. Matrix

Matrix and determinant, The operation of Matrix algebra- Addition, subtraction and Scalar multiplication, Multiplication of determinants (of third order). Diagonal Matrix, Scalar matrix, unit matrix, singular and Non- singular Matrix, Transpose matrix, Adjoint matrix Orthogonal matrix and its properties. Inverse of a Matrix, Solution of Homogeneous and Non-homogeneous linear equations.

B. Vector

Introduction to Vector, Addition and subtraction of two vectors, Dot and cross products of two vectors, unit vectors, scalar and Vector products of unit vector, The gradient, Divergence and curl.

C. Calculus

Differential calculus: Rules of Differentiation, Exact and inexact differential with their applications to Thermodynamic properties, Maxima and Minima (Examples related to Bohr radius and most probable velocity from Maxwell's distribution etc).

Integral Calculus: Basic rules for integration-Integration by parts, Partial fraction and substitution. Definite integrals and their evaluations.

UNIT-2 Operators:

Linear and non-linear operators, Hamiltonian operator, Hermitian operator and its significance, operators and commutation relations, Angular momentum operators and their commutation relations, operator using ladder operators.

UNIT-3 (a) Electronic structure of free atoms/ions-L-S coupling & J-J coupling

Schemes, Determination of term symbols of p^n and d^n ($n=1,2,3$) systems, Hund's rule for deciding relative energies of terms, Selection rules for electronic transitions.

UNIT-3(b) VSEPR theory-shapes of inorganic molecules/ions, Bent's rule and energetic of hybridization, Role of p and d orbitals in bonding and their implications, Simple reactions of covalently bonded molecules.

UNIT-3 (c) Hard and soft acids and base, Classifications of acids and bases into hard and soft categories, Acid-Base strength and hardness and softness. Symbiosis, Theoretical basis of hardness and softness, Electronegativity and hardness and softness.

UNIT-4: Symmetry elements, Symmetry operations, Point groups, Systematic approach to determine the point group of molecules/ions, Multiplication of symmetry operations, Multiplication table for C_{2v} , C_{2h} and C_{3v} Point groups (C_{2h} and C_{3v}), Use of character table in vibrational spectroscopy, Point group symmetry in the determination of dipole moment and optical activity of molecules.

UNIT-5(a) REACTION INTERMEDIATES

Generation, structure, stability and reactivity of Carbocations, Carbanions, Free radicals, Carbenes, Nitrenes and Benzyne. Application of NMR in detection of carbocations.

UNIT-5(b) REACTION MECHANISM: STRUCTURE AND REACTIVITY Types of mechanism, types of reactions Thermodynamic and kinetic requirements, kinetics thermodynamic control, Hammond's postulate. Curtin Hammett principle, Potential energy diagram, transition states and intermediates, methods determining mechanism, isotopic effects, Hard Soft acid and bases. Effect of structure reactivity – resonance and field effects, stereo effect, Hammett equation and linear free energy relationship, substitution and reaction constants.

UNIT-5(c) 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 level of molecular orbitals, annulenes, antiaromaticity, aromaticity, homoaromaticity.

BOOKS SUGGESTED:

1. Mathematical Methods for Physical and Analytical Chemistry" by David Z. Goodson
2. Reactive Intermediates" by Matthew B. Smith: Oxford University Press
3. Reactive Intermediates in Organic Chemistry: Structure, Mechanisms, and Reactions" by Maya Shankar Singh, Wiley-VCH
4. Mathematics for Physical Chemistry" by Robert G. Mortimer Publisher: Academic Press

M.Sc. Chemistry
Semester-I
Inorganic Chemistry

Paper-II
Full Marks:70

CHEC-02
Time:3 hrs.

UNIT-1

Pont symmetry group Schonflies Symbols, representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} . D_{nh} etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

UNIT-2 Stereochemistry And Bonding In Main Group Compounds **10 Hrs**

VSEPR, Walsh diagrams (tri- atomic molecules of type AH_2), dp pp bonds, Bent rule and energetic of hybridization, some simple reactions of covalently bonded molecules, Atomic Inversion, Betty Pseudorotation.

UNIT-3(a) METAL-LIGAND EQUILIBRIA IN SOLUTION **08 Hrs**

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory.

UNIT-3(b) METAL-LIGAND BONDING

Step wise 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 binary formation constants by pH-metry and spectrophotometer.

UNIT-4(a) METAL IONS IN BIOLOGICAL SYSTEMS **03 Hrs**

Essential and trace metals.

Na^+/K^+ Pump

Role of metals ions in biological processes,

UNIT-4(b) BIOENERGETICS AND ATP CYCLE **04 Hrs**

DNA polymerization, glucose storage, metal complexes In transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water Model System.

UNIT-5(a) TRANSPORT AND STORAGE OF DIOXYGEN **05 Hrs**

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper.

UNIT-5(b) ELECTRON TRANSFER IN BIOLOGY

05 Hrs

Structure and function of metalloproteins in electron transport processes – cytochromes and iron-sulphur proteins, synthetic models

Nitrogenase

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other nitrogenases model systems.

BOOKS SUGGESTED:

1. Principles of Structure and Reactivity” by James E. Huheey, Ellen A. Keiter & Richard L. Keiter; Pearson Education
2. Advanced Inorganic Chemistry: Volume I” by Gurdeep Raj: Krishna Prakashan Media
3. *Inorganic Chemistry* by J. Derek Woollins (also covered in Huheey's & Miessler's books); Oxford University Press / Elsevier (varies by edition)
4. *Bioinorganic Chemistry* by Asim K. Das: Books and Allied Pvt. Ltd. (India)

M.Sc. Chemistry
Semester-I
Organic
Chemistry

Paper-III
Full Marks:70

CHEC-03
Time:3 hrs.

UNIT-1 : STEREOCHEMISTRY OF ORGANIC COMPOUNDS

Optical isomerism: Fischer, Newman Sawhorse and Flying – Wedge projections and their interconversions, molecular symmetry and point groups, asymmetry and dissymmetry, stereochemical, descriptors, centre of chirality, assigning of absolute stereochemistry, CIP rules, isotopic asymmetry, variation of specific rotation in sign and magnitude under different conditions, optical isomerism of compounds containing more than one asymmetric carbon atoms, number of stereoisomers, prochirality-topacity- homotopic and heterotopic, prostereo isomerism.

Geometrical isomerism: Nomenclature of geometrical isomers (E-Z notation) of compounds with one and more double bonds in acyclic system, methods of determination of the configuration of geometrical isomers in acyclic and cyclic system, interconversion of geometrical isomers.

Stereochemistry of aldoximes and ketoximes- naming, types of isomerism, methods of determining configurations.

Annulenes- Binary number methods of designing the stereochemistry of annulenes.

UNIT-2: ELECTROPHILIC SUBSTITUTION REACTIONS

(a) **Aliphatic electrophilic substitution:** Bimolecular mechanism SE_2 , SE_1 and SE_i mechanism Electrophilic substitution accompanied by double –bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

(b) **Aromatic electrophilic substitution:** The arenium ion mechanism, orientation and reactivity, energy profile diagrams, The ortho para ratio, ipso attack, orientation in other ring system. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Gattermann Koch reaction, Vilsmeier reaction.

UNIT-3: NUCLEOPHILIC SUBSTITUTION REACTIONS

(a) **Aliphatic nucleophilic substitution:** The SN^2 , SN^1 , mixed SN^1 and SN^2 mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds.

(b) The S_{N}^1 mechanism Nucleophilic substitution at an allylic aliphatic trigonal and at vinylic carbon. Reactivity effect of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity.

