



# बिलासपुर विश्वविद्यालय, बिलासपुर (छत्तीसगढ़)

## SEMESTER SYLLABUS

### M.Sc. CHEMISTRY

#### SCHEME OF EXAMINATION & DISTRIBUTION OF MARKS

##### SEMESTER - I

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
1.	Inorganic Chemistry	20	80		100
2.	Organic Chemistry, Stereochemistry & Pericyclic Reaction	20	80		100
3.	Physical Chemistry- I	20	80		100
4.	Spectroscopy And Mathematics/Biology For Chemists	20	80		100
LAB-I	Organic Chemistry				100
LAB-II	Analytical Chemistry				100
<b>TOTAL</b>					<b>600</b>

##### SEMESTER - II

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
1.	Inorganic Chemistry	20	80		100
2.	Organic Chemistry	20	80		100
3.	Physical Chemistry	20	80		100
4.	Spectroscopy, Diffraction Methods & Computer For Chemists	20	80		100
LAB-I	Inorganic Chemistry				100
LAB-II	Physical Chemistry				100
<b>TOTAL</b>					<b>600</b>

##### SEMESTER - III

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
<b>COMPULSORY FOR GROUP A, B &amp; C</b>					
1.	Applications Of Spectroscopy	20	80		100
2.	Chemistry Of Bio-Inorganic & Bio-Organic	20	80		100
LAB-I	General (Compulsory)			200	200
<b>OPTIONAL GROUP-A INORGANIC</b>					
3.	Organotransition Metal Chemistry	20	80		100
4.	Photo inorganic Chemistry	20	80		100
<b>OPTIONAL GROUP- B ORGANIC</b>					
3.	Physical Organic Chemistry	20	80		100
4.	Chemistry Of Heterocyclic Compounds	20	80		100
<b>OPTIONAL GROUP-C PHYSICAL</b>					
3.	Chemistry Of Materials	20	80		100
4.	Advanced Quantum Chemistry	20	80		100
<b>TOTAL</b>					<b>600</b>



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## SEMESTER SYLLABUS

### M.Sc. CHEMISTRY

#### SEMESTER - IV

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
<b>COMPULSORY FOR GROUP A, B &amp; C</b>					
1.	Photochemistry & Solid State Chemistry	20	80		100
2.	Bio-Physical & Environmental Chemistry	20	80		100
<b>OPTIONAL GROUP-A INORGANIC</b>					
3.	Bioinorganic Chemistry & Supra-Molecular Chemistry	20	80		100
4.	Analytical Chemistry	20	80		100
LAB-I	Special			200	200
<b>OPTIONAL GROUP- B ORGANIC</b>					
3.	Medicinal Chemistry	20	80		100
4.	Chemistry Of Natural Product	20	80		100
LAB-I	Special			200	200
<b>OPTIONAL GROUP-C PHYSICAL</b>					
3.	Liquid States	20	80		100
4.	Computation Chemistry	20	80		100
LAB-I	Special			200	200
<b>TOTAL</b>					<b>600</b>
<b>GRAND TOTAL</b>					<b>2400</b>



**UNIT-I**

Stereochemistry and Bonding in Main group Compounds – VSEPR theory, Walsh Diagram (Tri and Pentatomic-Molecules)  $d\pi - p\pi$  bonds, bent rule and energetic of hybridisation, some simple reaction of covalently bonded, molecules.

**UNIT-II**

Metal Ligand Bonding – Limitation of Crystal field Theory, Molecular orbital theory, octahedral, Tetrahedral and square planar complexes.  $\pi$  Bonding & molecular orbital theory.

**UNIT-III**

Electronic spectra of transition metal complexes – Energy levels in an atom, coupling of orbital angular momentum, determination of ground state term, derivation of term symbols. Electronic spectra of Transition metal complexes, Orgel and Tanabe- sugano-diagrams for Transition metal complexes.

**UNIT-IV**

- Magnetic Properties of transition metal complexes- Anomalous magnetic moment, Magnetic Exchange coupling and spin crossover, charge transfer spectra.
- Symmetry and Matrix representation- Symmetry Element & Symmetry operation, point Symmetry Group, schoenflies symbols, Matrix Representation of Symmetry Operations, Multiplication Table.

**UNIT-V**

Group Theory in Chemistry- Definition of group subgroup, relation between orders of a finite group and its sub group. Conjugate relation and classes, reducible & irreducible representations (Representation for  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nv}$ ,  $D_{nh}$  etc. Groups to be worked out-explicitly)

**Books Suggested-**

- Group Theory - Bhattacharya
- Advance Inorganic Chemistry – F.A. Cotton and Wilkinson: John Wiley.
- Inorganic Chemistry – J.E. Huhey Harpes & Raw
- Chemistry of the elements – N.N. Greenwood & A Earnshaw Pergamon.
- Inorganic Electronic Spectroscopy – A.B.P. Lever, Elsevier.
- Magneto Chemistry – R.L. Carlin Springer Verlag.
- Comprehensive Co-ordination Chemistry, G. Wilkinson R.D. Gillar's and J.A. Mccleverty Pergamon.
- Chemistry Applications of Group Theory – F.A. Cotton.



SEMESTER-I

PAPER - II

ORGANIC CHEMISTRY, STEREOCHEMISTRY & PERICYCLIC REACTION

**UNIT- I**

**Reaction Intermediates:** Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes, and benzyne. Application of NMR in detection of carbocations.

**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  $\pi$  molecular orbitals, annulenes, homo-aromaticity, PMO approach.

**UNIT- II**

**Stereochemistry:** Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereo selective synthesis. Asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes). Chirality due to helical shape. Stereo chemistry of the compound containing nitrogen, sulphur and phosphorus.

**UNIT- III**

**Reaction Mechanism: Structure and Reactivity:** Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate. Potential energy diagrams, transition states and intermediates, methods of determining mechanism, isotope effects. Hammett equation and linear free energy relationship, substituent and reaction constants.

**UNIT- IV**

**Pericyclic Reactions:** Molecular orbital symmetry, frontier orbitals of ethylene 1,3-butadiene, 1,3,5- hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions, Conrotatory and disrotatory motions,  $4n$ ,  $4n+2$  and allyl systems. Cycloadditions - antarafacial and suprafacial additions,  $4n$ ,  $4n+2$  systems,  $2+2$  addition of ketenes, 1,3 dipolar cyclo additions and cheletropic reactions. Sigmatropic rearrangements - Suprafacial and antarafacial shifts of H. sigmatropic shifts involving carbon moieties 3,3 and 5,5- Sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Fluxional tautomerism, Ene reaction.

**UNIT- V**

**Molecular rearrangement:** General mechanistic approach to molecular rearrangement reactions, carbocation rearrangement- migratory aptitude and memory effects. Brief study of following rearrangement reactions. Favoroskii, Baeyer-Villiger oxidation, Stork enamine reaction, Shapiro reaction, Sommelet rearrangement, Wittig's rearrangement, Grovenstein-Zimmerman rearrangement.

**Books Suggested:**

1. Advanced Organic Chemistry - Reaction Mechanism and Structure, Jerry March, John Wiley.



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## SEMESTER SYLLABUS

### M.Sc. CHEMISTRY

2. Advanced Organic Chemistry - F.A. Carey and R.K. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry- Peter Syke longman.
4. Structure and Mechanism in organic chemistry - C.K. Ingold, Cornell University Press.
5. Organic Chemistry - R.T. Morrison and R.N. Boyed Prentice - Hall.
6. Modern Organic Reactions - H.O. House, Benzamic.
7. Principles of Organic Synthesis - R.P.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Pericyclic Reaction - S.M. Mukherji.
9. Reaction Mechanism in Organic Chemistry - S.M. Mukherji and S.P. Singh Macmilan.
10. Stereochemistry of Organic compounds - D. Nasipuri New age International.
11. Stereochemistry of Organic Compounds - P.S. Kalsi, New Age International.



**UNIT- I Quantum Chemistry:**

**Introduction in Exact Quantum Mechanical Result:** The Schrodinger equation and the postulates of quantum mechanics. Discussion of solution of the Schrodinger equation to some model systems, viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

**Approximate methods:** The various theorems, linear variation principle. Perturbation theory (first order and non – degenerate). Application of variation method and perturbation theory to the Helium atom.

**Angular Momentum:** Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Eigenvalue of angular momentum, operator using ladder operators, addition of angular momenta, spin anti-symmetry and Pauli Exclusion Principle.

**UNIT- II Atomic Chemistry:**

**Electronic Structure of Atoms:** Electronic configuration, Russell – Saunders term and coupling scheme. Slater – Condon parameters, term separation energies of  $p^n$  configuration, term separation energies for  $d^n$  configurations, magnetic effects: spin – orbital coupling and Zeeman splitting, introduction to the method of self- consistent field, the virial theorem.

**Molecular Orbital Theory:** Huckel theory conjugated system, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. introduction to extended Huckel theory.

**UNIT- III Chemical Dynamics:**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory, ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov - Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and nuclear magnetic resonance method, Dynamics of molecular motions, probing the transition state, dynamics of barrier less chemical reactions in solution, dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice- Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

**UNIT- IV Surface Chemistry:**

**Adsorption:** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Calvin equation), and Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film on liquids (Electro-Kinetic phenomenon), catalytic activity of surfaces.

**Micelles:** Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factor affecting the CMC of surfactants, counter ions binding to micelles, thermodynamics of micellization – phase separation and mass action models, solubilization, micro emulsion, reverse micelles.



**UNIT- V**

**Macromolecules:** Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetic of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering method), sedimentation, chain configuration of macro molecules, calculation of various chain structures.

**Books Suggested:**

1. Physical Chemistry; P. W. Atkins, ELBS.
2. Introduction to Quantum Chemistry; A. K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry; Ira. N. Levine, Prentice Hall.
4. Coulson`s Valence; R. Mc Weeny, ELBS.
5. Micelles Theoretical and Applied Aspects; V. Moroi, Plenum.
6. Introduction to Polymer Science; V. R. Gowariker, N. V. Vishwanathan and J. Sridhar, Wiley Eastern.
7. Physical Chemistry of Surface; A. W. Anderson and A. Gast, Wiley.
8. Surfaces; G. Attard and C. Barnes, Oxford Univ. press.
9. Introduction to Solid state physics. Kittel, Wiley.
10. Crystal structure determination; W. Clegg, Oxford University Press.



SEMESTER I

PAPER – IV

SPECTROSCOPY AND MATHEMATICS/BIOLOGY FOR CHEMISTS

SECTION- A

UNIT- I

**spectroscopy**

**Unifying Principles:** Electromagnetic radiation, Interaction of Electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and Natural line width and natural line broadening. Transition Probability, results of the time dependent perturbation theory, transition moment. Selection rules, intensity of spectral lines. Born-Oppenheimer approximation, Rotational, Vibrational and Electronic Energy Levels.

UNIT- II

**Microwave Spectroscopy:** Classification of Molecules, rigid rotor model effect of isotopic substitution on the transition frequencies, Intensities, non-rigid rotor. Stark effect, Nuclear and Electron spin Interaction .

**Raman Spectroscopy:** Classical & Quantum Theories of Raman Effect. Pure rotational, vibrational & vibrational rotational Raman Spectra, Selection rules, Mutual exclusion Principle, Resonance Raman Spectroscopy, Coherent, Antistokes, Raman Spectroscopy (CARS).

UNIT- III

**Vibrational Spectroscopy: Infrared Spectroscopy** - Review of linear harmonic oscillator, vibrational energies of diatomic molecules, Zero point energy, force constant and bond strengths anharmonicity, morse potential energy diagram, vibrational, rotation spectroscopy. P.Q.R. branches. Breakdown of oppenheimer approximation. Vibration of poly atomic molecules. Selection rules, normal modes of vibration, group frequencies overtones hot bands factors affecting the band positions and intensities for IR region.

SECTION- B

MATHEMATICS FOR CHEMISTS

(For Students without Mathematics in B.Sc.)

UNIT- IV

**Vector and Matrix Algebra**

**Vectors:** - Vector dot, cross and triple products etc. The gradient divergence and curl. Vector calculus, gauss Theorem divergence Theorem etc.

**Matrix Algebra:** - Addition and Multiplication, Inverse, adjoint and transpose of matrices. Special matrices. (Symmetric, Skew symmetric, diagonal, unitary etc.) And their properties, matrix equation, Homogeneous, Non Homogeneous linear equations.

**Differential Calculus:** Functions, continuity and differentiability rules for differentiation, Applications of differential calculus. Including maxima and minima. Exact & Inexact differentials with their Application to thermodynamics properties. Integral calculus, basic Rules for Integration, Integration by parts, partial fraction and substitution. Reduction formulae, Applications of integral calculus. Functions of several variables.

UNIT- V

**Elementary differential equations:** Variables-Separable and Exact First-order, differential equation, homogeneous, Exact and linear equation. Applications to Chemical Kinetics, Secular Equilibrium quantum chemistry.

