

# **Govt. Bilasa Girls' P.G. (Autonomous) College**

**BILASPUR (C.G.)**

## **SYLLABUS**

**M.Sc.**

**CHEMISTRY**

**SEMESTER: I, II, III, IV**

**2019-2020**

**UGC MODEL CURRICULUM**

# M.Sc. CHEMISTRY SEMESTER – I

## Paper I - INORGANIC CHEMISTRY 68 Hrs.

### 1. Stereochemistry and Bonding in Main group Compounds 12Hrs

VSEPR, Walsh Diagram (Tri and Pentatomic-Molecules)  $d\pi - p\pi$  bonds, bent rule and energetics of hybridisation, some simple reaction of covalently bonded, molecules.

### 2. Metal Ligand Bonding 14 Hrs

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

### 3. Electronic spectra and magnetic properties of transition metal complexes 22 Hrs

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, Anomalous magnetic moment, Magnetic Exchange coupling and spin crossover, charge transfer spectra.

### 4. Symmetry and Group Theory in Chemistry. 12 Hrs

Symmetry Element & Symmetry operation, definition of group subgroup, relation between order's of a finite group and its sub group Conjugate relation and classes point symmetry group, Schoenflies symbols, Representations of group by matrix. (Representation for  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nv}$ ,  $D_{nh}$  etc. groups to be worked out-explicitly) character of a representation. The great orthogonality theorem.

#### Seminar - 8 Hours

Books Suggested :- 1. Group Theory :- Bhattacharya.

2. Advanced Inorganic chemistry:- F.A.Cotton and Wilkinson : John Wiley.

3. Inorganic Chemistry : J.E. Huhey Harpes & Raw

4. Chemistry of the elements: N. N. Greenwood & A Earnshaw Pergamon.

5. Inorganic Electronic Spectroscopy :- A..B.P. Lever, Elsevier.

6. Magneto Chemistry :- R.L. Carlin Springer Verlag.

7. Comprehensive Co-ordination Chemistry

G. Wilkinson, R.D. Gillar's and J.A. McCleverty Pergamon.

8. Chemistry Applications of Group Theory - F.A. Cotton.

# M.Sc. CHEMISTRY SEMESTER – I

## PAPER - II

### ORGANIC CHEMISTRY

#### STEREOCHEMISTRY & PERICYCLIC REACTION

**68 HRS**

**1. Reaction Mechanism : Structure and Reactivity : 10Hrs**

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.

**Reaction Intermediates :**

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes, and benzynes. Application of NMR in detection of carbocations.

**2- Stereochemistry 14Hrs**

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.

**3. Nature of Bonding in Organic Molecules 10Hrs**

Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyperconjugation, Steric effect, 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.

**4 . Pericyclic Reactions : 18Hrs**

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.

## **5. Molecular rearrangement**

**08 Hrs**

General mechanistic approach to molecular rearrangement reactions, - migratory aptitude and memory effects.

Brief study of following rearrangement reactions. carbocation rearrangement Favoroskii, Baeyer-Villigers oxidation, Stork enamine reaction, Shapiro reaction, Sommelet rearrangement, wittig's rearrangement, Grovenstein-Zimmerman rearrangement.

### **Seminar- 8 Hrs**

Book 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 Syke 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. 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.

# M.Sc. CHEMISTRY SEMESTER – I

## PAPER - III

### PHYSICAL CHEMISTRY

68HRS

#### 1. Quantum Chemistry :-

15Hrs

A. Introduction to exact quantum mechanical result . The Schrodinger equation and the postulates of quantum mechanics. Applications of Schrodinger equation to particle in 1-dimensional box, 3dimensional box, harmonic oscillator and hydrogen atom.

B. **Approximate methods** :- The variation theorem, Perturbation theory, application of variation and perturbation theory to hydrogen atom.

#### 2. Thermodynamics

15Hrs

A. **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 significance. Determinations of these quantities. Concept of fugacity and determination of fugacity.

B. **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.

#### 3. Chemical Dynamics

12Hrs

Methods of determining order of reaction, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory, Kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, decomposition of acetaldehyde & ethane), photo chemical chain reactions (hydrogen - bromine and hydrogen chlorine reactions)

#### 4. Surface Chemistry

8Hrs

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

#### 5. Electrochemistry

10Hrs

**Theory of strong electrolyte** :- Debye - Huckel theory, Test of Debye Huckel theory, Extension of Debye Huckel equation, Derivation of Onsager equation, Validity of Onsager equation, Deviation from Onsager equation.