(c) Aromatic Nucleophilic Substitution: The $\text{S}_{\text{N}}^{\text{Ar}}$, S_{N}^1 , benzyne and S_{RN}^1 mechanism. Reactivity effect of substrate structure. Leaving group and attacking nucleophile. The von Richter and Smiles rearrangement.

UNIT-4 (a) ADDITION TO CARBON- CARBON MULTIPLE BONDS

Mechanism and stereochemical aspects of addition reactions involving electrophiles, Nucleophiles and Free radicals, region and Chemoselectivity, Orientation and reactivity, Addition to cyclopropane ring. Hydrogenation of double and triple bonds. Hydrogenation of Aromatic rings. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

UNIT-4 (b) ADDITION TO CARBON-HETERO-MULTIPLE BONDS

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters nitriles. Addition of Grignard's reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Mechanism of condensation reactions involving enolates Aldol. Knoevenagel, Claisen, Mannich, Perkin and Stobbe reactions. Hydrolysis of ester and amides.

UNIT-5 (a) ELIMINATION REACTIONS

The E_2 , E_1 , and $\text{E}_{1\text{CB}}$ mechanism and their spectrum, orientation of double bond. Reactivity-effects of substrate, Structures, attacking base, the leaving group and the medium.

UNIT-5 (b) MOLECULAR REARRANGEMENT REACTIONS

General mechanistic approach to molecular rearrangement reactions, Carbocation rearrangement, Migratory aptitude and Memory effects, Brief study of following rearrangement reactions Pinacol-Pinacolone, Favorskii, Baeyer-Villiger oxidations, Amdt-Eistert synthesis, Beckmann, Hofmann, Curtius, Fries and Claisen rearrangement.

BOOKS SUGGESTED:

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry – F.A Carey and R.J. Sundberg, plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry-C.S. Ingold, Cornell University Press.
5. Organic Chemistry- R.T. Morrison and R.N. Boyd, Prentice- Hall
6. Modern Organic Reactions- H.O., House, Benjamin.

7. Principles of Organic Synthesis – R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry- S.M. Mukherji and S.P. Singh, Macmillan.
9. Stereo Chemistry of Organic Compounds- P.S. Kalsi, New Age International. 10. Stereochemistry of Organic Compounds – P.S. Kalsi, New Age International.
11. Advance organic chemistry, J. Singh and L.D.D. Yadav, Pragati Prakash, Meerut.

M.Sc.
Chemistry
Semester-I
Practical

Paper-IV
Full Marks:70

CHEP-04
Time:6 hrs.

Two practicals are to be done selecting one each from two groups carrying
Equal marks each have to be set in the examination

Group A

1. Quantitative Analysis — involving two of the following in Ores, Alloys or mixture in Solution, one by Volumetric and other by Gravimetric methods Ag, Cu, Fe, Cr, Mn, Ni, Zn, Ca, Mg, Cl and SO_4^{2-} .
2. Determination of COD and Hardness of water volumetrically.
3. Preparation of selected Inorganic Complex compounds.
 - i) Cis $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})]$
 - ii) $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
 - iii) $\text{K}[\text{Fe}(\text{C}_2\text{O}_4)_3]$
 - iv) $[\text{Ni}(\text{NH}_3)_4]\text{Cl}_2$
 - v) $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3]$

Group B

4. **Organic Synthesis** One Step organic Synthesis
 - (i) Benzophenone Oxime from Benzophenone
 - (ii) Benzanilide from Benzophenone oxide (Beckmann" Rearrangement)
 - (iii) Phthal imide from Phthalic anhydride
 - (iv) Anthranilic Acid from Phthalimide (Hoffmann reaction)
 - (v) Ortho chloro benzoic acid from Anthranilic acid
(Sandmeyer's reaction)
- Benzil from Benzoin (Oxidation) Dibenzyl from Benzil (Reduction)
- (VI) Phenyl azo 9-naphthol from Aniline @diazo coupling)
- (VII) 1-amino-2-hydroxy naphthalene from Phenyl azo@ naphthol @reduction)

- (viii) Benzylic Acid from Benzil.
- (ix) Fluorescein from Phthalic anhydride.
- (x) m-nitro aniline from m-dinitro benzene (Reduction)
- (xi) Picric acid from phenol (nitration)
- (xii) Cinnamic acid from Benzaldehyde and malonic acid
- (xiii) (Knoevenagel reaction)
- (xiv) Dibenzal acetone from Benzaldehyde (Claisen Schmidt reaction)
- (xv) acetanilide Aom Acetanilide.

Group C

1. Distribution Law

- (a) To determine the partition coefficient of Benzoic acid or acetic acid between Benzene and water.
- (b) To study the complex formation between Cu^{+2} and Ammonia and to determine the formula of the complex.
- (c) To determine the equilibrium constant of the reaction $\text{KI} + \text{I}_2 \rightleftharpoons \text{KI}_3$

2. Chemical Kinetics

- (a) To determine the velocity constant of hydrolysis of methyl acetate catalyzed by HCl by titrimetric method.
- (b) To determine the velocity constant of saponification of Ethyl acetate conductometrically
- (c) To determine the acid catalyzed reaction between I_2 and Acetone

3. Viscosity

- (a) To determine the radius of molecules from viscosity measurement.
- (b) To determine the composition of a liquid mixture Visco metrically.

Viva-Voce	16 marks
Note Book	04 marks
Experiment	50 marks
Internal Assignment	20 marks
Day to day internal Assignment	10 marks

Chemistry
M.Sc. Semester- II
(Skill Development)

Paper-V (A)

Full Marks:70

CHES-05 (A)

Time:3 hrs.

This is a theory-cum –laboratory course with more emphasis on laboratory work.

UNIT-1 Introduction to Computers and Computing

Basic structure and functioning of computers with a PC as an illustrative example, Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data Processing, principles of programming. Algorithms and flow-charts.

UNIT-2 Use of Computer Programmes

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Packages- MS-Word, MS-Excel, FOXPRO, MATLAB.

UNIT 3: Potentiometric analysis

Reversible cells, Types of cells, Liquid – Junction potential, Primary and secondary reference electrodes, measurement of E.M.F., Determination of (i) solubility and solubility product of sparingly soluble salts (ii) pH of a soluble salt. (iii) instability constant of a complex. Potentiometric titrations.

UNIT-4: Spectrophotometric analysis

UV- visible, Lambert-Beer law, use of spectrophotometer in the determination of (a) Percentage composition of a mixture.
(b) Ionisation constant of acid- base indicator (c) Composition of complex (Job's method)

UNIT-5: Conductometric analysis

Conductance, Equivalent conductance, molar conductance, Factor affecting different kinds of conductance of electrolytes. Principle of Conductometric titrations,

Determination of

1. Dissociation constant of weak acid
2. Basicity of weak acid.
3. Hydrolysis constant of salt derived from a weak base and strong acid.

4. Velocity constant of saponification of ethyl acetate.

Books Suggested

1. Comdex Computer Course kit (XP Edition), Vikas Gupta, Dreamtech, New Delhi
2. Fox Pro For DOS & Windows, R.K. Taxali, BPB Publication.
3. Programming in ANSIC, E. Balaguruswamy, Tata McGraw Hill
4. Compute for Chemist Bansal, Pragati Prakashan

Chemistry
M.Sc. Semester- II
(Skill Development)

Paper-V (B)

CHES-05 (B)

Full Marks:70

Time: 3 hr.

UNIT 1 : ENVIRONMENTAL MONITORING

- (a) Monitoring of water quality — Method of Sampling, Principle and procedure of the monitoring BOD, COD, DO, Nitrite, Nitrate, Fluoride and Iron and Total Hardness of water as in water samples.
- (b) Analysis of Soil Samples - Principle and Procedure of the analysis of moisture, salinity, soil colloids, cation and anion exchange capacity.
- (c) Air pollution Monitoring — Sampling, Analysis of air pollutants such as SO₂, NO₂, NO, and suspended particulate matter (SPM).