**Permutation and Probability:** Permutations and combinations, probability and probability theorem, probability curves, average, root mean square and most probable errors, examples from kinetic theory of gases.





OR

SECTION- B

BIOLOGY FOR CHEMISTS

(For Student without Biology In B.Sc.)

#### UNIT- IV

**Cell Structure and Functions:** Structure of prokaryotic and eukaryotic cells Intercellular organelles and their functions. Comparison of Plant and animal cells. Overview of metabolic processes- catabolism and anabolism. ATP- The biological Energy currency. Origin of life - unique properties of carbon, Chemical evolution and rise of living systems. Introduction to bio molecules, building blocks of Bio-macromolecules.

**Carbohydrates:** Conformation of mono-saccharides, structure and function of important derivatives of monosaccharide. Like glycosides-deoxy sugar myoinositol, Aminosugar, disaccharides and polysaccharides structural. Poly saccharides cellulose and chitin. Storage polysaccharides starch and glycogen. Carbohydrate of glyco-protein and glycolipids. Role of sugar in biological recognition. Blood group substances. Ascorbic Acid, Carbohydrate metabolism, Krebs cycle, Glycolysis, Glycogenesis and Glycogenolysis, Gluconeogenesis, pentose phosphate pathway.

#### UNIT- V

**Lipids:** Fatty acids, essential fatty acids, structure and function of triglycerals glycerophospholipids, Sphingolipids cholesterol, bile acids, prosta-glandins lipoproteins- composition and function role in atherosclerosis. Properties of lipid aggregates micelles bilayers. Liposomes and their possible biological functions, Biological membranes, fluid mosaic model of membrane spectra liquid metabolism.  $\beta$ -Oxidation. of fatty acids.

**Amino acids, Peptides and Proteins:** Chemical & enzymatic hydrolysis of proteins to peptides, Amino Acid sequencing, secondary structure of proteins, forces responsible for holding of secondary structure.,  $\alpha$ -helix,  $\beta$ -sheets super secondary structure, triple helix structure of collagen, Tertiary structure of protein folding and domain structure. Quaternary structure. Amino Acid metabolism, degradation and biosynthesis of Amino acid. Sequence determination. Chemistry of Oxytocin and tryptophane releasing hormones (TRH)

**Nucleic Acid:** Purine, Pyrimidine, bases of Nucleic acid, base pairing, via H-bonding, structure of Ribo Nucleic Acid (RNA) & D.N.A. deoxy ribonucleic acid, double helix model of DNA and forces responsible for holding at chemical and Enzymatic Hydrolysis of Nucleic Acid. The Chemical bases of heredity, an overview of replication of DNA. Transcription, translation and genetic code, chemical synthesis of mono and Trinucleosides.

#### Book Suggested for Spectroscopy :

1. Modern Spectroscopy - J.M. Hollas Hohnwiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windowi and F.L. Ho Willey interscience.
3. NMR, NQR, ESR and mossbaure spectroscopy in Inorganic chemistry :- R.V. Parish, Ellis Harwood.
4. Physical Method in Chemistry - R.S. Drago, Saunders College.
5. Introduction to Molecular Spectroscopy - G.M. Barrow, Mcgraw Hill.
6. Basic Principle of Spectroscopy- R. Chang Mcgraw Hill.
7. Theory and Application of Uv Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford.
8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.



9. Introduction to magnetic Resonance. A. Carrington and A.D. MacLachalan Harper & Row.

10. H. Kaur, Spectroscopy, Wiley.

**Books: Mathematics for chemists:**

1. The Chemistry Mathematics Book: E.Steiner, Oxford University Press.

2. Mathematics for Chemistry - Doggett and Sectcliffe longman.

3. Mathematical preparation for physical chemistry - F. Daniels Mcgrow Hill.

4. Chemical Mathematics - D.M. Hirsl- Longmann.

5. Applied Mathematics for Physical Chemistry - J.R. Barrate, Prentice Hall.

6. Basic Mathematics for Chemists Tebbutt Wiley.

**Books –Biology for chemists**

1. Principles of Biochemistry, A. L. Lehninger, Worth Publishers.

2. Biochemistry, L.Stryer, W. H. Freeman.

3. Biochemistry, J. David Rawn, Neil Patterson

4. Biochemistry, Voet & Voet John Wiley

5. Biochemistry, Jain & Jain. S. Chand.



SEMESTER I  
LABORATORY COURSE - I  
ORGANIC CHEMISTRY

**1. Qualitative Analysis:-**

Separation, Purification and Identification of compounds of Binary Mixture, T.L.C. and Column chromatography. I.R. Spectra may be used for functional group identification of compound by suitable derivatives preparation and determination of their melting points.

**2. Organic Synthesis:-**

1. Bromination - Preparation of p-Bromo Aniline from Acetanilide.
2. Nitration - Preparation of p-Nitro Aniline from Acetanilide
3. Hoffman Bromide Reaction. Preparation of Anthranilic Acid from Pthalic anhydride.
4. Aldol Condensation - Dibenzal acetone from Benzaldehyde.
5. Sandmeyer Reaction -
  - o-Chloro Benzoic Acid from Anthranilic Acid.
  - p- Chloro toluene from Toluene.
6. Friedel Craft Reaction - p-Benzoyl Propionic Acid from Succinic Anhydride and Benzene.
7. Oxidation - Adipic Acid by Chromic Acid oxidation of cyclohexanol.
7. Diazotization:-
  - Preparation of methyl orange from Sulphanilic Acid.
  - Phenyl Azo- p-Naphthol from Aniline.
8. Preparation of Acridone from N- Phenyl anthranilic acid.
9. Grignard's reaction: Synthesis of triphenyl Methanol from Benzoic acid.

**Note:** Two stage preparation. Preparation of pure and crystalline compound based on any two of above principals with confirmation of melting point.

**3. Quantitative Analysis:-**

1. Determination of the percentage or number of Hydroxyl group in an organic compound by Acetylation method.
2. Estimation of Amines/Phenols using Bromate - Bromide Solution / or Acetylation method.
3. Determination of equivalent- weight of carboxylic compound.
4. Estimation of carboxyl group by titration / silver salt-method.
5. Estimation of Carbonyl group by Hydrazone method.
6. Estimation of Glycine by titration.

**Instruction to Practical Examiners in Chemistry Semester –I**

1. The Board of Examiners; one external and one internal for each branch will meet to decide the exercises and other matter in connection with the conduct of practical examinations

S. No.	Lab. Course (branch)	Max. Marks	Duration
1.	I- Organic Chemistry	100	5 hrs.
2.	II- Analytical Chemistry	100	5 hrs.

2. The distribution of marks is as under. Marks of Ex-students are given in parentheses.

(a) Qualitative Analysis of mixture containing two Organic compounds	30 (40) marks
(b) Preparation	10 (15) marks
(c) Estimation	20 (25) marks
(d) Viva voice	20 (20) marks
(c) Sessional	20 (-) marks

Total-100 (100) marks

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises.



SEMESTER I  
LABORATORY COURSE II  
ANALYTICAL CHEMISTRY  
SECTION- A  
INSTRUMENTATION AND COMPUTERS

1. Error Analysis & Statistical data Analysis:-  
Errors, types of errors, Minimization of Error, Statistical treatment for error analysis, standard deviation, Relative standard deviation, Linear least square. Calibration of volumetric apparatus burrettes pipette, standard flask, weight box etc.
2. Volumetric Analysis:-  
Basic Principles, determination of  $I_2$  and saponification values of oil sample determination of DO, COD, BOD, Hardness of water samples.
3. Chromatography:-  
Separation of Cations and anions by (A) Paper Chromatography, (B) Column Chromatography.

SECTION- B

4. pH Metry / Potentiometry / Conductometry titration :-  
Determination of strength of acid etc.
5. Flame Photometry / AAS/FIA/Colorimetry :-  
Determination of Cations / anions and metal ions eg.  $Na^+$ ,  $K^+$ ,  $Ca^{2+}$ ,  $SO_4^{2-}$ ,  $NO_2^-$ , Fe, Mo, Ni, Cu, Zn etc.
6. Spectro Photometry :-  
Verification of Beer - Lambert Law. Molar Absorptivity calculation, Plotting graph to obtain  $\lambda_{max}$  etc. effect of pH in aqueous coloured system. Determination of metal ions eg. Fe, Cu, Zn, Pb etc
7. Nephelometry / Turbidimetry :- Determination of chlorine, sulphate phosphate turbidity etc.
8. Application of Computer in Chemistry:- As Specified in Theory paper in section II (A).

**For Lab. Course –II (Analytical Chemistry):**

- |  |                 |
|--|-----------------|
| (a) Two practical exercise (one from each section)<br>(at least one of these will be based on instrumental analysis) | 60 (80) marks   |
| (b) Viva voice   | 20 (20) marks   |
| (c) Sessional  | 20 (-) marks    |
| Total-   | 100 (100) marks |

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises. Sessional marks will be awarded by External Examiner in consultation with the internal Examiner



Note: - Two questions will be asked from each Unit and student will have the choice to attempt any one question from each unit.

### Unit- 1

**metal ligand Equilibrium in solution:** - Step wise & overall formation constants and their interaction, trends in step wise formation constants, factors affecting the stability of Metal Complexes with reference to nature of metal ion and ligand.

### Unit- 2

**Reaction mechanism of transition metal complexes:-** Energy profile of a reaction, reactivity of metal complexes, Inert and Labile complexes. Kinetic application of valence bond & crystal field theories. Kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis. Base hydrolysis, Anation reactions, Reactions without metal ligand bond cleavage, substitution reactions in square planar complexes. The trans effect.

### Unit- 3

#### Metal Complexes:

(A) Mechanism of the substitution reaction, Redox reactions, Electron transfer reactions, mechanism of one electron transfer reaction.

(B) Metal Clusters- **Higher** boranes, carboranes, metalboranes and metallocarboranes, Metal carbonyl.

### Unit- 4

(A) Metal Carbonyls, Structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls.

(B) Nitrosyl :- Preparation, bonding, structure & important reactions of transition metal nitrosyl, dinitrogen complexes, tertiary phosphine as ligand.

### Unit- 5

**Isopoly and Heteropoly Acid & salt:** Isopoly acids of transition metals Mo, W, V, Nb, Ta.

Heteropoly acids and salt of Mo, W, Structure of heteropoly acids

#### Books Suggested:-

1. Advanced Inorganic chemistry: - F.A. Cotton and Wilkinson: John Wiley.
2. Inorganic Chemistry : J.E. Huhey, Harpes & Row
3. Chemistry of the elements: N. N. Greenwood & A Earnshaw Pergamon.
4. Inorganic Electronic Spectroscopy – A..B.P. Lever, Elsevier
5. Magnetochemistry - R.L. Carlin, Springer Verlag.
6. Comprehensive Co-ordination Chemistry G. Wilkinson, R.D. Gillars and J.A. McCleverty Pergamon.
7. Chemistry Applications of Group Theory - F.A. Cotton.
1. Group Theory: - Bhattacharya.



SEMESTER-II

PAPER - II

ORGANIC CHEMISTRY  
(REACTION MECHANISM)

UNIT- I

**Electrophilic substitution reactions:-**

**Aliphatic electrophilic substitution:** - Bimolecular mechanism:  $SE^2$ ,  $SE1$ , and  $SE_i$  mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

**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- II

**Nucleophilic Substitution reactions:-**

**Aliphatic nucleophilic substitution:** The  $S_N2$ ,  $S_N1$ , mixed  $S_N1$  and  $S_N2$  and SET mechanism. The neighbouring group mechanism, neighbouring group participation by  $\pi$  and  $\sigma$  bonds. The  $S_Ni$  mechanism. Nucleophilic substitution at an allylic aliphatic trigonal and at a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile.

**Aromatic Nucleophilic substitution:** The  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms, Reactivity-effect of substrate structure. Leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangement.

UNIT- III

**Free Radical reactions**

Types of free radical reactions, Free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance, Reactivity for aliphatic and aromatic substrates at a bridge head. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement, Hunsdiecker reaction.

UNIT- IV

**(a) Addition to Carbon-Carbon Multiple Bonds**

Mechanism and stereo chemical aspects of addition reactions involving electrophiles, Nucleophiles and Free radicals, regio and chemoselectivity, Orientation and reactivity, Addition to cyclopropane ring. Hydrogenation of double and triple bonds. Hydrogenation of Aromatic rings. Hydroborations Michael reaction, epoxidation.

**(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, Benzoin, Perkin and Stobbe reactions, Hydrolysis of ester and amides, Ammonolysis of esters.

UNIT- V

**Elimination reactions:**

The  $E_2$ ,  $E_1$  and  $E_{1cB}$  mechanism and their spectrum, orientation of double bond. Reactivity-effects of substrate structures, attacking base, the leaving group and the medium.