Unit-2. PRINCIPLE OF ANALYSIS OF FOOD

- (a) Principles and procedures of food analysis: proteins, lipids, and pesticide residues
- (b) the pharmaceutical analysis of Aspirin, Vitamin A, Vitamin B1, and Vitamin G (likely a typo for Vitamin B2, or Riboflavin).
- (c) Clinical Analysis —principles and procedures for the clinical analysis of urea, fructose, albumin, sodium, and potassium, with a specific focus on flame photometry for sodium and potassium analysis.

UNIT- 3 : ANALYSIS OF METALS & MINERALS

- (a) Principles and procedures for the analysis of brass, steel, limestone, and cement.
- (b) Application of UV-visible spectroscopy in qualitative and quantitative analysis
- (c) Electroanalytical techniques: voltammetry, polarography, conductometry, and chromatography.
- (d) Coal — Ultimate and proximate analysis, bleating and values, grading of coals.

UNIT - 4: RISKS & HAZARDS OF CHEMICALS AND PROCEDURES

- (a) Hazards of Handling ordinary chemicals, Fire hazards, Handling corrosive chemicals, Poisons chemicals.

(b) Carcinogens Toxicity of Cd, Pb, Hg, As, Se, Pt, Oxides of Nitrogen & Sulphur, Benzene, halogenated hydrocarbons, Aromatic amino compounds, benzopyrene and related compounds, Plastic Waste Management.

(c) Role of incineration in the production of carcinogens like dioxides,

(d) Treatment of Hazardous waste and its disposal, Radiochemical wastes & technique of safe disposal of them.

UNIT- 5 FUNDAMENTALS OF AGRICULTURAL TOXICOLOGY

Toxicology, poison & poisoning, the toxicity of pesticides, threshold value dose or T.L V. for some common clinical toxic substances and lethal dose, lethal dose, Toxicity indices (LD-50, ED-50 etc.) Penetration of poisonous substances into cell-action on enzymes, Metabolism of poison in organism, Toxicity of pesticides to harmful organism factors determining

References:

1. Environmental Chemistry, S.E. Manahan and Timothy Lewis.
2. Environmental chemistry, A. K. De, New Age International.
3. Environmental pollution Analysis, S. M Khopkar, Wiley Eastern.
4. Environmental Toxicology, Fied, Golden and Sridhar: Science publication.

Chemistry
M.Sc. Semester-II
(Physical Chemistry)

Paper-VI
Full Marks:70

CHEC-06
Time:3 hrs.

UNIT 1: Thermodynamics

A. Classical Thermodynamics: Concept of free energy and entropy. Partial molar volume, Partial Molar entropy and Partial Molar free energy, Chemical potential. Effect of pressure and temperature, Chemical potential, Determination of Partial molar quantities by Graphical method and method of intercepts. Fugacity, change of fugacity with temperature and pressure, calculation of fugacity (a) by graphical method (b) through Poynting factor and (c) from equation of state.

B. Non-ideal systems:

Activity and activity co-efficient, Debye Huckel Theory for activity coefficient of electrolytic solutions, determination of activity co-efficient, Ionic strength.

UNIT 2: Statistical Mechanics:

Stirling's approximation and Derivation of Boltzmann distribution laws, partition function and its Physical significance, relation between partition function and their molar quantities e.g. Internal energy, Entropy, Work function, Gibbs energy and Heat capacity. Statistical formulation of Third law of Thermodynamics, Derivation of relation between entropy and thermodynamics probability ($S = k \ln w$) and Residual entropy. Translational Partition function for a monoatomic Ideal gas, Entropy and translational Partition function (Sackur Tetrode equation), Partition Function for Rotational and Vibrational energy.

UNIT 3: Chemical Kinetics

Kinetics of Reversible First and second order reactions, kinetics of sequential first order reaction and parallel reactions. Derivation of Arrhenius equation, Activation energy and its experimental determinations, Frequency factor, Collision theory of reaction. or collision theory, transition state theory) strength of the reaction rates – Primary and secondary salt effects.

The stationary State (steady state) steady-state approximation) in chemical kinetics — Hydrogen — Bromine reaction, Decomposition of ethane and ethanal. Kinetics of Photochemical Reactions-Hydrogen Chlorine and Hydrogen — Bromine reactions, oscillatory reactions — Belsusov- Zhabotinsky (BZ) reaction), Enzyme catalysts, kinetics of enzyme catalysis — Michaelis — Menten equation and Its importance

UNIT 4: Electrochemistry;

Huckel limiting Law of activity coefficient, verification and limitations of Debye-Huckel theory and its extension

Inake allowance for finite size and ionic ascciatfcn parameter

Measurement of activity co-efficient by solubility, freezing point depression and E.M.f methods, Effect of ion- solvent interaction on activity co-efficient of ions (Robinson stroke treatment). Overpotential,

Exchange current density, Derivation of Butler-Volmer equation and Tafel plot.

Unit 5 Surface Chemistry

5(a) Derivation of Gibbs adsorption Equation, Surface film, Langmuir Theory of Adsorption. Derivation of the BET equation and Estimation of surface area. Thermodynamics & statistical Mechanics of Adsorption. Chemical Reaction of Surface- Unimolecular reactions, Bimolecular reactions and Langmuir – Hinshelwood mechanism, Langmuir – ideal mechanism.

5(b) : Laws of Photochemistry, Quantum yield, Reasons for high and low quantum yield Photolysis of HI and its kinetics, fluorescence, Phosphorescence, Chemical reactions and their quantum yields, Photosensitization, Photosynthesis, Photo stationary state, Chemiluminescence and Thermoluminescence, Photography, Photochemical cells, The Carbon monoxide oxygen Reaction, Kinetics of collisional quenching – Stern- Volmer equation and deviation from stern- Volmer equation and deviation from stern- Volmer equation, E- type P-type delayed fluorescence.

BOOK SUGGESTED:

1. Physical Chemistry — P.W. Atkins, ELBS.
2. A. Text Book of Physical Chemistry — S. Glasstone, McMillan.
3. Physical Chemistry Alberty and Daniels.
4. Chemical kinetics — K.J. hardier, 1\le Grow Hill.

5. Modern Electro Chemistry Vol.-I & Vol.-II — JOM Bockris A AKN Reddy, Plenum.
6. Mathematics for Chemistry — Doggett and Sutcliffe, Langman.
7. Basic Mathematics for Chemists
8. Physical Chemistry A. molecular Approach, McQuarrie and J.D Simon; Viva Books Pvt. Lid.

Chemistry M.Sc.
Semester-II
(Theoretical Chemistry)

Paper-VII
Full Marks:70

CHEC-07
Time:3 hrs.

UNIT - 1 Quantum Mechanical Results:

Solution and discussion of the Schrodinger equation to some model systems viz. Particle in three-dimensional box, Particle on a ring, The harmonic oscillator, The rigid rotor, The hydrogen atom, simple and generalized treatment.

UNIT - 2 Approximate Methods:

First order time independent Perturbation theory for non-degenerate states. The variation theory, Application of variational methods perturbation theory to helium atom.

UNIT- 3 Huckel Molecular orbital Theory

Huckel theory of conjugated systems, application of HMO to Ethene, 1, 3-butadiene, and Cyclic polyenes radical. Bond order and charge density cations.

UNIT-4 Microwave spectroscopy

Classification of molecules, Rotational energy levels, Isotope effect in Rotational spectra, Intensity of rotational lines, Non-rigid rotator, vibrational Excitation! Effect, Symmetric Top molecules, A symmetric top molecules, Stark effect, Information derived from Rotational spectra.

UNIT — 5(a) Infra-red spectroscopy

Vibrational Energy of a diatomic molecule, zero point energy, force constant, Anharmonicity, Morse potential energy diagram, Vibration—rotation spectroscopy, P, Q, R Branches, Vibrations of poly atomic molecules, normal modes of vibration, overtones, factors affecting the band positions and, intensity.

UNIT - 5(b) Raman Spectroscopy

Classical and quantum theories of Raman Spectrum,, 'Rotational Raman Spectra Linear molecules, Symmetric Top molecules, Vibrational Raman Spectra, Pauli Exclusion Principle.

BOOKS SUGGESTED:

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1. Modern Spectroscopy by J. Michael Hollas (John Wiley & Sons)
2. Introduction to Molecular spectroscopy, G.M. Barro
3. Molecular structure & spectroscopy, O. Aruldas, P
4. Modern Molecular Spectroscopy, H S Randhawa McMillan.
5. Introduction to Quantum Chemistry by A.K. Chandra and Lata (Tata McGraw Hill)
6. Quantum Chemistry by Ira N. Levine (PHI Learning)

**Chemistry M.Sc.
Semester-II
(Practical)**

**Paper-VIII
Full Marks:70**

**CHEP-08
Time:6 hrs.**

Two practicals selecting one from each of the two groups carrying 25 marks each have to be set in the examination.

Group A

1. Qualitative Analysis of mixture containing 8 radicals including some less common metal ions and interfering radicals from among the following by common method (Preferably Semi Micro)

The basic radicals to be identified are:

Pb, Cu, Cd, Bi, Sn, Fe, Al, Cr, Zn, In, Co, Ni, Ba, Sr, Ca, Li, Na, K, NH₄.

Acid radicals

Carbonate, Sulphate, Sulphite, Nitrite, Acetate, Fluoride, Chloride, Bromide, Iodide, Nitrate, Borate, Oxalate, Phosphate, Silicate, Chromate, Arsenite, Arsenate, Permanganate.

Group B

2. Estimate of Glycine
3. Estimate of Glucose
4. Determination of saponification value of given oil/ fat.
5. Estimation of Phenol
6. Estimation of Hydroxyl groups
7. Determination of equivalent wt of carboxylic acid by Titration method.
8. Determination N-acetyl group in organic compound.

Group C

Conductometry

9. Determination of the velocity constant, order of reaction and of activation of Saponification of Ethyl acetate by NaOH conductometrically
10. Determination of solubility and solubility product of sparingly soluble salts. (e.g. PbSO₄, BaSO₄, etc.) conductometrically.

11. To study the effect of solvent on the conductance of AgNO_3 Acetic Acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixture (DMSO, DMF, Dioxane, aceton, water) and to test the Validity of Debye — Onsager 'equation.
12. Determination of the activity coefficient of Zn^{2+} in a 0.02 M ZnSO_4 solution using potentiometry and the Debye-Hückel limiting law
- Potentiometry/pH Metry**
13. Acid — Base titration' in a non-aqueous medium using pH meter.
14. Determination of strength of strong and weak acids in a mixture using potentiometry/pH meter and Abbe's refractometer
15. Determination of refractive index and molecular refractivity of a liquid.

Viva-Voce	16 marks
Note Book	04 marks
Experiments	50 marks
Internal Assignment	20 marks
Day to day Internal Assignment	10 marks

Chemistry M.Sc.
Semester-III
(Choice based Elective)

Paper-IX (A)
Full Marks:70

CHE-A-09 (A)
Time:3 hrs.

METAL-LIGAND EQUILIBRIUM IN SOLUTION AND INORGANIC REACTION MECHANISM

UNIT 1 : Stability of complexes in aqueous solution

Stability of complexes, Stepwise and overall stability constants and their relationship, Kinetic versus thermodynamic stability, Trends in stepwise formation constants, Factors affecting stability of complexes, Chelate effect and its thermodynamic origin, Experimental methods for the determination of stability constant and composition of complexes by spectrophotometric method, Job's method & Bjerrum method.

UNIT 2: Ligand substitution reactions in octahedral complexes

Reactivity of metal complexes, Inert and labile complexes, Valence bond and crystal field interpretation of lability and inertness of the complexes, Rate laws and their interpretation The Eigen Wilkins mechanism & Fuoss Eigen equation, The activation of octahedral complexes, Mechanism of ligand substitution reactions in octahedral complexes, Hydrolysis reaction acid hydrolysis (SN1 mechanism), base hydrolysis (SNLCB mechanism) Evidences in favour of SN1CB mechanism.

UNIT 3: Ligand substitution reactions

The trans effect, theories of trans effect, Difference between trans effect and trans influence, Trans effect series, Mechanism of ligand substitution reactions in square planar complexes, Factors affecting the rate ligand substitution reactions in square planar complexes, Applications of trans effect.

UNIT 4 : Electron transfer-reactions

Basic concepts of oxidation and reduction, reactions, Electron transfer reactions in coordination compounds by outer sphere and inner sphere mechanisms, The marcus theory and

the factors affecting the rate of electron transfer reactions by outer sphere mechanism, complementary and non-complementary electron transfer reactions.

UNIT 5 : Photochemical reactions

Basic concepts of photochemistry, Photochemical and thermal excitation of complexes of complexes and fates of excited complexes, Photochemical reactions of cobalt (III) and chromium (III) complexes, photo-oxidation, Photo reduction, intervalence transitions.

BOOKS SUGGESTED:

1. Elements of Inorganic Photochemistry (W.J. Ferraudi, Wiley)
2. Inorganic Chemistry, Shriver and Atkins, Oxford University, Press
3. Concepts of Inorganic Photochemistry, A.W. Adamson (Adamson & Fleischauer, Wiley)
4. selected Topics in Inorganic Chemistry, Madan, Malik & Tuli, S. Chand

Chemistry M.Sc.
Semester-III
(Choice based Elective)

Paper-IX (B)
Full Marks:70

CHE-A-09 (B)
Time:3 hrs.

UNIT-1 Selectivity

Types of selectivity Regio, Stereo and Chemoselectivity, Reagents for reduction of alkenes, alkynes, arenes and carbonyl compounds, mechanism of action dissolving metal reduction, Removal of functional groups, reduction of benzene rings and alkynes, Protection of aldehydes, ketones, alcohols and amines, carrying out reaction at less reactive group in the presence of more reactive group. Reagents for chemo selective oxidation of (a) C-C double bonds e.g. peracids, osmium tetroxide, ozone etc. and (b) alcohols and carbonyl compounds e.g. Cr(VI) and Mn(VII) compounds Peptide synthesis The Cbz protection group and removal, t-Boc protection group and removal, and the Fmoc protection and removal - Merrifield approach.

Unit-2 Making new C-C bond

- a. Alkylation of nitroalkanes, alkyl nitriles, Lithium enolates of carbonyl compounds such as ketones, esters, and carboxylic acids. Alkylation of aldehydes and ketones using specific enol equivalents such as enamines (Stork enamine reaction), silyl enol ethers, azaenolates derived from imines. Regioselective formation of enolates from ketones, thermodynamic enolates and kinetic enolates alkylation of β -dicarbonyl compounds. Regioselective reduction of enones; formation of enolates regiospecifically, conjugate addition to enones to give enolates regiospecifically

b. Acylation at Carbon

Directed C-acylation of enols and enolates, Acylation of enols under acidic conditions, acylation at nucleophilic carbon (other than enols and enolates)

c. Conjugate addition of enolates -

Conjugate addition (i) Under thermodynamic control (ii) Under kinetic control condition, Conjugate addition of (i) enols (ii) enolates (iii) enamines (iv) silyl enol ethers : Electrophilic alkenes exo-methylene ketones a component obtained from Mannich reaction, nitroalkanes, Robinson's annulation reaction, Use of Lithium dimethyl cuprate.