बिलासपुर विश्वविद्यालय, बिलासपुर (छत्तीसगढ़)

SEMESTER SYLLABUS

M.Sc. CHEMISTRY

**Books Suggested.**

1. Advanced Organic Chemistry - Reaction Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry - F.A. Carey and R.K. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry Peter Sykes- longman.
4. Structure and Mechanism in organic chemistry - C.K. Ingold, Cornell University Press.
5. Organic Chemistry - R.T. Morrison and R.N. Boyd, Prentice - Hall.
6. Modern Organic Reactions H.O. House, Benzamic.
7. Principles of Organic Synthesis - R.P.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Reaction Mechanism in Organic Chemistry - S.M. Mukherji and S.P. Singh Macmillan



SEMESTER-II

PAPER - III

PHYSICAL CHEMISTRY

KINETICS & ENERGETICS

**UNIT- I**

**THERMODYNAMICS: Classical Thermodynamics:** Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions. Activity, Activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength. Application of phase rule to three component systems, second order phase transitions.

**UNIT- II**

**Statistical Thermodynamics:** Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions - translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function, application of partition function. Heat capacity behavior of solids - chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and application to metal. Bose-Einstein statistics - distribution law and application to helium.

**Non Equilibrium Thermodynamics:** Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electro kinetic phenomena, diffusion electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

**UNIT- III**

**ELECTROCHEMISTRY:** Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions, Debye-Huckel Jerum mode. Thermodynamics of electrified interface equations, derivations of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Graham-Devanathan - Mottwatts, Tobin, Bockris, Devanathan models. Over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes- solution interfaces, quantization of charge transfer, tunneling. Semiconductor interfaces - theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light a semi-conductor solution interfaces.

**UNIT- IV**

Electro-catalysis - influence of various parameters, Hydrogen electrode. Bio-electrochemistry, threshold membrane phenomena, Nernst-Plank equation. Hodges-Huxley equation, core conductor models, electrocardiograph. Polarography theory, Ilkovic equation, half wave potential and its significance, Introduction to corrosion, homogenous theory, forms of corrosion monitoring and prevention methods.





**UNIT- V**

**(a) ELECTRON DIFFRACTION-**

Scattering intensity vs. scattering angle. Wierl equation, measurement technique, Elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surface.

**(b) NEUTRON DIFFERACTON-**

Scattering of neutron by solid and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

**Book Suggested**

1. Physical Chemistry - P.W. Atkins, ELBS
2. Introduction to Quantum Chemistry - A.K.Chandra, Tata McGraw Hill
3. Quantum Chemistry - Ira N.Levine, Prentice Hall
4. Coulson's Valence - R. McWeeny, ELBS
5. Chemical Kientics - K.J. Laidler, McGraw Hill
6. Kinetics and mechanism of chemical transformation - J.Rajaraman and J.Kuriacose; McMillan.
7. Micelles, Theoretical and Applied Aspects - V. Moroi, Plenum.
8. Modern Electrochemistry Vol.I and II - J.O.M. Bockris and A.K.N.Reddy, Plenum.
9. Introduction of Polymer Science - V.R.Gowarikar, N.V.Vishwanathan and J.Sridhar Wiley Easter



**UNIT- I**

**Electronic Spectroscopy:-**

**A. Atomic Spectroscopy:** - Energy of Atomic orbitals, Vector Representation of momenta & vector coupling, spectra of Hydrogen atom, alkali metal atom.

**B. Molecular Spectroscopy:** - Energy levels, Molecular orbitals, vibration transition, vibrational progression and geometry of the excited states, Franck-Condon principle, Electronic spectra of polyatomic, molecules, Emission Spectra.

**C. Photo Electronic Spectroscopy :-** Basic principles, Photo-electric effect Ionisation process, Photo Electron Spectra of simple molecules, E.S.C.a., Chemical Information of E.S.C.A., Auger Electron Spectroscopy-basic idea.

**UNIT- II**

**Magnetic Resonance Spectroscopy:-**

**A). Nuclear Magnetic Resonance Spectroscopy :-** Nuclear Spin, Nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors Influencing chemical shift, deshielding, spin-spin interaction. Factors Influencing coupling constant "J", classification (ABx, AMx, ABC, A<sub>2</sub>B<sub>2</sub> etc), spin decoupling basic ideas about instruments.

**B. Electron Spin Resonance Spectroscopy:** - Basic principle, Zero field splitting and orbital energy degeneracy, factors affecting the 'g' value, isotopic and anisotropic hyperfine coupling constant. Spin densities and Applications of ESR

**C. Nuclear Quadrupole Resonance Spectroscopy** quadrupole nuclear, quadrupole moment electric field gradients, coupling constant splittings, Applications.

**D. Photoacoustic Spectroscopy :-** Basic principle of photoacoustic spectroscopy (PAS), PAS-gases and condensed-systems, chemical & surface application.

**UNIT- III**

**X-ray Diffraction:-**

Bragg's condition, Miller indices, Laue-method, Bragg's method, Debye-scherrer method of X-ray structural analysis of crystals. Index- Reflections identification of unit cell from systematic absences in diffraction pattern structure of simple lattices and X-Ray Intensities structure factor and its relation to intensity and electron density. Phase problem. Description of the procedure for an X-Ray structure analysis, Absolute configuration of molecules.

**UNIT- IV**

**Introduction to Computer and Computer Programming in "C"**

**Computer Fundamental;** - Introduction to Computer organisation. Operating System, DOS, Introduction to UNIX and Window. Computer Languages Principle of programming Algorithm and flow charts.

**Programming in C :-** Structure of a C Programming, constants, variables, operators and Expressions, data Input & output, decision making, branching and looping statements arrays, well defined functions pointers structure and unions, Format statement. Termination statements. Branching statements such as IF of GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBROUTINE. COMMON and DATA statements.



## UNIT- V

### Programming in Chemistry and use of Computer Programmes.

1. Development of small computer codes Involving simple formulae in Chemistry such as Vander waals Equation, pH Titrations, Kinetic. Radioactive Decays. Evaluation of Lattice Energy and Ionic radii secular equation (within Huckel Theory), Elementary structural features, such as, bond lengths, bond Angle, dihedral angles etc. Of molecules extracted from a database.
2. Introduction and use of computer package MS-Word and Excel. Preparation of graphs and Charts.

### Book Suggested for Spectroscopy

1. Modern Spectroscopy - J.M. Hollas John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Window and F.L. Ho Willey interscience.
3. NMR, NQR, ESR and Mossbauer spectroscopy in Inorganic chemistry: - R.V. Parish, Ellis Harwood.
4. Physical Method in Chemistry - R.S. Drago, Saunders College.
5. Introduction to Molecular Spectroscopy - G.M. Barrow, McGraw Hill.
6. Basic Principle of Spectroscopy- R. Chang McGraw Hill.
7. Theory and Application of UV Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford.
8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.
9. Introduction to magnetic Resonance. A. Carrington and A.D. MacLachlan Harper & Row.
10. Spectroscopy by Kalsi

### Books suggested for Computers

1. Computer and Common Sense: - R. Hunt and J. Shelley Prentice Hall.
2. Computational Chemistry A.C. Norris.
3. Micro Computer Quantum Mechanics. J.P. Killingbeck. Adam Hilger.
4. Computer Programming in Fortran IV V. Rajaraman, Prentice Hall.
5. An Introduction to Digital Computer Design, V.Rajaraman and T. Radha Krishnan Prentice Hall.



SEMESTER-II  
LABORATORY – COURSE I  
INORGANIC CHEMISTRY

**Note- Students is accepted to complete all exercises.**

1. Qualitative analysis of mixture containing eight radical including some less common metal ions among the following by common method (Preferably semi-micro method)

**Group-A**

Basic Radicals : - {Ag, Pb, Hg, Cu, Cd, Bi, As, Sb, Sn, Fe, Al, Cr, Zn, Mn, Co, Ni, Ba, Sr, Ca, Mg, Na, K, NH<sub>4</sub> ,}

Acid Radicals: - {CO<sub>3</sub>, SO<sub>4</sub>, SO<sub>3</sub>, NO<sub>3</sub>, F, Cl, Br, I, NO<sub>2</sub>, BO<sub>3</sub>, C<sub>2</sub>O<sub>4</sub>, PO<sub>4</sub>}

**Group- B**

Basic Radicals: - {Ce, Th, Zr, W, Te, Ti, Mo, U, V, Be, Li, Au, Pt.}

Acid Radicals :-{SiO<sub>4</sub>, Thiosulphate, Ferrocynide, Ferricyanide, Chromate, Arsenite , Arsenate, Permanganate }

**Note** – The mixture to be analysed by the students must contain at least one basic and one acid radical from Group B.

**2. Quantitative Analysis:-**

Involving two of the following in ores, alloys or mixture in solution- one by volumetric and other by gravimetric method Ag, Cu, Fe, Cr, Mn, Ni, Zn, Ca, Mg, Chloride, Sulphate.

**3. Estimation of:-**

(A) Phosphoric acid in Commercial ortho phosphoric acid.

(B) Boric Acid in Borax.

(C) Ammonium Ion in Ammonium Salt.

(D) MnO<sub>2</sub> in pyrolusite

(E) Available Chlorine in bleaching powder.

(F) H<sub>2</sub>O<sub>2</sub> in commercial sample.

Students are expected to perform at least three exercises From above during laboratory work.

4. Preparation of selected Inorganic compounds and study of their properties by various method including IR, Electronic Spectra, Mossbauer, ESR. Spectra+ Magnetic susceptibility etc.

(i) VO(acac)<sub>2</sub>

(ii) cis K [Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>],

(iii) [Co(NH<sub>3</sub>)<sub>6</sub>]Cl<sub>3</sub>

trans K [Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>].2H<sub>2</sub>O

(iv) Na [Cr (NH<sub>3</sub>)<sub>2</sub> (SCN)<sub>4</sub>]

(v) Mn (acac)<sub>3</sub>

(vi) K<sub>3</sub>[Fe(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>]

(vii) Prussian Blue Turnbull's Blue.

(viii) [Co(NH<sub>3</sub>)<sub>6</sub>] [Co(NO<sub>2</sub>)<sub>6</sub>]

(ix) Hg [Co (SCN)<sub>4</sub>]

(x) [Ni(NH<sub>3</sub>)<sub>4</sub>]Cl<sub>2</sub>, [Ni(NH<sub>3</sub>)<sub>4</sub>]Cl<sub>2</sub>

(xi) Ni (DMG)<sub>2</sub>(xii)[Cu(NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>

(xii) K<sub>3</sub>[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>].3H<sub>2</sub>O

(xiii) [Cu(NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>



SEMESTER-II  
LABORATORY COURSE- II  
PHYSICAL CHEMISTRY

1. Adsorption:-

- Verification of Freundlich's Adsorption Isotherm.
- To study surface tension – concentration relationship for solutions (Gibbs equation).

2. Phase Equilibria:

- Determination of congruent composition and temperature of binary system e.g. diphenylamine – benzophenone system.
- Determination of glass transition temperature of given salt e. g.  $\text{CaCl}_2$  conductometrically.
- To construct the phase diagram for three component system e. g. chloroform, acetic acid and water.

3. Chemical Kinetics

- Hydrolysis of an ester/ ionic reactions.
- Determination of the velocity constant of hydrolysis of an ester. Determination of effect of (a)change of temperatures, (b)change of concentration of reactants and catalyst and(c)ionic strength of the media on the velocity constant of media.
- Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide
- Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ions oxidized by persulphate ion).

4. Conductometry

- Determination of solubility of sparingly soluble salt (eg,  $\text{PbSO}_4$ ,  $\text{BaSO}_4$ ) Conductometrically.
- Determination of the strength of strong and weak acids in a given mixture conductometrically.
- Determination of dissociation constant of weak electrolyte by conductometer.
- Determination of velocity constant, Order of reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide.

5. pH Metry/Potentiometry

- Determination of the strength of strong and weak acid in a given mixture using pH meter/potentiometer.
- Determination of dissociation constant of weak acid by pH meter.
- Determination of concentration of acid in given buffer solution by pH meter.
- Determination of strength of halides in a mixture potentiometrically.
- Determination of the valency of mercurous ions potentiometrically.
- Determination of the strength of strong acid, weak acids in a given mixture using a potentiometer/ pH meter.
- Determination of temperature dependence of EMF of a cell.
- Determination of the formation constant of silver- ammonia complex and stoichiometry of the complex potentiometrically.
- Determination of activity and activity coefficient of electrolytes.
- Determination of thermodynamic constant.  $\Delta G, \Delta S$  and  $\Delta H$  for the reaction by e.m.f. method.  $\text{Zn} + \text{H}_2\text{SO}_4 = \text{ZnSO}_4 + \text{H}_2$
- Determination of the dissociation constant of monobasic / dibasic acid

6. Polarimetry:-

Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.  
Enzyme kinetic – inversion of sucrose.



**7. Solutions:**

- Determination of molecular weight of non-volatile and non- electrolyte/electrolytes by cryoscopy method and to determine the activity coefficient of an electrolyte.
- Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

**Instructions to Practical Examiners in Chemistry.**

- The Board of Examiners - one external and one internal for each branch will meet to decide the exercises and other matter in connection with the conduct of practical examinations.

S.No.	Branch	Marks	Duration
(i).	Lab Course-I Inorganic Chemistry	100	10 hours
(ii)	Lab Course-II Physical Chemistry	100	05 hours

- Sessional marks will be awarded by External Examiner in consultation with the Internal Examiner.
- The distribution of marks is as under. Marks for Ex-students are given in parentheses.

**For Lab. Course –I (Inorganic Chemistry):**

- Qualitative analysis of mixture containing not more than 8 radicals by semi-microMethod only. 32 (42) marks
  - Quantitative analysis (involving separation) of a solution containing 2 metals, one of these is to be estimated gravimetrically and the other volumetrically. 18 (23) marks
  - (c) Preparation 10 (15) marks
  - (d) Viva voce and manipulation 20 (20) marks
  - (e) Sessional 20 (-) marks
- Total 100 (100) marks

**For Lab. Course –II (Physical Chemistry):**

- One practical exercise 60 (80) marks
  - Viva voce and manipulation 20 (20) marks
  - Sessional 20 (-) marks
- Total 100 (100) marks

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises.



SEMESTER III

COMPULSORY FOR GROUP A, B & C

PAPER- I

APPLICATIONS OF SPECTROSCOPY

**UNIT- I INORGANIC CHEMISTRY**

Vibrational Spectroscopy: Symmetry and shape of AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub>, AB<sub>6</sub> mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly metallo-proteins.

Electron Spin Resonance spectroscopy: Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one, unpaired electron) including biological systems and to inorganic free radicals.

Nuclear Magnetic Resonance of Paramagnetic substances in solution: Factors affecting nuclear relaxation, some applications including biological systems, an overview of NMR of metal nuclides with emphasis <sup>195</sup>Pt and <sup>119</sup>Sn NMR.

**UNIT- II ORGANIC CHEMISTRY**

Ultraviolet and Visible Spectroscopy: Instrumentation and sample handling various electronic transition (185-800 nm) Beers-Lambert law, effect of solvent on electronic transitions, ultra-violet bands for carbonyl compounds, dienes, conjugated Polyenes, Fieser- Woodward rule for conjugated dienes and carbonyl compounds, ultra-violet spectra of aromatic and Heterocyclic compounds, steric effect in biphenyls.

Infra-Red Spectroscopy: Instrumentation and Sample Handling characteristic, vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohol, ethers, phenols and amines. Detailed study of Vibrational frequencies of carbonyl compounds (Ketones, aldehydes, esters, amides, acids, anhydrides, lactones, Lactams and conjugated carbonyl compounds), Effect of Hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance FT IR. IR of gaseous, solids and polymeric materials

**UNIT- III**

Nuclear Magnetic Resonance Spectroscopy: General introduction and definition, chemical shift, spin-spin interaction, Shielding mechanism, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, mercaptol) complex, spin-spin interaction between two, three, four and five nuclei (first order spectra) vicinal coupling, stereochemistry, Hindered rotation, Karplus curve, variation of coupling constant with dihedral angle. Solvent effect, Fourier Transform Technique, Nuclear overhauser effect (NOE).

**UNIT-IV**

Carbon-13 NMR Spectroscopy- General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, Heteroaromatic and carbonyl carbon) coupling constants.

Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) - Definition, deduction of absolute configuration, octant rule for ketone.

**UNIT-V**

Mass Spectrometry- Introduction, ion production-EL, CL, F.D Factors affecting fragmentation, ion analysis. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, Nitrogen rule, Examples of mass special fragmentation of organic compounds with respect to their structure determination.



**Books Suggested-**

1. Modern Spectroscopy- J.M. Hollas Hohnwiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windowi and F.L. Ho Willey interscience.
3. NMR, NQR, ESR and Mossbaure spectroscopy in Inorganic chemistry- R.V. Parish, Ellis Harwood.
4. Physical Method in Chemistry – R.S. Drago, Saunders College.
5. Introduction to Molecular Spectroscopy – G.M. Barrow, Mcgraw Hill.
6. Basic Principle of Spectroscopy – R. Chang Mcgraw Hill.
7. Theory and Application of UV Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford.
8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.
9. Introduction to magnetic Resonance. A. Carrington and A.D. Maclachalan Harper & Row.
10. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Raniin and Cradock, ELBS.
11. Progress in Inorganic Chemistry, Vol. 8 Ed. F.A. Cotton Vol. 15 Ed. S.J. Lippard Wiley.





SEMESTER III

COMPULSORY FOR GROUP A, B, C

PAPER- II

CHEMISTRY OF BIO-INORGANIC & BIO-ORGANIC

**UNIT- I BIO-INORGANIC CHEMISTRY:**

Metal Ions in Biological Systems- Essential and trace metals. Na<sup>+</sup>/K<sup>+</sup> pumps- Role of metal ions in biological processes. Bio-energetic and ATP cycle- DNA polymerization, glucose storage, metal complexes in transmission of energy, chlorophylls, Photosystem-I and Photosystem-II in Cleavage of water. Model systems.

**UNIT- II**

Transport and Storage of Dioxygen- Heme protein and oxygen uptake, structure and function of Hemoglobin Myoglobin. Hemocyanins and hemerythrin, model synthetic complexes iron, cobalt and copper. Electron Transfer in Biology- Structure and function of metalloproteins in electron transport processes, Cytochromes and iron-sulphur proteins, synthetic models. Nitrogenase- Biological nitrogen fixation, Mo-Nitrogenase spectroscopic and other evidences. Other nitrogenases and model systems.

**UNIT-III BIO-ORGANIC CHEMISTRY**

Introduction- Basic considerations, Proximity effects and molecular adaptation. Enzymes- Introduction and historical perspective, Chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extractions and purification, Fischer's lock and key and Koshland's induced Fit hypothesis, Concepts and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics. Michaelis- Menten and Lineweaver- Burk plots. Reversible and irreversible inhibition.

**UNIT-IV**

Kinds of Reaction catalysed by Enzymes- Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer to sulphase, addition and elimination reactions, enolic intermediates in isomerisation reactions, Beta-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Co-Enzyme Chemistry- Cofactors as derived from vitamins, coenzymes, prosthetic groups, apo-enzymes structure and biological function coenzyme A thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, Lipoic acid. Vitamins B12 Mechanisms of reactions catalysed by above cofactors.

**UNIT-V**

Enzyme Models- Host-guest chemistry, chiral recognition and catalysis. Molecular recognition. Molecular asymmetry and prochirality. Biomimetic chemistry, Crown ethers, cryptates, cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes or synzymes.

Biotechnological Application of Enzymes- Large scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, use of enzymes in food and drink industry-brewing and cheese making syrup from corn starch, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy. Enzymes and recombinant DNA technology.



**Book Suggested-**

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg. University Science Book.
2. Bioinorganic Chemistry I. Bertuni, H.B. Gray, S.J. Lippard and J.S. Velentine, University Science books.
3. Inorganic Biochemistry Vol. I and II Ed. GL Eichhron. Elsevier.
4. Progress in Inorganic Chemistry Vol. 18 and 38 Ed. JJ Lippard Wiley.
5. Bioinorganic Chemistry. A Chemical approach to Enzyme action. Hprmann Dugas and C Penny Spnnger Veralg.
6. Understanding Enzymes. Travor Palmer Hall.
7. Enzyme Chemistry Impact and application Ed. Collin J Suckling. Chapmad and Hall.
8. Enzyme Mechanisms Ed M.I. Page and A Williams, Royal Society of Chemistry.
9. Fundamentals of Enzymology. N.C. Price and L. Sievens Oxford University Press.
10. Immobilised Enzyme- An introduction and application in Biotechnology Michael D TreVan John Wiley.
11. Enzymatic Reaction Mechanisms- C Walsh W.H. Freeman.
12. Enzyme structure and Mechanism – A Fersht. W.H. Freeman.
13. Biochemistry-The Chemical Reactions of living cells. DE Metzler. Academic press.
14. Principles of Biochemistry- A.L. Lehinger. Worth Publisher.
15. Biochemistry L. Stryer W.H. Freeman.
16. Biochemistry J. David Rawn. Neil Patterson.
17. Biochemistry Voiet and Voiet. John Wiley.
18. Outlines of Biochemistry. EE. Conn and PK Stumpt. John Wiley.
19. Biochemistry- L.Stryer, W.H. Freeman
20. Biochemistry- J.David Rawn, Neil Patterson
21. Biochemistry- Voet & Voet John Wiley
22. Biochemistry- Jain & Jain, S. Chand
23. Bio-Inorganic Chemistry By Kalsi



बिलासपुर विश्वविद्यालय, बिलासपुर (छत्तीसगढ़)

SEMESTER SYLLABUS

M.Sc. CHEMISTRY

SEMESTER III

GROUP- A

INORGANIC CHEMISTRY

PAPER- III

ORGANOTRANSITION METAL CHEMISTRY

#### UNIT- I

**Alkyls and Aryls of Transition Metals-** Types, routes of synthesis, stability and decomposition pathways. organocopper in organic synthesis.

#### UNIT- II

**Compounds of transition Metal-Carbon multiple bonds-** Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

#### UNIT- III

**Transition Metal  $\pi$  – Complexes-** Transition metal  $\pi$ -complexes with unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

#### UNIT- IV

**Transition Metal Compounds with Bonds to Hydrogen-**

Transition metal compounds with bonds to hydrogen.

**Fluxional Organometallic Compounds-**

Fluxionality and dynamic equilibria in compounds such as  $\eta^2$  olefin  $\eta^2$  allyl and dienyl complexes.

#### UNIT- V

**Homogeneous Catalysis-**

Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxoreaction) oxopalladation reactions, actions of C-H bond.



SEMESTER III

GROUP- A

INORGANIC CHEMISTRY

PAPER- IV

PHOTOINORGANIC CHEMISTRY

**UNIT- I Basic of Photochemistry -**

Absorption, excitation, photochemical laws, quantum yield, electronically excited states-life times-measurements of the times, Flash photolysis, stopped flow techniques, Energy dissipation by radiative and non-radiative processes absorption spectra Franck-Cordon principle, photochemical states- primary and secondary processes.

**UNIT- II Properties of Excited States-**

Structure, dipole moment, acid-base strengths, reactivity, photochemical kinetics-calculation of rates of radiative processes, Bimolecular deactivation quenching.

**UNIT- III Excited States of Metal Complexes-**

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge transfer spectra..

**UNIT- IV Ligand field Photochemistry-**

Photo-substitution, photo-oxidation and photo-reduction, lability and selectivity. Zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states.

**Metal Complex Sensitizers-**

Metal Complex sensitizer, electron relay, metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

**UNIT- V Redox reactions by excited Metal Complexes**

Energy transfer under conditions of weak interaction and strong interaction exciplex formation: Conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (e.g. 2'-bipyridine and 1, 10-phenanthroline complexes), illustration of reducing and oxidizing character of Ruthenium<sup>2+</sup> (bipyridal complex), comparison with Fe (bipy)<sub>3</sub> role of spin-orbit coupling life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes transformation of low energy reactants into high energy products, chemical energy into light.

**Book Suggested-**

1. Principle and application of Organotransition Metal Chemistry, J.P. Collman, L.S. Heegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree John Wiley.
3. Metallo-organic Chemistry, A.J. Pearson Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.
5. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischaur, Wiley.
6. Inorganic Photochemistry, J. Chem, Educ, Vol 60 No.- 10, 1983.
7. Progress in inorganic Chemistry vol 30ed, S.J. Lippard, Wiley.
8. Coordination Chem Revs., 1981, Vol 39, 121, 131, 1975, 15, 321, 1990, 97, 313.
9. Photochemistry of Coordination compounds, V. Balzan and V. Carassiti Academic Press.
10. Elements of Inorganic Photochemistry, G.J. Ferraudi Wiley.



SEMESTER III

GROUP-B

ORGANIC CHEMISTRY

PAPER-III

PHYSICAL ORGANIC CHEMISTRY

UNIT - I

**Concepts in Molecular orbital (MO) and Valence Bond (VB) Theory:**

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics. semi empirical methods and ab initio and density functional methods.

Qualitative MO theory - Huckel molecular orbital (HMO) method as applied to ethane allyl and butadiene. Qualitative MO theory - ionization potential. Electron affinities. MO energy levels. Orbital symmetry. orbital interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group. conjugation and hyperconjugation aromaticity. valence bond (VB) configuration mixing diagrams. hyperconjugation aromaticity. valence bond (VB) configuration mixing diagrams. relationship between VB configuration mixing and resonance theory. reaction profiles. potential energy diagrams curve-crossing model - nature of activation barrier in chemical reactions.