- d. Carbon bond formation using radicals, Tributyltinhydride, nucleophilic and electrocyclic radical, Comparison of reactivity pattern of radicals and polar reagents, Comparison between Intermolecular and Intra molecular radical reactions, Barton and Hoffmann — Löffler — Freytag reaction.

Unit -3 The Aldol reaction

Introduction, acid and base catalysed reactions, Aldol reaction of unsymmetrical ketones, crossed condensation Conditions of successful crossed aldol reaction. Controlling aldol reactions with specific enol equivalents; use of following enolates in aldol reactions lithium enolates, silylenol ethers, zinc enolates, aza enolates, enamines; use of conjugated Wittig reagents as specific enol equivalents in aldol reaction. Specific enol equivalent for (a) carboxylic acid derivatives, (b) free carboxylic acids, (c) aldehydes and (d) ketones preparation of (i) kinetic and (ii) thermodynamic enolates. Intramolecular aldol reaction, Overview of equilibrium and directed aldol methods.

Unit -4 Creative Chemistry

Retrosynthetic analysis, Synthons, classification of synthons, Different terminologies, Umpolung reactions, Disconnections Guidelines for good disconnections, Functional group interconversions, C-C disconnection, Two group C-C disconnection :- 1,3 difunctionalized compounds, 1,2 difunctional compounds, 1,4 difunctional compounds.

Synthesis of (i) Penicillin (V) and Ceftriaxone with emphasis on retrosynthetic analysis. (ii) Ibuprofen — emphasis on stereocontrol of the synthesis.

UNIT - 5

Synthesis using reagents containing Phosphorous, Sulfur or boron.

1. Phosphorous containing reagents:

Reactions of phosphorous ylides; Reductive cyclization of nitro compounds;

Synthesis of alkenes from 1, 2 diols, Conversion of alcohols into aldehydes.

2. Sulfur containing reagents:

Reactions of sulfur ylides, sulfoxide elimination, use of dithioacetals, reversed polarity of carbonyl compounds, Julia reaction.

3. Boron containing reagents:

Reactions of organoboranes from alkenes: Oxidation to alcohols, conversion into primary amines, carbonylation — synthesis of 1° and 3° alcohols, Ketones and aldehydes.

Cyanidation and synthesis of esters. Reactions of organoboranes from alkynes; Synthesis of ketones and aldehydes, synthesis of E and Z alkenes, Synthesis of conjugated dienes and synthesis of bromoalkenes.

BOOKS SUGGESTED:

- (1) Organic chemistry : Clayden, Greeves, Warren and Wothers Oxford university Press
- (2) Organic Synthesis : R.O.C. Norman & Coxan
- (3) Modern methods of organic synthesis W. Camither

**M.Sc.
Chemistry
Semester-III
(Choice Based Elective)**

**Paper-IX (C)
Full Marks:70**

**CHE-A-09 (C)
Time:3 hrs.**

UNIT 1 Band Theory & Electronic Properties

Band theory of solids, conductor, Insulator and Semi-conductor, Propagation of Broglie waves in solids, Brillouin Zones, Distribution of density of states.

Semi-conductors: Intrinsic semi-conductors, Number of electrons in a conduction Band, Extrinsic Semi-conductor, The p-n junction, The p-n junction as a rectifier, super-conductors, Photoelectric Effect, Thermocouples, The Hall effect.

UNIT 2 Organic Solids

Electrically conducting organic solids, organic metals — conjugated systems — Doped poly acetylene, Polyparaphenylene, poly pyrrole, organic charge transfer complexes — New Superconductors.

UNIT 3 Phase Transitions

Thermodynamic classification of Phase transitions, Applications of G — T diagram; Stable phases and instable phases, kinetics of Phase transitions, critical size of nuclei, Rate equations — Nucleation Rate, overall transformation rate — Avrami equation, Factors that influence the kinetics of Phase transitions, order — disorder transitions.

UNIT 4 Properties of Insulators

Electrical Properties — Dielectric Properties, polarization density and electric susceptibility, Lorentz force and field, Clausius Mossoni equation, piezoelectricity, Ferroelectricity, Ionic conductivity and ionic diffusion, Electric breakdown, magnetic properties: Antiferromagnetism, Curie Temperature, ferrimagnetism and magnetic resonance.

UNIT 5 Crystal defect and Reciprocal lattice

Crystal defects - Point, line and plane defects, Schottky defect, Frenkel defect, Thermodynamics of Schottky and Frenkel defect, formation of colour centres.

Reciprocal lattice: reciprocal lattice and its properties, Bragg's equation in reciprocal lattice

UNIT-6

Specific Heat of Solid, Einstein theory of specific heat and its limitation, Debye Continuous model-Debye T^3 law. Deviation from the Debye Theory

BOOKS SUGGESTED:

1. Physical Chemistry — R.A. Alberty Wiley Eastern Ltd.
2. Solid State Chemistry and Its Applications, Anthony R. West
3. Introduction to Solids by Leonid V. Azaroff, Tata McGraw-Hill (TMH)
4. Physical Chemistry by Gordon M. Barrow, Tata McGraw-Hill (TMH)

M.Sc
Chemistry
Semester-III
(Inorganic Chemistry)

Paper- X
Full: 70

CHEC- 10
Time: 3 hrs

UNIT 1:

Chemistry of main group elements, Synthesis, properties and structure of Boranes, Carboranes, Borazines, Silicates, Silicones Phosphazenes and S-N ring & chain compounds.

UNIT-2;

Crystal field theory splitting of d orbitals in low symmetry, environments (square planar, square pyramidal & trigonal bipyramidal fields), structural effects of orbital splitting, Jahn-Teller effect and its implications, thermodynamic effects, crystal field stabilization energies for octahedral and tetrahedral complexes, correlation of CFSE with related thermodynamic properties such as lattice energies, enthalpy of hydration, stabilization of unusual oxidation states, CFSE and structure of spinels.

UNIT-3:

Limitations of crystal field theory, evidences in favour of M-L orbital overlap Nephelauxetic effect, Molecular orbital theory, Molecular orbital diagram of tetrahedral and octahedral complexes with and without bonding, Studies of spectral properties transition metal complexes, splitting of terms of d' and d' ions in octahedral, tetrahedral and square planar fields, Orgel diagram, Tanabe-Sugano diagram, Racah parameters and their calculation,

UNIT 4:

Complexes with acceptor ligands, Metal carbonyls-mononuclear, binuclear, trinuclear & polynuclear carbonyls and their preparation, properties, structure, bonding & applications, Reactions of coordinated CO Metal nitrosyls-preparation, reactions, bonding & structure, Reactions of coordinated NO. Dinitrogen and dioxygen complexes

UNIT — .5:

Metal metal bonding and intermetal cluster compounds : M-M multiple bonds, Factors favouring the formation of M-M bond, Evidences in support of M-M bond, Metal Clusters-

classification-dinuclear clusters, trinuclear clusters, tetranuclear clusters & trinuclear cluster,
Synthesis and important reactions of metal clusters

Book recommended

1. Advanced Inorganic Chemistry by F. Albert Cotton and Geoffrey Wilkinson,
by John Wiley & Sons
2. Inorganic Chemistry: Principles of Structure and Reactivity by James E.
Huheey, Ellen A. Keiter, and Richard L. Keiter, by HarperCollins College
Publishers
3. Modern Inorganic Chemistry, William L. Jolly, published by McGraw-Hill

M.Sc.
Chemistry
Semester-III
(Organic Chemistry)

Paper-XI
Marks:70

CHEC- 11 Full
Time:3 hrs.