UNIT - II

**Solvation and Solvent Effects & Acids, Bases, Electrophiles, Nucleophiles, Catalysis:**

Qualitative understanding of solvent-solute effects on reactivity. thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria. various empirical indexes of solvation based on physical properties. solvent-sensitive reaction rates. spectroscopic properties and scales for specific solvation use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model. Acid-base Dissociation, Electronic and structural Effects, acidity and basicity, acidity functions and their application. hard and soft acids and bases. nucleophilicity scales. nucleofugacity. The alpha-effect. Ambivalent nucleophiles. Acid-Bases catalysis-specific and General Catalysis. Bronsted catalysis. nucleophilic and electrophilic catalysis. Catalysis by non covalent binding-micellar catalysis.

UNIT - III

**(a) Principles of Reactivity:** Mechanistic significance of entropy enthalpy and Gibb's free energy. Arrhenius equation. transition state theory. Uses of activation parameters. Hammond's postulate Bell-Evans-Polanyi principle potential energy surface model. Marcus theory of electron transfer. reactivity and selectivity principles.

**(b) Radical and Pericyclic Reactions:** Radical stability, polar influences, solvent and steric effects a curve crossing approach to radical addition. Factor affecting barrier heights in additions regioselectivity in radical reaction. Reactivity specificity and periselectivity in pericyclic reactions.

UNIT - IV

**Nucleophilic and Electrophilic Reactivity:**

Structural and electronic effects on  $S_N$  1 and  $S_N$  2 reactivity. Solvent effects. Kinetic isotope effects. Intramolecular assistance. Electron transfer nature of  $S_N$  2 reactions. Nucleophilicity and  $S_N$  2 reactivity based on curve-crossing model. relationship between polar and electron transfer reactions.  $S_{RN}$  1 mechanism. electrophilic reactivity. general mechanism kinetic of  $S_E$  2 Ar reaction. structural effects on rates and selectivity Curve-crossing approach to electrophilic reactivity.



**UNIT - V**

**Steric and Conformational Properties:**

Various types of steric strain and their influence on reactivity. Steric acceleration. Molecular measurement of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

**Book Suggested:**

1. Molecular mechanics U Burkert and N.L. Allinger ACD Monograph 177. 1982.
2. Organic Chemists Book of Orbirals. L. Salem and W.L. Jorgensen, Academic Press.
3. Mechanism and Theory in Organic Chemistry, T.H.Lowry and K.C. Richardson. harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular Modeling. W.B. smith VCH.Weinheim.
5. Physical Organic Chemistry. N.S. Isaacs.ELBS/ Longman.
6. Supramolecular Chemistry Concepts and Perspectives, J.M. Iehn. VCH.
7. The physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.



SEMESTER-III

GROUP-B

ORGANIC CHEMISTRY

PAPER-IV

CHEMISTRY OF HETEROCYCLIC COMPOUNDS

**UNIT - I**

**(a) Nomenclature of Heterocycles -**

Replacement and systematic nomenclature (Hantzsch - Widman system) for monocyclic, fused and bridged heterocycles.

**(b) Aromatic Heterocycles -**

General chemical behaviour of aromatic heterocycles. Classification (structure type) criteria of aromaticity (bond lengths, ring current and chemical shift in <sup>1</sup>H-NMR spectra, Empirical resonance energy, delocalisation energy and Dewar resonance energy, Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

**UNIT - II**

**Non aromatic Heterocycles -**

Strain-Bond angle and torsional strain and their consequences in small ring heterocycles. Conformation of six membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1, 3 diaxial interaction, stereo-electronic effect, anomeric effect, Attractive interaction hydrogen bonding and intermolecular nucleophilic-electrophilic interactions.

**UNIT - III**

**(a) Heterocyclic synthesis -**

Principle of heterocyclic synthesis involving cyclisation reactions and cyclo addition reactions.

**(b) Small Ring Heterocycles**

Three membered and four membered Heterocycles - synthesis and reactions of Aziridines, oxirane, thirane, Azetidines, Oxitanes and Thietanes.

**UNIT - IV**

**(a) six membered Heterocycles with one Hetero atom**

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium and thiopyrylium salts and pyridones. coumarins and chromones.

**(b) six membered Heterocycles with two or more Hetero atoms**

Synthesis and reactions of diazines, Triazines and Thiazines.

**UNIT - V**

**(a) Benzo-fused five membered Heterocycles**

Synthesis and reaction including medicinal application of Benzo-pyrrole, Benzo-furans and Benzo-thiophenes.

**(b) Seven and large membered Heterocycles**

Synthesis and reaction of azepines, thiepines, diazepines, Thiazepines.

**Book Suggested:**

1. Heterocyclic Chemistry by J.A. Joule, K. Mills and G.F. Smith. Chapman & Hall
2. Heterocyclic Chemistry by T.L. Gilchrist, Longman Scientific Technical.
3. An Introduction to Heterocyclic Chemistry by R.M. Acheson. John Wiley.
4. Organic Chemistry Vol. II by I.L. Finar ELBS



# बिलासपुर विश्वविद्यालय, बिलासपुर (छत्तीसगढ़)

## SEMESTER SYLLABUS

### M.Sc. CHEMISTRY

5. Rodds Chemistry of Carbon Compounds Ed. S. Coffery Elsevier
6. Natural Products chemistry and Biological Significance by J. Mamm, R.S. Davidson, J.B. Hobbs, J.B. harborne, Longman, Essex.
7. Heterocyclic Chemistry, Vol. 1 to 3, by R.D. Gupta, -----Kumar and v. Gupta. Springer Verlag.
8. Chemistry of Heterocycles, by T. Eicher and S. Hanpalmann. Thieme.
9. Contemporary Heterocyclic Chemistry by G.R. Newkome,





SEMESTER III  
GROUP-C  
PHYSICAL CHEMISTRY  
PAPER – III  
CHEMISTRY OF MATERIALS

**UNIT – I**

**Multiphase Materials**

Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

**Glasses, Ceramics, Composites and Nanomaterial's**

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications.

Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites. Nano crystalline phase, preparation procedures, special properties, applications.

**Thin Films and Langmuir – Blodgett Films**

Preparation techniques; evaporation/sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and applications of thin and LB films.

**UNIT – II**

**Liquid Crystals**

Mesomorphic behaviour, thermo tropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic – nematic transition and clearing temperature – homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

**UNIT – III**

**Polymeric Materials**

Molecular shape, structure and configuration, crystallinity, stress-strain behaviour, thermal behaviour, polymer types and their applications, conducting and ferro-electric polymers.

**Ionic Conductors**

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion super ionic conductors, examples and applications of ionic conductors.

**UNIT – IV**

**High  $T_c$  Materials**

Defect perovskites, high  $T_c$  superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multi gap structure in high  $T_c$  materials, applications of high  $T_c$  materials.

**Materials for Solid State Devices**

Rectifiers, Transistors, capacitors –IV-V compounds, low-dimensional quantum structures: optical properties.



**UNIT –V**

**Organic Solids, Fullerenes, Molecular Devices**

Conducting organics, organic superconductors, magnetism in organic materials.

Fullerenes – doped, fullerenes as superconductors.

Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches – sensors.

Nonlinear optical materials: nonlinear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility – materials for second and third harmonic generation.

**Books Suggested**

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D. Callister, Wiley.
3. Principles of the Solid State, H.V. Keer, Wiley Eastern.
4. Material Science, J.C.Anderson, K.D.Leaver, J.M. Alexander and R.D.Rawlings, ELEBS
5. Thermotropic Liquid Crystals, Ed., G.W.Gray, John Wiley.
6. Handbook of Liquid Crystals, Kelker and Hatz, ChemieVerlag.



SEMESTER III

GROUP-C

PHYSICAL CHEMISTRY

PAPER – IV

ADVANCED QUANTUM CHEMISTRY

**UNIT – I**

**Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory**

Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-Condon rules, Hartree-Fock equation, Koopmans and Brillouin theories, Roothan equation, Gaussian basis sets.

**UNIT – II**

**Configuration Interaction and MC-SCF**

Introduction to CI: full and truncated CI theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods.

**UNIT – III**

**Semi-Empirical Theories**

A review of the Huckel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic and properties. An introduction to MOPAC and AMI with hands on experience on personal computers.

**UNIT – IV**

**Density Functional Theory**

Derivation of Hohenberg-Kohn Theorem, Kohn-Sham formulation, N- and V- represent abilities; review of the performance of the existing local (e.g. Slater Xa and other methods) and non-local functions, treatment of chemical concepts with the density functional theory.

**UNIT – V**

**Computer Experiments**

Computer experiments using quantum chemistry – software packages such as GAUSSIAN/GAMESS/MOPAC and modelling software e.g. MM2/ AMBER/CHARM etc.

**Books Suggested**

1. Modern Quantum Chemistry, N.S.Ostlund and A. Szabo, McGraw Hill.
2. Methods of Molecular Quantum Mechanics, R. McWeeny and B.T.Sutcliffe, Academic Press.
3. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford.
4. Exploring Chemistry with Electron Structure Methods, J.B. Foresman and E. Frish, Gaussian Inc.
5. Semi-empirical MO Theory, J.Pople and D.L.Beveridge.



SEMESTER - III  
COMPULSORY FOR GROUP - A, B & C  
LABORATORY COURSE - I (GENERAL)

MM-200

Duration-12 hrs.

Note: The laboratory course (general) will be of 12 hours duration spread over two days. The examinee will have to perform three experiments. These experiments will be of 40 marks each 40 marks each will be allotted for viva - voce and Sessional work.

**PHYSICAL CHEMISTRY**

**A. Conductometry**

- Verify Debye Huckel and Onsager limiting law for strong electrolyte
- Determine the degree of hydrolysis and hydrolysis constant of  
(a)  $\text{CH}_3\text{COONa}$  (b)  $\text{NH}_4\text{Cl}$  (c) Aniline hydrachloride
- Determine the basicity of an organic acid by conductometric measurements.
- Determine the equivqlent conductance of an electrolyte and determine the dissociation constant.
- Determine solubility of sparingly soluble salts.

**B. Colorimetry**

- Determine the composition of  $\text{K}_2\text{Cr}_2\text{O}_7$  and  $\text{KMnO}_4$  using spectrophotometer
- Determine the dissociation constant of methyl red by Spectrophotometric method.
- To verify additivites of absorbances of a mixture of a coloured substance of  $\text{K}_2\text{Cr}_2\text{O}_7$  and  $\text{KMnO}_4$  using spectrophotometer.

**C. pH metry**

Determine pK value of given dibasic and tribasic acid by pH meter.

**D. Potentiometry**

Titrate ferrous ammonium sulphate against  $\text{K}_2\text{Cr}_2\text{O}_7$  and  $\text{KMnO}_4$  and determine redox potential of ferric system.

**E. Distribution coefficient**

- Determine the equilibrium constant of the reaction  $\text{KI} + \text{I}_2 \rightleftharpoons \text{KI}_3$  by distribution method.
- Determine the formula of complex formed between cupric ion and ammonia by distribution method.

**F. Partial molar volume:**

Determine the partial molar volume of Na Cl in aq. Solution at room temperature.

**INORGANIC CHEMISTRY**

**A. Instrumental method and Analytical Technique**

Spectrophotometric determination

- Manganese/Chromium/Vanadium in steel sample.
- Iron-salicylic acid complex by Job's method of continuous variation of concentration
- Zirconium-Alizarin red-s-complex; Mole ratio method.
- Copper Ethylenediamine Complex; Slope ratio method.

**B. Separation & determination of two metal ions:** Cu - Ni Zn-Ni-Mg-Ni involving volumetric & gravimetric method.

**C. Polarography**

Composition and stability constant of complexes

**D. Flame Photometric determination**

- Sodium and Potassium when present together
- Lithium/Calcium/Barium/Strontium
- Cadmium and Magnesium in tap water

**E. Quantitative & Qualitative Analysis:**



- a. Paper chromatography - Cadmium and Zinc and Magnesium
  - b. Thin layer chromatography-separation of Nickel, Manganese, Cobalt and Zinc. Determination of  $R_f$  values.
  - c. Ion Exchange.
  - d. Solvent Extraction
  - e. Electrophoretic separation.
- F. (i) Analysis of Dolomite.  
(ii) Estimation of available oxygen in  $H_2O_2$  by Iodometry.

### ORGANIC CHEMISTRY

#### A. Quantitative organic analysis Analytical Techniques.

- a. Estimation of Sulphur by messengers method.
- b. Estimation of Nitrogen by Kjeldahl method.
- c. Estimation of Halogen by Fusion method.
- d. Estimation of carbon and hydrogen by combustion method

#### B. Functional Group Estimation -

- a. Estimation of Aniline
- b. Estimation of Amino group by Acetylation method
- c. Estimation of Hydroxyl group by Acetylation method
- d. Estimation of Carboxyl group by Hydrazone formation method.
- e. Estimation of Glucose
- f. Estimation of Sucrose
- g. Estimation of methoxy group.