UNIT — 1: PHOTOCHEMISTRY :

1. Basic concepts, Electronic transitions, Jablonski diagram, Intersystem crossing, Energy transfer, Molecular orbital view of excitation.
2. Photochemistry of Alkenes: Intermolecular reactions of olefinic bond, geometrical isomerism, cyclisation reactions, rearrangement of (1,4) — and (1,5) — dienes, di - methane rearrangement.
3. Photochemistry of Carbonyl : Compounds : Iner-molecular reactions of Carbonyl Compounds, saturated cyclic and acyclic, α , β unsaturated and α , γ unsaturated compounds, cyclohexadienone Intermolecular cycloaddition reactions, Dimerization and oxetane formation.
4. Photochemistry of Aromatic compounds : Isomerization, Additions, substitutions.
5. Miscellaneous Photochemical reactions : Photo Fries reactions of anilldes, Photo Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions, Photochemistry of vision.

UNIT — 2: PERICYCLIC REACTIONS :

Molecular orbital symmetry, Frontier orbital of ethylene, 1, 3 —butadiene, 1,3,5- hexatriene and allyl system. Classification of Pericyclic reactions. Woodward — Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions, Conrotatory motions, $4n$, $4n+2$ and allyl systems, (2+2) addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangement suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, (3,3) and (5,5) Sigmatropic rearrangements. Claisen, Cope and aza-cope rearrangement. Fluxional tautomerism, Ene reaction.

UNIT — 3: SPECTROSCOPY — APPLICATIONS IN ORGANIC CHEMISTRY :

1. UV-VIS Spectroscopy : Electronic transitions of Enes, enones and arenes. Woodward-Fieser rules. Effect of solvent polarity on UV absorption, Application of Woodward-Fieser rule for calculating absorption maxima in cyclic and acyclic conjugated dienes

and enones. Problems based on the above rules. Carbonyl chromophores, Steric hindrance and coplanarity — distinction between cis and trans isomers.

2. FTIR Spectroscopy: Vibration-rotation spectrum Theory of molecular vibrations, stretching, bending vibrations. Hydrogen bond and efficiency distinction between inter and intramolecular hydrogen bonding. Finger print region. Characteristic group frequencies of OH group in alcohols and phenols, CO group in aldehydes, ketones, acid chlorides, acid anhydrides, amides and esters. Simple problems based on these data.
3. NMR Spectroscopy: Chemical shift, anisotropic effect and coupling constants in organic compounds. Spin-spin interactions in typical systems. Effect of magnetic field strength on sensitivity and resolution. Karplus relationship of J on dihedral angle. C^{13} chemical shifts. Spectral interpretation and structure identification. Solving of structural problems on the basis of numerical and spectrum-based data.
4. Mass Spectroscopy: Fragmentation pattern, molecular ion peak, metastable peak, McLafferty rearrangement, Examples of mass spectral fragments of organic compounds Solving of Structural problems
5. Combined applications of UV-Visible, IR, NMR and Mass spectroscopy in structure determination of organic compounds.

BOOKS SUGGESTED:

1. W. Kemp, "Organic Spectroscopy", Longman.
2. Jerry March, "Advance Organic Chemistry"
3. Organic Spectroscopy by Y.R. Sharma
4. Introduction to Organic Spectroscopy, Silverstein
5. Fundamentals of Photochemistry by K.K. Rohatgi Mukherjee
6. Organic Chemistry by Cleyden, Oxford University Press
7. Organic Reaction & Mechanism by Singh & Mukherjee
8. Pericyclic & Photochemistry-Yadav Singh
9. Spectroscopy Kalsi, Pragati Prakashan
10. Conservation of Orbital Symmetry Woodward & Hoffman.

M.Sc.
Chemistry
Semester-III
(Practical)

Paper-XII
Full Marks:70

CHEP- 12
Time:06hrs.

Two practicals selecting one from two groups carrying 25 marks each have to be set in the examination.

Group A

1. Determination of standard deviation and correlation coefficient.
2. Plotting of graph by least square method.
3. Quantitative calculation based on Beer's law.
4. Analysis of Dolomite, Pyrolusite and Haematite.

Group B

5. Identification of organic compounds containing not more than two functional groups, (Ten compounds are to be identified in the lab work.)

Group C

6. To determine the equivalent conductance of an electrolyte at infinite dilution and determine the dissociation constant.
7. To determine the pK_a of given dibasic and tribasic acids pH incrementally.
8. To determine the pH of various mixtures of acetic acid and Na- acetate in aqueous solutions and hence the dissociation constant of the acid.

9. Titrate ferrous ammonium sulphate against $\text{K}_2\text{Cr}_2\text{O}_7$ / KMnO_4 , and determine redox potential of $\text{Fe}^{2+} / \text{Fe}^{3+}$ system potentiometrically
10. To determine ionization constant of polybasic acid potentiometrically.

Viva - voce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

**M.Sc.
Chemistry
Semester-IV
(ELECTIVE-1)**

**Paper-XIII(A)
Full Marks:70**

**CHEP- 13(A)
Time:03 hrs.**

Organometallic and Bioinorganic Chemistry

UNIT 1: Alkyls and Aryls of transition metals

Stability of transition metal alkyls, classification of σ -bonded hydrocarbyls, general methods of preparation, general characteristics, structure and bonding organocopper compounds.

UNIT 2: Transition metal - π complexes,

Transition metal π complexes with unsaturated organic molecules /group alkenes, alkynes, allyl, dienes, dienyl, trienyl, arenes-synthesis, nature of bonding and structural features, Important reactions, relating to nucleophilic and electrophilic attack on coordinated ligand.

UNIT 3: Reactions of organometallic compounds

Substitution reactions of carbonyl complexes, Oxidative addition reaction, Reductive elimination reaction, Insertion reaction and Deinsertion reaction.

UNIT 4: Catalysis by organometallic compounds

General features of catalysis, Types of catalysis, Catalytic steps, Hydrogenation of alkenes (Wilkinson's catalyst), Hydroformylation of alkenes, Ziegler-Natta polymerization of alkenes, Wacker process, Monsanto acetic acid synthesis, Water gas shift reaction, Fischer-Tropsch synthesis. Hydrosilylation, Activation of C-H bond.

UNIT5(a)Metal ions in biological systems

Role of alkali and alkaline earth metals in biological systems, -potassium pump, Active transport of cations across the membrane Transport and storage of dioxygen Haeme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin and haemocyanin. Electron transfer in biological systems Structure and function of

metalloproteins, Vitamin B₁₂ and mechanism of electron transfer in ferredoxin and cytochrome.

UNIT T5 (b) Metals in medicines

Metal deficiency and disease, Toxic effect metals, Metal complexes in chemotherapy as drugs and anticancer agents.

BOOKS SUGGESTED:

1. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International Publishers
2. Organometallic Compounds, I. Kumar, Pragati Prakashan
3. Principles of Bioinorganic Chemistry, S.J. Lippard, J.M. Berg
Unkv. Science Books

**M.Sc.
Chemistry
Semester-IV
(ELECTIVE-1)**

**Paper-XIII(B)
Full Marks:70**

**CHEP- 13(B)
Time:03 hrs.**

Unit 1: Stereochemistry

- (A) Stereospecific and stereoselective reactions Definition and examples.
- (B) Review of the stereochemical aspects of SN_1 , SN_2 , SN_i (Mitsunobu reaction) E_1 , E_2 , E_{1cB} , and neighbouring group participation reactions. Role of stereochemistry in rearrangement reactions, Tiffeneau Demjanov rearrangement, Bayer Villiger rearrangement and Beckmann rearrangement and Favorskii Rearrangement.
- (C) Conformational analysis of cyclohexanes and decalins including their reactivities of the axially and equatorially substituted conformers.
- (D) Conformations of saturated heterocycles. The anomeric effect and the double anomeric effect, stability of 2-substituted pyrones.

Unit 2: Fragmentation reaction:

Definition, Factors affecting fragmentation Polarization of C-C bond, electron push and pull, Stereochemical requirement. Fragmentation of (a) Three (b) Four (c) six membered rings, Ring expansion by fragmentation -Eschenmoser fragmentation; Beckmann fragmentation

Unit 3: Asymmetric Synthesis:

Definition, Different methods of asymmetric Synthesis Resolution, Chiral pool, Chiral auxiliary, Chiral reagent and Chiral catalyst CBS reagent, Sharpless asymmetric epoxidation, Sharpless asymmetric dihydroxylation; Baker's yeast.

Unit 4: Synthesis of single geometrical isomers of double bonds:

- a. Stereoselective formation of olefins: The Julia olefination, Stereoselectivity of olefination through E , E_2 and E_{1cB} mechanism, Wittig reaction, E selective and Z selective Wittig reaction, Transformation of alkynes to Z and E selective alkenes, Synthesis of Z and E selective enolates.
- b. Stereospecific formation of olefins: E_1 , E_2 elimination-Formation of Cis substituted alkenes, The Peterson reaction. Formation by fragmentation of cyclic compounds.

Unit-5 (a) Stereoselective reaction of cyclic systems

Stereoselective reactions on (a) Four (b) Five (c) Six membered rings with (i) one trigonal carbon (ii) two or more trigonal carbons (e) bicyclic Fused, bridged and spiral systems (f) more hindered face - (i) tetrahedral nucleophilic (ii) cyclic transition state mediated approach.

Unit 5(b)

- (A) Stereospecific alkene transformations: (a) Bromination (b) Iodolactonization (c) Epoxidation (d) cis -1, 2 diol and (e) trans 1,2-diol formation (f) hydroboration.
- (B) Stereoselective chiral alkene transformations: (a) epoxidation of chiral alkene (b) alkylation of chiral enolates Explanation by the Houk model.
- (C) Stereoselective addition of carbonyl group with adjacent stereogenic centre, Cram's rule, Felkin Anh model, Effect of electronegative atoms and chelation on stereoselectivity.

BOOKS SUGGESTED:

1. Principle of Organic Synthesis — Norman & Coxan
2. Organic synthesis — M.B. Smith
3. Organic Chemistry — I.L. Finar Vol.-2
4. Organic Chemistry — Clayden, Greeves, Warren and Wothers
5. Organic synthesis The disconnection approach S. Warren

**M.Sc.
Chemistry
Semester-IV
(Advanced Quantum Chemistry, Elective - I)**

**Paper- XIII (C)
Full Marks:70**

**CHEE-13 (C)
Time:3 hrs.**

UNIT 1 Energy of Molecules & Wave Functions

The hydrogen molecule ion, Evaluation of U and $9J^2$. Electronic Energy of molecules, Hybrid orbitals — Combination of 1s and one 2p orbital, Combination of 2s and two 2p orbitals, combination of one 2s and three 2p orbitals.

UNIT-2 Hartree Fock Theory

Born Oppenheimer Approximation, Frank Condon Rules. Hartree-Fock Equation. Koopman's Theorem and Roothaan's Equation.

UNIT 3 Semi Empirical Theories

Application of HMO Theory to Benzene. Heteronuclear conjugated systems Pyrrole and Pyridine. Extended Huckel theory. The pariser Parrpople (PPP) method and its treatment to Ethene and Butadiene

UNIT 4 Density Functional Theory

Hohenberg Kohn Theorems. Kohn-sham Equations Density functional theory and its applications.

UNIT 5 Scattering Theory

Scattering Cross — section, Scattering length, Low energy scattering Theory, charged particle scattering and coulomb wave function,

Resonance scattering Breit-wigner Formula, Levinson's Theorem.

Application of Scattering theory in (a) square well potential, (b) Bound States (c) Resonance (d) Proton — Proton Scattering.

BOOKS SUGGESTED:

1. Quantum Chemistry, T. Veszpremi and M. Feher, Springer.
2. Quantum Chemistry, J.P. Lowe and K.A. Peterson.
3. Elementary Quantum Chemistry, F.A.Pilas, McGraw Hill International Editions.
4. Quantum Chemistry, D.A. Mc Quarrie, Viva Books Pvt. Ltd.
5. Quantum Chemistry, M.R. Awode, S. Chand & Company Ltd.

**M.Sc.
Chemistry
Semester-IV
(Elective -I I)**

**Paper- XIV (A)
Full Marks:70**

**CHEE-14 (A)
Time:3 hrs.**

UNIT 1: Application IR spectroscopy in the elucidation of structure of metal carbonyls, nitrosyls & dinitrogen complexes and complexes with ambidentate ligands such as NO_2 , SCN , CN , etc.

UNIT 2: Study of the spectral properties of metal complexes, Splitting of terms of d^1 and d^2 ions in (i) octahedral (ii) tetrahedral and (iii) square planar crystal fields. Orgel diagram, Tanabe-Sugano diagram, Selection rules for electronic transitions, Racah parameters and their calculation, Charge transfer spectra.

UNIT 3: ESR spectroscopy Basic principle, Presentation of spectrum. Hyperfine splitting in some simple systems, g- value, Zero field splitting, Kramer degeneracy, Simple applications ESR spectroscopy.

UNIT 4 : Application of ^1H , ^{19}F , ^{13}C and ^{31}P NMR spectroscopy in the elucidation structure of inorganic molecules/ions.

UNIT 5: Mossbauer spectroscopy Basic principle, Instrumentation, Spectral parameters isomer shift, quadrupole splitting, magnetic hyperfine interaction, Applications (i) oxidation states of metals in their compounds (ii) structure determination (iii) nature of chemical bonding in Prussian blue / Prussiates (iv) covalently bonded molecules (v) magnetically ordered compounds.

BOOKS SUGGESTED:

1. Physical methods in Inorganic Chemistry, R.S. Drago
2. IR Raman Spectroscopy of Inorganic & Coordination compounds, K. Nakamoto John Wiley & Sons
3. Electronic Spectroscopy, A.B.P. Lever, Oxford University Press
4. Instrumental methods, Willard, Merritt and Dean, East-West Press
5. Molecular Spectroscopy, C.N. Banwell, TMH

**M.Sc.
Chemistry
Semester-IV
(Elective -I I)**

**Paper- XIV (B)
Full Marks:70**

**CHEE-14 (B)
Time:3 hrs.**

Unit 1: Special Techniques of organic synthesis:

Polymer supported reagents and synthesis introduction properties of polymer support, advantages of polymer supported reagents, choice of polymer, Classification of reactions involving polymers. Synthesis of peptides, solid state Edman degradation, Asymmetric synthesis of aerotactic acid Example of increased stereoselectivity; use of Ploy-N-Bromo succinimide, polystyrene carbodiimide in organic synthesis, use of Polymer supported photosensitizer and polymer supported phase transfer catalysts and crown ethers.

Unit 2: Microwave induced organic synthesis:

Introduction, microwave oven, reaction, vessel, reaction medium, advantages, limitations, precautions, applications: Synthesis of chalcones (use of solvent), enaminketones (support catalysis), Knoevenagel reaction (without solvent).