#### C. Chromatography -separation and identification of sugars present in the given mixture of glucose, Fructose, and sucrose by paper chromatography and determination of $R_f$ value.

### ANALYTICAL CHEMISTRY

1. Preparation of Homo and Hetero-Polyacids of Sb, V, Nb, Ta, Cr, Mo, W etc and study their properties
2. Determination of  $P_k a$  of weak acids by pH metric and spectrophotometric methods.
3. Purification of water by using natural materials, i. e. silica, alumina, iron oxide and zirconite, dolomite, charcoal etc.
4. Determination of distribution ratio and distribution co-efficient of organic and inorganic compounds.
5. Determination of percentage Extraction of Species of Interest.
6. Separation of organic compounds by the chromatographic technique i. e. TLC, paper Chromatography, column chromatography, column chromatography, Electrophoresis.
7. Analysis of carbohydrates, Amino acids, protein, alkaloid etc.
8. Analysis of pharmaceutical materials.
9. Analysis of surfactants, Detergents, Soap, oil etc.
10. Analysis of ore minerals, alloy, soil sediment
11. Application of Redox titration for analysis of Sn (iv), Fe (iii), Cr (VI), Mn (vii).
12. Analysis of water.
13. Collection, sampling, digestion and extraction of volatile materials.
14. Determination of equilibrium constant and composition of complexes.
15. Determination of dimerization/polymerization constant.



SEMESTER – IV

PAPER – I

COMPULSORY FOR GROUP - A, B & C

PHOTOCHEMISTRY & SOLID STATE CHEMISTRY

A – PHOTOCHEMISTRY

UNIT – I

**Photochemistry Reaction:** Interaction of electromagnetic radiation with matter, Types of excitation, Fate of excited molecule. Quantum yield. Transfer of excitation energy.

**Determination of reaction mechanism:** Rate constant and life time of reactive energy states, determination of rate constant of reaction. Effect of light intensity on the rate of photochemical reactions. Types of photo-chemical reactions. Photo-dissociation.

UNIT – II

**Photochemistry of Alkenes:** Intermolecular reactions of olefinic bond, geometrical isomerism. Cyclisation reaction, Rearrangement of 1,4 and 1,5-dienes.

**Photochemistry of Carbonyl compounds:** Intra-molecular reaction of Carbonyl compounds, saturated cyclic and acyclic,  $\beta,\gamma$ - unsaturated and  $\alpha,\beta$ - unsaturated compounds, cyclohexadienone. Inter-molecular cyclo addition reactions. Dimerization and Oxitane formation.

UNIT – III

**Photochemistry of Aromatic compounds:** Isomerisation, Addition, Substitution.

**Miscellaneous photochemical reactions:** Photo fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog.

B – SOLID STATE CHEMISTRY

UNIT –IV

**Solid State Reactions:** General principles. Experimental procedures methods, kinetics of solid state reactions.

**Crystal Defects and Non-stoichiometry :** Perfect and imperfect crystals, intrinsic and extrinsic defects, point defects, line and plane defects, Vacancies - Schottky defects and Frenkel defects. Thermodynamics and defect formation, colour centres, non-stoichiometry and defects.

UNIT – V

**Electronic properties and Band Theory:** Metals, insulators and semiconductors, Electronic structure of solids – band theory – band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semi-conductors, doping semiconductors, p-n junctions, optical properties – Photoconduction, photoelectric effects. Magnetic properties – Classification of materials. Effect of temperature. Calculation of magnetic moment. Magnetic domains. Superconductivity and organic solids, Occurrence, Principle and uses of conventional, organics and New super conductors.

**Books suggested:**

1. Solid State chemistry and its application – A.R.West, Plenum.
2. Principles of the Solid State, H.V.Keer, Wiley Eastern.
3. Solid State Chemistry, N.B.Hannary
4. Solid State Chemistry, D.K. Chakraborty, New Age International
5. Fundamentals of photochemistry, K.K.RohtagiMukherji, Wiley Eastern.
6. Essentials of molecular photochemistry, A. Gilbert and J. Baggott, Molecular photochemistry, N.J. Turro, W.A. Benjamin.
7. Introductory photochemistry, A. Cox and T. Camp, McGraw-Hill.
8. Photochemistry, R.P.Kundall and Gilbert, Thomson Nelson.
9. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.



SEMESTER – IV

PAPER – II

COMPULSORY FOR GROUP - A, B & C

BIO-PHYSICAL & ENVIRONMENTAL CHEMISTRY

A. BIO-PHYSICAL CHEMISTRY

UNIT-I

**Biological cell and its constituents:** Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems. Helix coil transition.

**Bioenergetics:** Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

**Statistical mechanics in biopolymers:** Chain configuration of macromolecules, statistical distribution end to end dimensions. Calculation of average dimensions for various chain structures, polypeptide and protein structures, introduction to protein folding problem.

UNIT-II

**Biopolymer interactions:** Forces involved in biopolymer interactions, Electrostatic changes and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibrium and various types of binding processes in biological systems. Hydrogen ion titration curves.

**Thermodynamics of biopolymer solutions:** Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical systems.

**Cell Membrane and Transport of Ion:** Structure and function of Cell membrane, ions transport through Cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.

UNIT-III

**Biopolymer and their Molecular Weights:** Evaluation of size, shape, molecular weight and extent of hydration of biopolymer by various experimental techniques, Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation viscosity, electrophoresis and rotational motions.

**Diffraction Methods :** Light scattering, low angle X-ray scattering X-ray diffraction and photo correlation spectroscopy. ORD.

B. ENVIRONMENTAL CHEMISTRY

UNIT-IV

**Environment:** Introduction, Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S, and Bio distribution of elements.

**Hydrosphere:** Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle, Aquatic pollution-inorganic, organic. Pesticide, agricultural industrial and sewage, detergents, oil spills and oil pollutants.

UNIT-V

**Water quality parameters** - Dissolved oxygen, biochemical oxygen demand, solids, metals, sulphate, phosphate, Nitrate, fluoride Micro-organism and their hazardous effects on life. Water quality standard. Analytical methods for measuring BOD, DO, COD, F oils, metals (As, Cd, Cr, Hg, Pb, Se etc.) Residual chloride and chlorine demand. Purification and treatment of water (Students must be well acquainted with the physiological effects and chemical principles involved in their estimation.)

**Industrial pollution :** Chemists overview of pollution and its possible solutions caused by industries such as Cement, sugar, distillery, paper and pulp, thermal power plants. Nuclear power plants. Metallurgy, polymers, drugs etc. Radionuclide analysis, Disposal of wastes and their management.



**Books Suggested:**

1. Bioorganic Chemistry. A Chemical Approach to Enzyme Action, H.Dugas and C. Penny. Springer-verlag.
2. Macromolecules. Structure and Function, F. Word, Prentice Hall
3. Environmental Chemistry. S.E. Manahan. Lewis Publishers.
4. Environmental Chemistry, Sharma and Kaur, Krishna Publishers.
5. Environmental Chemistry, [A.K.De](#). Wiley Eastern.
6. Environmental Pollution Analysis S.M.Khopkar, Wiley Eastern.
7. Standard Method of Chemical Analysis, F.J.Welcher. Vol III, Van Nostrand Reinhold Co.
8. Environmental Toxicology, Ed. J Rose. Gordon and Breach Science Publication.
9. Elemental Analysis of Airborne Particles, Ed. S. Lansberger and M Cretchman. Gordon and Breach Science Publication.
10. Environmental Chemistry, C.Baird, W.H.Freeman.





SEMESTER IV

GROUP- A

PAPER- III

BIOINORGANIC CHEMISTRY & SUPRA-MOLECULAR CHEMISTRY

**UNIT- I**

**Metal Storage Transport and Bio-mineralization-** Ferritin, Transferring and siderophores.

**Calcium in Biology-** Calcium in living cells, transport and regulation molecular aspects of intermolecular processes, extracellular binding proteins.

**UNIT- II**

**Metalloenzymes-** Zinc enzymes- carboxy-peptidase and carbonic anhydrase. Iron enzymes Catalase.

**Peroxidase and cytochrome p-450. Copper enzymes-** superoxide dismutase Molybdenum oxatransferase enzymes- xanthine oxidase. Coenzyme vitamin B12.

**UNIT- III**

**Metal-Nucleic Acid Interactions-** Metal ions and metal complex interactions, metal complexes-nucleic acids.

**Metals in Medicine--** Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs.

**UNIT- IV**

**Molecular recognition--** Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co-receptor molecules and multiple recognition. Supra-molecular reactivity and catalysis.

**UNIT- V**

Transport processes and carrier designs.

Supra-molecular devices, Supra-molecular photochemistry, supra-molecular electronic, ionic and switching devices, some examples of self-assembly in supra-molecular chemistry.



SEMESTER- IV

GROUP- A

PAPER- IV

ANALYTICAL CHEMISTRY

**UNIT- I**

**Introduction-**

Role of analytical chemistry. Classification of analytical method- classical and instrumental. types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operation and practices. Analytical balance. Techniques of weighing errors. Volumetric glasswares-cleaning and calibration of glasswares ,sample preparation-dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents, Laboratory notebooks, Safety in the analytical laboratory.

**UNIT- II**

**Error and Evaluation-**

Definition of terms in mean and median, Precision- standard deviation, relative standard deviation. Accuracy- absolute error, relative error. Types of errors in experimental data determinate (Systematic), indeterminate (or random) and gross Source of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data- indeterminate errors. The uses of Statistics.

**UNIT- III**

**Food Analysis:**

Moisture, ash, crude protein, fat, crude fiber, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration- common adulterants in food, contamination of food stuffs. Pesticide analysis in food products. Extraction and purification of sample. HPLC Gas chromatography for organophosphates. Thin- layer chromatography for identification of chlorinated pesticides in food products.

**UNIT- IV**

**Analysis of Water Pollution:**

Origin of waste water, types, water pollutants and their effects. Sources of water pollution- domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objective of analysis, parameter for analysis - color, turbidity. total solids, conductivity acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica phosphates and different forms of nitrogen. Heavy metal pollution- public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic General survey of instrumental technique for the analysis of heavy metal in aqueous systems.

**UNIT- V**

**Analysis of Soil Fuel -**

(a) Analysis of Soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

(b) Fuel analysis: Solid, liquid, and gas, Ultimate and proximate analysis ,heating values-grading of coal. Liquid fuels- flash point, aniline point octane number and carbon residue. Gaseous fuels- producer gas and water gas-calorific values.

**Book Suggested-**

1. Principle of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg University Science Books.



# बिलासपुर विश्वविद्यालय, बिलासपुर (छत्तीसगढ़)

## SEMESTER SYLLABUS

### M.Sc. CHEMISTRY

2. Bioinorganic Chemistry, I Bertini, H.B. Gray. S.J. Lippard and J.S. Valentine University Science Book.
3. Inorganic Biochemistry vols I and II ed. G. L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed., J.J. Lippard Wiley.
5. Supramolecular Chemistry, J.M. Lehn VCH.
6. Analytical Chemistry, G.D. Christian, J. Wiley.
7. Fundamentals of Analytical Chemistry, D.A. Skoog. D.M. West and F.J. Holler, W.B. Saunders.
8. Analytical Chemistry- Principle, J.H. Kennedy, W.B. Saunders.
9. Analytical Chemistry- Principle and Techniques, L.G. Hargis, Prentice Hall.
10. Principles of Instrumental Analysis, D.A. Skoog and J.L. Loary, W.B. Saunders.
11. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
12. Quantitative Analysis, R.A. Day, Jr, and A.L. Underwood. Prentice Hall.
13. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
14. Basic Concept of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
15. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.



SEMESTER-IV

GROUP-A

LABORATORY COURSE (SPECIAL)

PHOTO INORGANIC & ORGANO-TRANSITION CHEMISTRY

12 hrs. (In two days)

200 marks

Note: Special Practical Course for Group 'A' will be of 8 hrs duration spread over two days. The examinee will have to perform three experiments (one each from Section A, B, and C). These experiments will be of 20 marks each 20 marks each will be allotted for viva-voce and Sessional work.

SECTION-A

**A. Preparation:**

Preparation of selected inorganic compounds and their study by IR, electronic spectra, Mossbauer, ESR, and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines. Selection can be made from the following.