Unit 3: Sonochemistry: The use of ultrasound in organic synthesis:

Introduction, instrumentation physical aspects, types of sonochemical reactions, homogenous reactions, heterogeneous liquid-liquid reactions, heterogeneous solid-liquid reactions, synthetic applications.

Unit 4: Phase-transfer catalyst:

Introduction, factors affecting use of PTC, mechanism of PTC reactions types of PTC, advantages, types of phase transfer catalyzed reactions, preparation of phase transfer catalyst, important applications of PTC in organic synthesis.

Units(a) Carbocyclic ring synthesis:

- i. Three membered rings, use of carbene intermediates -Simmon smith reaction, use of diazoketone.
- ii. Four membered rings : Photochemical (2+2) cycloaddition regioselectivity, synthesis of ionic reactions, expansion of three membered ring, use of ketenes.
- iii. Five membered rings: From 4 dicarbonyl compounds, from 1, 6 dicarbonyl compounds, Pericyclic rearrangement dienone to cyclopentenone, vinyl cyclopropane to cyclopentene rearrangement. Synthesis via intramolecular radical intermediates cyclization.

iv. Six membered rings: carbonyl condensations, Robinson annelation, Diels Alder reactions, partial / total reduction of aromatic compounds.

V. Large rings:-

- a) Intramolecular cyclization of dinitriles Ziegler's method.
- b) Intramolecular cyclization of diketenes: Blomquist method
- c) Acyloin Synthesis.

Unit 5(b) Heterocyclic synthesis:

(A) Synthesis of saturated Heterocycles:-

Introduction case of ring closure, Baldwin's rules for ring closure Retrosynthetic analysis.

Synthesis of three membered rings, four membered rings - ionic and pericyclic pathway.

BOOKS SUGGESTED:

1. Advanced Organic Chemistry: Part B – Reactions and Synthesis by Francis A. Carey & Richard J. Sundberg
2. Organic Synthesis: Special Techniques by V.K. Ahluwalia & Renu Aggarwal; Narosa Publishing House (Indian Author)
3. Sonochemistry: Theory, Applications and Uses of Ultrasound in Chemistry by T.J. Mason; Ellis Horwood / Wiley
4. Green Chemistry and Engineering by Mukesh Doble & Anil Kumar Kruthiventi (Indian Context); Academic Press / Elsevier

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**M.Sc.
Chemistry
Semester-IV**

(Molecular Dynamics, Elective-II)

Paper- XIV (C)

Full Marks:70

CHEE-14 (C)

Time:3 hrs.

UNIT 1: INTRODUCTION TO MOLECULAR REACTION DYNAMICS

Dynamics of reaction, mechanism of activation, concept and shape of potential energy surfaces, rate of reaction on theoretical Potential energy surfaces, determination of position and properties of the transition state on the surfaces, Dynamic calculation Vs Transition state theory.

UNIT 2: KINETICS OF CONDENSED PHASE REACTION

Factors determining reaction rate in solution, diffusion controlled reactions and activation controlled reactions, collision on solution encounter, Transition state theory in solution, kinetics of ionic reactions, Single and double spherical model, kinetics of dipole-dipole reaction, ion-dipole reactions, Dependence of rate constant on ionic strength and dielectric constant of the medium, Bronsted - Bjerrum equation.

UNIT 3: CATALYSIS AND OSCILLATORY BEHAVIOUR

General mechanism and kinetics of catalytic reactions, Arrhenius intermediates, Vant Hoff intermediates, Theory of acid-base catalysis, Effect of salt on acid-base catalysis, Bronsted Catalysis law, linear free energy relationship, Hammett equation, Oscillatory reactions, Lotka-Volterra model, B-Z reactions and its mechanism.

UNIT 4: STUDY OF FAST REACTIONS

Flash photolysis, relaxation technique, NMR method, Molecular beam and shock tube kinetics, stop flow method, Isomerisation, Photo dissociation and recombination reactions.

UNIT 5: KINETICS OF ELECTRODE REACTIONS

Faradaic and Non-faradaic current, Rate law in faradaic process, current density, factors affecting electrode reaction rate, Nernst diffusion layer treatment, Exchange current density, stoichiometric number and transfer coefficient, energy barrier for multistep reactions, effect of double layer structure on electrode reaction rates.

UNIT 6: ELECTRODE DEPOSITION AND CORROSION PROCESS

Electrocatalysis, Electrocatalytic rate, electrocatalysis in redox system, Total deposition, current density, Time variation of the overpotential and rate determining step in electrode deposition.

References:

1. Advanced Concepts in Physical Chemistry, Kaufman, International Studel Edn.
2. Chemical Kinetics, K.J. Laidler, TMH.
3. Advanced Chemical Kinetics - K.N. Upadhayay
4. Physical Chemistry, Barrow, TMH.
5. Physical Chemistry, Atkins, Oxford
6. Physical Chemistry - A molecular Approach, Viva-books Pvt. Ltd.

**M.Sc.
Chemistry
Semester-IV
(Laboratory course- Inorganic Chemistry)**

Paper- XV (A)

Full Marks:70

CHEE-15(A)

Time:3 hrs.

Two practicals are to be set.

1. Quantitative analysis of a mixture containing not more than three metal ions using volumetric or gravimetric techniques, or 20 marks Spectrophotometric determination of metal ions/ anions, or Quantitative estimation of major constituents of any one of the following.

- a) Dolomite
- b) Brass
- c) Stainless steel
- d) Bronze
- e) Solder

Analysis of two cation system using complexometric method, or Determination halide or silver ion by indirect EDTA titration.

2. Synthesis, purification and crystallization of coordination compounds of any of the following Cu(II), Cr(II), Co(II) and Fe(III) ions. 20 marks

3. Analysis of inorganic mixture containing not than six radicals including rare earths, interfering radicals and insoluble compounds 20 marks

Viva – voce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

**M.Sc.
Chemistry
Semester-IV
(Laboratory course- Organic Chemistry)**

Paper- XV (B)

CHEE-15(B)

Two practicals are to be set.

1. Qualitative analysis

Separation, purification and identification of the components of binary mixture of organic compounds

2. Two step synthesis of organic compounds

p-nitroaniline from Acetanilide

p-Chlorotoluene from p- toluidine

p - amino azobenzene from aniline

Benzilic acid from Benzoin

Benzanilide from Benzophenone

Any other two step synthesis may also be carried out.

3. Identification of simple organic compounds by the analysis of their spectral data
(UV, IR, PMR, CMR and MS Recorded spectral graphs/data will be supplied.

Viva – voce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

**M.Sc.
Chemistry
Semester-IV
(Laboratory course- PHYSICAL Chemistry)**

Paper- XV (C)

CHEE-15(C)

1. To determine the critical solution temperature above in Phenol-water system.
2. To determine the Eutectic temperature and the composition of the Eutectic mixture.
3. To determine the order of reaction between I, and CH_3COCH_3 , catalyzed by acids.
4. To study the adsorption of acetic acid on charcoal.
5. To determine K_r of camphor and the molecular wt. of solute by Rast's method.
6. To determine the water equivalent of calorimeter and heat of solution of KCl
7. To determine the heat of neutralization of HCl against caustic soda and heat of ionization of acetic acid.
8. To determine the basicity of succinic acid thermochemically.
9. To verify Beer's law and to determine the concentration of a coloured solution spectrophotometrically
10. To determine the ionization constant of an indicator spectrophotometrically.

Viva – voce	16 marks
Note Book	04 marks
Experiment	50 marks
Interval Assignment	20 marks
Day to day interval Assignment	10 marks

**M.Sc.
Chemistry
Semester-IV
(Dissertation/Project)**

**Paper- XVI
Full Marks: 100**

**CHEE-16
Time: 6 hours**