1. Sodium amide. Inorg. Synth. 1946, 2, 128
2. Synthesis and thermal analysis of group II metal oxalate hydrate, J. Chem. Ed., 1988.65, 1024.
3. Atomic absorption analysis of Mg and Ca.
4. Trialkoxyboranes - Preparation, IR, and NMR spectra.
5. PhBCl<sub>2</sub> Dichlorophenylborane -Synthesis in vacuum line.
6. Preparation of Tin (IV) iodide, Tin (IV) chloride and Tin (II) iodide Inorg. Synth. 1953.4.119.
7. Relative stability of Tin (IV) and Pb (IV). Preparation of ammonium hexachlorostannate (NH<sub>4</sub>)<sub>2</sub> s-et, ammonium hexachloroplumbate (NH<sub>4</sub>) PbCl<sub>6</sub>.
8. Hexa - bis (4- nitrophenoxy) cyclotriphosphazene.
9. Synthesis of Trichlorodiphenylantimony (V) hydrate. Inorg. Synth. 1985, 23, 194.
10. Sodium tetrathionate Na<sub>2</sub>S<sub>4</sub>O<sub>6</sub>.
11. Metal complexes of Dimethyl sulfoxide (IR): CuCl<sub>2</sub> 2 DMSO, PdCl<sub>2</sub>• 2DMSO, RuCl<sub>2</sub>, 4DMSO, Chem. Edu, 1982.59.57.
12. Synthesis of metal acetylacetonate : Magnetic moment, IR, NMR Inor, Synth. 1957.5.130: 1963. 1. 183.
13. Bromination of Cr (acac); J.Chem. Edu., 1986,63,90.
14. Magnetic moment of Cu (acac) 2Hp
15. Cis and Trans [Co (en) 2Cl<sub>2</sub>].
16. Separation of optical isomer of cis-[Co (en) 2 Cl<sub>2</sub>] J.Chem. Edu. 1960, 4369
17. Ion Exchange separation of oxidation state of vanadium. J. Chem.Edu, 1980, 57 316; 1978, 55, 55
18. Determination of Cr (III) complexes. [Cr (Hp)<sub>6</sub>] NOI<sub>3</sub>HP; [Cr (Hp)<sub>4</sub>] Cl<sub>2</sub>HP; [Cr(en)<sub>3</sub>] Cl<sub>3</sub>, Cr (acac); Inorg. Synth. 72.13.184.
19. Preparation of N, N bis (salicylaldehyde) ethylene, salen H<sub>2</sub>, Co (Salen) J. chem. Educ., 1977, 54, 443; 1973, 50,670. Determination of O<sub>2</sub> absorption by Co (salen) Acct. Cem.Res.1975, 8,384. Reaction of oxygen adduct with ChCl<sub>3</sub> (deoxygenation).



20. Preparation of Fe (II) Chloride use it as Friedel-Craft chlorination source. J.Org.Chem., 1978,43,2423; J. Che. Edu., 1984,61,645; 1986,63,361.
21. Reaction of Cr (III) with a multidentate ligand: a kinetic experiment (Visible spectra Cr - EDTA complex) JAC.S. 1953, 75, 5670.
22. Preparation of [Co (phenanthroline - 5, 6-quinone)]. J. Chem.Soc.,A, 1970,447. J. Chem. Edu., 1977, 54,710.
23. Preparation and use of Ferrocene. J. Chem.edu., 1966, 43, 73; 1976, 53,730.
24. Preparation of copper glycine complex - cis and trans bis [glycinato Copper (II)] J. Chem. Soc. Dalton, 191979, 1901, J.Chem. Edu. 1982,59,1052.
25. Preparation of phosphine  $\text{Ph}_3\text{P}$  and its transition metal complexes.
26. Any other experiment such as conversion of p-xylene to terephthalic Acid catalyzed by  $\text{CoBr}_2$  (homogeneous catalysis).

### SECTION - B

1. **Inorganic Reaction Mechanism:** Kinetics and mechanism of following reactions:
  - i. Substitution reactions in octahedral complexes (acid hydrolysis and base hydrolysis).
  - ii. Redox reaction in octahedral
  - iii. Isomerisation reaction of octahedral.
2. **Bio-Inorganic chemistry:**
  - i. -Extraction of chlorophyll from green leaves of student's choice. Separation of chlorophylls and their electronics spectral study.
  - ii. Complexation study of Cu (II) ion with biologically important amino acids.
3. **Inorganic Photochemistry:**
  - i. Synthesis of potassium ferrioxalate and determination of the intensity of radiation.
  - ii. Photo-oxidation of oxalic by  $\text{UO}_2$  sensitization.
  - iii. Photodecomposition of HI and Determinant of its quantum yield.

### Books Suggested-

1. A.W. Adamson and P.D. Fleischer: Concept of inorganic Photo Chemistry.
2. V Balani and V. Carassilli: Photochemistry of Coordination compounds.
3. K.K. Rohatagi Mukherjee: Fundamentals of Photochemistry.
4. Quarterly Reviews 21,213 (1967).
5. coordination Chemistry Reviews: 3,169 (1968)
6. Quarterly Reviews: 8,422 (1954)
7. G.L. Eichhorn: Inorganic BioChemistry, Vols. I, II.
8. M.W. Hughes inorganic Chemistry of Biological Process.
9. Purcell and Kotz: Inorganic Chemistry.
10. R.C. Mehrotra and A Singh : Organometallic Chemistry : An Introduction.
11. J.J. Lagowski: Modern Inorganic Chemistry.
12. Cotton and Wilkinson (Vth) Edition: Advanced Inorganic Chemistry.



SECTION-C

**1. Complete analysis of alloys, ores and mineral-**

- (a) Ni Al Alloy (b) Ag, Cu, Ni, and Zn alloy
- (c) Cu, Ni and Zn Alloy (d) Stainless steel
- (e) Dolomite Silica Sesquioxide, CA, Mg
- (f) Haematite, Silica, Al, Ca & Mg
- (g) Bauxite Silica Fe, Be.

**2. Inorganic preparation of advanced nature:**

Complex salt of Cobalt and chromium with various coordination spheres. Barium tetrathio carbonate, Ammonium tetrathio cupprato potassium perchlorate Red. Mercuric sulphide, Ammonium meta Vana-date, tin (VI) Iodide, Silicotungestic acid.

**3. Experiments baed on the following instrumental techniques:**

- (a) Colorimetry and spectrophotometr, Beer's law, stimation of inorganic ions, pH various of indicators and study of complexes by various methods Absorption spectra in visible and ultraviolet region.
- (b) Potentiometry- Dissociation constant of acids, Redox potentials and study of complex formation.
- (c) pH metry- Dissociation constants of acids, study of complex.
- (d) Dissociation constants of acids and quantitative determination of mixture of halides.
- (e) Polarography. Use of dropping mercury and rotating platinum electrodes half wave potentials of Zn and cadmium and their determination in trace amount and study of complex.
- (f) Dipole moment measurement of dielectric constants of liquids, calculation of dipole moment.
- (g) Other experiments of Advanced Nature.

**Books Suggested.**

- 1. Cotton and wilkinson Advanced inorganic Chemistry 3rd Ed.
- 2. Dey and Selbin Theoretical Inorganic Chemistry 3rd Ed.
- 3. Emeleus and Anderson Modern Aspects of Inorganic Chemistry.
- 4. Barnar J. Theoretical Principles of Inorganic Chemistry.
- 5. Pauling The Nature of Chemical Bond
- 6. Gilerath Fundamental Concepts in Inorganic Chemistry.
- 7. Dongilas & Mecdaniel Concepts and Models in Inorganic Chemistry.
- 8. Harvey and Borter Introduction of Physical Inorganic Chemistry.
- 9. Durrant and Durrant Introduction to Advanced Inorganic Chemistry.
- 10. Drago, R.S. Physical Methods in Inorganic Chemistry.
- 11. Weddington Non Aqueous Solvent System Part I & II
- 12. Chemistry in Non-aqueous Solvents.
- 13. Satya Prakash Advanced Chemistry of Ray elements
- 14. Moeller Advanced Inorganic Chemistry.
- 15. Rabinso and Helsop Inorganic Chemistry.
- 16. Glenn and Seaorg The Transuranium Elements
- 17. Moeller The Chemistry of Lanthanides
- 18. JulJy N. SynthetiC Inorganic Chemistry.



19. Sheeds Maynard Comprehensive Inorganic Chemistry Vol. I to XIV
20. Eneidiander & Keennedy Introduction to Radio Chemistry Chemistry of Nuclear & Radiation Chemistry
21. Overman Basic Concepts of Nuclear chemistry
22. Vogel Text Book of Quantative Inorganic Analysis 4th Ed.
23. Meits and thoms Advanced Analytical Chemistry.
24. Ayres Quantitative Chemistry Analysis
25. Treadwell and hall Analytical Chemistry vol. t and II
- 26. Busev/poliankit The use of Organic Reagents in Inorganic Analysis
27. Figgis Introduction to Ligand Fields
28. Nettle Co-ordination Compounds
29. Jones Elementary Co-ordination Chemistry.
30. Bailer Chemistry of the Co-ordination Compounds
31. Liwis & Wilkins Modern Co-ordination Chemistry
32. Basalo & Perason Mechanism of Inorganic Reaction
33. Martell & Calvin Chemistry of Chelete compounds
34. Hahan University Chemistry
35. Malik tuli and Madan Selected topics of Inorganic Chemistry.
36. Benerjee Fundamental principles of Inorganic Chemistry.
37. Emeleus & Sharpe Modern Aspects of Inorganic Chemistry.
38. Bailars, Emeleus Comprehensive Inorganic chemistry Vol. I to V
39. Emeleus Inorga9ic Chemistry series on Vol. I to x.



### UNIT - I

#### Drug Design-

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity : occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free- Wilson analysis, Hansch analysis, relationship between Free-Wilson and Hansch analysis, LD-50, ED-50 (Mathematical derivations of equations excluded).

### UNIT - II

#### (a) Pharmacokinetics:

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention uses of pharmacokinetic in drug development process.

#### (b) Pharmacodynamics

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

### UNIT - III

#### (a) Antineoplastic Agents:

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors synthesis of mechlorethamine, cyclophosphamide, melphalan, uracil, mustards and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

#### Local Anti-infective drugs

Introduction and general mode of action-synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapson, aminosalicic acid, isoniazid, ethionamide, ethambutal, fluconazole, econazole, griseofulvin, Chloroquin and primaquin.

### UNIT-IV

#### Cardiovascular Drugs:

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators, synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, exiprenolol..

Cell wall bio synthesis, inhibitors, -lactam rings, antibiotics inhibiting protein synthesis. Synthesis, of penicillin-G penicillin-V, ampicillin, amoxicillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.





**UNIT-V**

**Psychoactive Drugs- The Chemotherapy of Mind-**

Introduction, neurotransmitters, CNS depressants, general anesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs-the neuroleptics, antidepressants, butyrophenones, serendipity and drug development stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium. glutethimide.

**Book suggested:**

1. Introduction to Medicinal Chemistry. A. Gringuage Wiley-VCH
2. Wilson and Gisvolds Text Book of Organic Medicinal and Pharmaceutical Chemistry ED. Robert F. Dorge.
3. An Introduction to drug design, S.S.Pandaya and J.R. Dimmock, New Age International.
4. Burgers Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch- 14) Ed ME Wolff, John Wiley.
5. Goodman and Gilman's Pharmacological Basis of Therapeutics McGraw-Hill.
6. The Organic Chemistry of Drug and Drug Action, R.B.Silverman Academic Press.
7. Strategies for Organic Drug Synthesis and Design D Lednicer, John Wiley.
8. Drug Design and Medicinal Chemistry by S.N. Pandaya.
9. Medicinal Chemistry by Ashutosh Kar.



SEMESTER-IV

GROUP-B

PAPER-IV

CHEMISTRY OF NATURAL PRODUCT

**UNIT - I**

**Terpenoids-**

Classification, nomenclature, occurrence, isolation, general methods of structure determination, Isoprene Rule,

Structure determination, stereochemistry, biosynthesis and synthesis of Citral, Geraniol,  $\alpha$ -Terpeneol, Menthol, Camphor,  $\alpha$ -pinene, Zingibarene, Phytol, abietic acid.

**UNIT -II**

**Alkaloids-**

Definition, nomenclature and physiological action, occurrence, isolation, general method of structure, elucidation, degradation, classification based on nitrogen heterocyclic ring. Role of alkaloids in plants. Structure elucidation, stereochemistry, synthesis and biosynthesis of Ephedrine (+) - coniine, Nicotine, Atropine, Quinine and morphine.

**UNIT - III**

**Steroids and Hormones-**

Occurrence, Nomenclature, Basic skeleton, Diels-Hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol, bile acids, Androsterone, Testosterone, Ergosterol, Sigmasterol, Oestrone, Progesterone, Aldosterone.

**UNIT - IV**

**Plan pigment-**

Occurrence, nomenclature, and general methods of structure determination. Isolation and synthesis of Bixin, Quercetin, Daidzein, Cyanin, Pelargonin chloride, Hirustidin.

Biosynthesis of flavonoids, Acetate pathway and shikimic acid pathway.

**UNIT - V**

**(a) Porphyrins & Carotenoids-**

Structure and synthesis of Haemoglobin and chlorophyll, spectral properties of porphyrins. Biosynthesis of Porphyrin, Phthalocynin, B-carotene and its relation with Vitamin A, Y carotene.

**Book Suggested-**

1. Natural Products: Chemistry and Biological Significance, J. Mann, R. S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
2. Organic Chemistry, Vol 2, I. L. Finar, ELBS.
3. Stereoselective Synthesis : A Practical Approach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed.S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic publishers.
7. New Trends in Natural Product Chemistry, Atta-urRahman and M.I. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, SukhDev, Harwood Academic publishers.



SEMESTER-IV  
GROUP-B  
LABORATORY COURSE (SPECIAL)  
ORGANIC CHEMISTRY

200 marks

Note: Laboratory course with Group 'B' will be of 12 hrs duration spread over two days. The examinee will have to perform three experiments. These experiments will be of 40 marks each. 40 marks each will be allotted for viva-voce and Sessional work.

**Qualitative Analysis**

Separation, Purification and identification of the components of a mixture of binary organic compounds & mixture of three organic compounds.

**Multi-step synthesis of Organic compounds (Three stage preparations. Preparation of pure crystalline product. By using any two following principals Conformation by melting point determination.)-**

The exercises should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

1. Photochemical reaction: Benzophenone- Benzopinacol- Benzpinacolone.
2. Beckmann rearrangement: Benzanilide from benzene, Benzene- benzophenone ,oxime- Benzanilide.
3. Benzilic acid rearrangement : Benzilic acid from benzoin, (Benzoin- Benzil- Benzilic acid)
4. Synthesis of heterocyclic compounds, Skraup synthesis: Preparation of quinoline from aniline, Skraup synthesis: Preparation of 2 phenyl-indole from phenyl hydrazine.
5. Sandmeyer Reaction: Preparation of o chlorobenzoic acid from anthranilic acid.
6. Ultman reaction - Preparation of N-Phenyl anthranilic acid from o-chlorobenzoic acid.
7. Preparation of Acridone from N-Phenyl anthranilic acid.
8. Preparation of p nitro aniline
9. Preparation of p bromo aniline
10. Preparation of methyl orange from aniline via sulphanilic acid.

**Extraction of Organic compounds from Natural sources-**

1. Isolation of caffeine from tea leaves
2. Isolation of casein from milk
3. Isolation of lactose from milk
4. Isolation of nicotine dipicrate from tobacco
5. Isolation of piperine from black pepper
6. Isolation of lycopene from tomatoes
7. Isolation of b-carotene from carrots.

**Paper Chromatography**

Separation and identification of the sugars, dyes and amino acids present in the given mixture of sugars, dyes and amino acids by paper chromatography and determination of RF values.

**Spectroscopy:**

Identification of organic compounds by the analysis of their spectral data (UV. IR. PMR, CMR & M) Spectrophotometric (UV/VIS) Estimations of

1. Amino acids
2. Proteins
3. Carbohydrates
4. Aspi



SEMESTER-IV

GROUP-B

LABORATORY COURSE (SPECIAL)

PHYSICAL CHEMISTRY

1. Study of kinetics of exchange between ethyl iodide and the iodide ion.
2. Determination of the solubility product of lead iodide.
3. Determination of the dissociation constant of barium nitrate.
4. Determination of relative strength of the acids by studying the hydrolysis of an ester.
5. Study the hydrolysis of methyl acetate catalysed by HCl and equimolar urea hydrochloride and hence the degree of hydrolysis of the salt.
6. Investigate the inversion of can-sugar in presence of an acid. Determine also the energy of activation of the reaction.
7. Study in inversion of can-sugar in presence of HCL and  $H_2SO_4$  and hence determine the relative strength of the acids.
8. Study the kinetics of hydrolysis of ethyl acetate by NaOH at two temperatures by conductance measurement, and hence the energy of activation of the reaction.
9. Study the kinetics of hydrolysis of tertiary amyl iodide, and determine the order and energy of activation of the reaction.
10. Investigate the reaction between  $H_2O_2$  and HI.
11. Study the kinetics of decomposition of benzene diazonium chloride at different temperatures.
12. Study the kinetics of reaction between  $K_2S_2O_8$  and KI.
  - (a) Determine and rat constant and order of reaction.
  - (b) Study of influence of ionic strength on the rate constant.
13. Investigate the kinetics of autocatalytic reaction between  $KMnO_4$  and Oxalic acid.
14. Determination of order of reaction between bromic acid and hydrobromic acids.
15. Determination of concentration f iodine in a given sample (KI) by isotope dilution technique.
16. Determination of effect of-
  - (a) Change of temperature.
  - (b) Change of concentration.
  - (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester.
17. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidised by persulphate ion.)
18. Investigate the adsorption of oxalic acid from aqueous solution by activated charcoal and verify Frenndlish and Langmuir's adospriton isotherms.
19. Determine adsopition isotherms of acetic acid from aqueous solution by charcoal.



SEMESTER IV  
GROUP C  
PHYSICAL CHEMISTRY  
PAPER III  
LIQUID STATES

**UNIT-I**

**General properties of Liquids**

a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations, internal pressure and its significance in liquids. Equations of state, critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids, additivity of pair potential approximation.

b) A classical partition function for liquids, correspondence principle, configuration, integral, configuration properties.

**UNIT-II**

**Theory of liquids**

Theory of liquids, partition function, method or model approach; single cell models, communal energy and entropy, LTD Model, significant structure model.

**UNIT-III**

**Distribution function and Related Equations**

Radial distribution method, equation of state in terms of RDF. Molecular distribution functions, pair function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, clusters expansion.

**UNIT-IV**

**Methods for Structure Determination and Computational Techniques**

Spectroscopic techniques for liquid dynamic structure studies. Neutron and X-ray scattering spectroscopy. Computation Techniques-Monte Carlo and molecular dynamics methods.

**UNIT- V**

**Super cooled and Ionic Liquids**

Super cooled and ionic liquids, theories of transport properties; non Arrhenius behaviour of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in super cooled liquids.

**Books Suggested**

1. An Introduction to Liquid State, P.A. Egelstaff, Academic Press.
2. The Dynamic Liquid State A.F.M. Barton, Longman.
3. Introduction to Statistical Thermodynamics, T.L. Hill, Addison Wiley .
4. The Liquid State J.A. Pryde.
5. Significant Liquid Structures, H. Eyring and M.S. John.



SEMESTER IV

GROUP C

PHYSICAL CHEMISTRY

PAPER IV

COMPUTATION CHEMISTRY

**UNIT - I**

**Fortran/c Programming and Numerical Methods** -Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopic considering the background of students, available time etc.

**Solution of Equations**-Bisection, regular falsi, Newton -Raphson and related methods for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning.

**Linear Simultaneous Equations**-Gaussian elimination, Gauss -Seidel method, Gauss-Jordan method, Pivoting strategy. Errors and ill conditioning.

**UNIT - II**

**Eigen values and Matrix Diagonalization**-Jacobi and Householder methods, analysis or errors.

**Interpolation**-Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. Polynomial wiggle problem.

**UNIT - III**

**Numerical Differentiation**-Solution of simple differential equations by Taylor series and Runge-Kutta methods.

**Numerical Integration**-Newton-Cotes formulae, Romberg integration, errors in integration formulae.

The Students should develop computer programs for some of the above numerical methods.

**UNIT - IV**

**Running of Advanced Scientific Packages**-The students are expected to get hands on experience of running a few selected advanced level scientific software packages after a brief introduction to the basic theory and methodology. ab initio quantum chemical packages such as GAUSSIAN/GAMES With carefully designed exercises for illustrating various features of the packages. Semi-empirical/Dynamics/simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design. etc.

**UNIT - V**

**Introduction to Networking and using Internet -Project**-The students will develop utilities such as analysis of spectra, simulation programmes which will supplement laboratory or theory exercises in physical, organic, inorganic chemistry or biochemistry. This list is only indicative and a variety of small projects designed by the teacher based on the interest of the student and capabilities should be worked out.

**Book Suggested**

1. Computational Chemistry, A.C. Norris, John Wiley.
2. Computer Programming in FORTRAN 77, R. Rajaraman, Prentice Hall.
3. Numerical Analysis, C.E. Froberg, Macmillan.
4. Numerical Analysis - A Practical Approach, M.J. Maron John Wiley.
5. Numerical Methods for Scientists and Engineers, H.M. Antia, Tata McGraw Hill.



SEMESTER IV  
GROUP C  
PHYSICAL CHEMISTRY  
LABORATORY COURSE (SPECIAL)

200 marks

Number of hours for each experiment: 3-4 hours

A list of experiments under different headings is given below. Typical Experiments are to be selected from each type.

### Thermodynamics

- (i) Determination of partial molar volume of solute (e.g., KCl) and solvent in a binary Mixture.
- (ii) Determination of the temperature dependence of the solubility of a compound in Two solvents having similar intermolecular interactions (benzoic acid in water and in DMSO- water mixture) and calculate the partial molar heat of solution.

### Spectroscopy

- (i) Determination of pKa of an indicator (e.g., methyl red) in (a) aqueous and (b) micellar media.
- (ii) Determination of stoichiometry and stability constant of inorganic (e.g. ferric - salicylic acid) and organic (e.g. amine-iodine) complexes.
- (iii) Characterization of the complexes by electronic and IR spectral data.

### Polarography

- (i) Estimation of  $Pb^{2+}$  and  $Cd^{2+}$  /Zn and  $Ni^{2+}$  ion in a mixture of  $Pb^{2+}$ /Zn<sup>+</sup> and  $Ni^{2+}$  by Polarography.
- (ii) Determination of dissolved oxygen in aqueous solution of organic solvents.

### Electronic

This lab course will have theory as well as practical and the lectures shall be delivered during lab hours.

### Basic Electronics

Notations used in an electric circuit, study of electronic components and colour codes, conversion of chemical quantities into electrical quantities. Transducer, illustration with electrodes, thermocouples and thermostats. Passive components: Resistors, capacitors and inductors with some emphasis on solid state properties of materials. Net works of resistors. Thevenin's theorem, superposition theorem, loop analysis R C circuits, L R circuits Illustration of the use of the circuits in NQR spectroscopy, Mossbauer spectroscopy, cyclic voltametry and in power supplies as filter circuits.

### Active Components

Introduction to ordinary diodes and Zener diodes with some emphasis on p-n junction as a solid state property. Use of diodes as rectifiers, clipping and clamping circuits. Power supplies. Transistors: An extension of p-n junction to p-n-p and n-p-n transistors. Characteristics of circuits. Derivation pairs, differential amplifiers.

### Operational Amplifiers

Ideal characteristics; inverter, summer, integrator, differentiator, voltage follower, illustrative use of operational amplifiers. Introduction to Fourier transform in instrumentation.



### List of Experiments in Electronics

1. Measurements of resistance with multimeter
2. To measure the resistance of the given ammeter
3. Voltage measurement with CRO
4. Familiarising with CRO
5. Use of a Wheatstone Bridge for accurate measurement of resistance
6. Capacitor as a charge storage device
7. To study the behaviour of parallel charged capacitors in series charged capacitors placed in parallel
8. The use of LCR Bridge
9. Response characteristics of RC network
10. Response characteristics of LR network
11. Response characteristics of LCR network
12. Verification of Kirchoff's law
13. To study the Lissajou's figures
14. Measurement of e.m.f. with thermocouple
15. To plot the characteristic curve of a diode
16. Half-wave and full-wave rectifier
17. Clipping and clamping circuits
18. Capacitor filter for full-wave rectifier
19. Voltage doubler, Zener stabilized bipolar power supply
20. Transistor characteristics
21. Differential amplifier
22. Transistor amplifier
23. Transistor amplifier
24. Introduction of an operational amplifier as a voltage follower
25. Op-Amp as non-inverting and inverting amplifier
26. Simple integration differentiation with Op-Amp 741
27. Op-Amp as comparator
28. Designing and fabrication of a printer circuit board
29. Setting up of a thermostat Constant temperature bath
30. Four-probe method for resistivity measurement

### Books Suggested

1. Inorganic Experiments, J. Derek Woollins VCH.
2. Micro scale Inorganic Chemistry, Z. Szafran, R.M. Pike and M.M. Singh, Wiley.
3. Practical Inorganic Chemistry, G. Marr and B.W. Rockett, Van Nostrand
4. The Systematic Identification of Organic Compounds, R L. Shriner and D. Y Curtin
5. Semi micro Qualitative Organic Analysis, N.D. Cheronis, J.B. Entrikin and E.M. Hodnett
6. Experimental Organic Chemistry M. P. Doyle and W.S. Mungall
7. Small Scale Organic Preparations, P.J. Hill.
8. Organ metallic Synthesis, J.J. Fisch and R.B. King, Academic.
9. Experimental Physical Chemistry, D.P. Shoemaker C.W. Garland and J.W. Niber, McGraw Hill Inter science.
10. Findlay's Practical Physical Chemistry revised B.P. Levitt, Longman.
11. Experiments in Physical Chemistry, J.C. Ghosh Brarati Bhavan.