## **SEMINAR - 8 Hrs**

### **Book Suggested :-**

1. Physical Chemistry - P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry - A.K. Chandra,, Tata Mc Graw Hill.
3. Quantum Chemistry - Ira N.Levine, Prentice Hall.
4. Chemical Kinetics - K.J. Laidler, Mc Graw Hill.
5. Kinetics and Mechanism of Chemical Transformation, J. Rajaraman and J. Kuriacore, McMillan.
6. Modern Electrochemistry Vol.I and Vol.II , J.O.M. Bockris and A.K.N. Reddy, plenum.
7. Introduction to Polymer Science - V.R. Gowarikar , N.V. Vishwanathan and J. Sridhar, Wiley Earthern.

# M.Sc. CHEMISTRY SEMESTER – I

## PAPER - IV

### SPECTROSCOPY AND MATHEMATICS/BIOLOGY FOR CHEMISTS

**68 HRS**

#### **A- SPECTROSCOPY**

**30 HRS**

##### **1. Unifying Principles :-**

10 Hrs

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.

##### **2. Microwave Spectroscopy :-**

05 Hrs

Instrumentation , 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 .

##### **3. Vibrational Spectroscopy :-**

15 Hrs

**A.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.

**B.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).

## **B-MATHEMATICS FOR CHEMISTS**

**30HRS**

**(for Students without mathematics in B.Sc.)**

### **1. Vector and Matrix Algebra 10Hrs**

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

**B. 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 ..

### **2. Differential Calculus :- 10Hrs**

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.

### **3. Elementary differential equations 7 Hrs**

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

### **4. Permutation and Probability 3 Hrs**

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

## **B-BIOLOGY FOR CHEMISTS**

**(For student without biology in B.Sc.)**

**30Hrs**

### **1. Cell Structure and Functions :- 5Hrs**

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 biomolecules, building blocks of Bio-macromolecules.



**2. Carbohydrates:- 8Hrs**

Conformation of monosaccharides, 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.

**3. Lipids :- 6Hrs**

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.

**4. Amino acids, Peptides and Proteins :- 6Hrs**

Chemical & enzymatic hydrolysis of proteins to peptides, Amino Acid sequencing, secondary structure of proteins, forces responsible for holding of secondary structure.,  $\alpha$ -hetix, B-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)

**5. Nucleic Acid :- 5Hrs**

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.

**Seminar-8Hrs**

**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. Mathamatics 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 .

# M.Sc. CHEMISTRY 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.

2. Organic Synthesis :-

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

3. Quantitative Analysis :-

1. Determination of the percentage or number of Hydroxyl group in an organic compound by Acetylation method.
1. Estimation of Amines/Phenols using Bromate - Bromide Solution / or Acetylation method.
2. 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.

# M.Sc. CHEMISTRY SEMESTER – I

## LABORATORY COURSE - II

### ANALYTICAL CHEMISTRY

#### (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 burettes 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.

**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).

## **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

<b>S. No.</b>	<b>Lab. Course (branch)</b>	<b>Max. Marks</b>	<b>Duration</b>
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.

### **For Lab. Course –I (Organic Chemistry) :**

(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.

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

(a)Two practical exercise (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

# M.Sc. CHEMISTRY SEMESTER – II

## Paper I - INORGANIC CHEMISTRY

68 Hrs.

### 1. Metal Ligand Equilibria in solution:-

8 Hrs

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.

### 2. Reaction mechanism of transition metal complexes:-

25Hrs

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

### 3. Metal $\pi$ -Complexes.

15Hrs

(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.

### 4. Metal Clusters.

6Hrs

Higher boranes, carboranes, metalloboranes and metallocarboranes, Metal carbonyl.

### 5. Isopoly and Heteropoly Acid & salt.

6Hrs

Isopoly acids of transition metals Mo, W, V, Nb, Ta.

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

**Seminar-8hours**

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.
8. Group Theory :- Bhattacharya.

# M.Sc. CHEMISTRY SEMESTER – II

## PAPER - II

### ORGANIC CHEMISTRY

#### REACTION MECHANISM

68Hrs

#### 1. Electrophilic substitution reactions :-

14Hrs

(a) Aliphatic electrophilic substitution :- Biomolecular mechanism :

$SE^2$ ,  $SE^1$ , and  $SE^1$  mechanism, electrophilic substitution accompanied by double bond shifts. effect of substrates, leaving group and the solvent polarity on the reactivity.

#### (b) Aromatic electrophilic substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring system. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Gattermann Koch reaction, Vilsmeier reaction.

#### 2. Nucleophilic Substitution reactions :-

14Hrs

(a) Aliphatic nucleophilic substitution : The  $S_N2$ ,  $S_N1$ , mixed  $S_N^1$  and  $S_N^2$  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.

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

#### 3. Free Radical reactions

10Hrs

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.



**5. Addition to Carbon-Carbon Multiple Bonds 8Hrs**

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.

**6. Addition to Carbon-Hetero Multiple bonds : 9Hrs**

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.

**7. Elimination reactions : 5Hrs**

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.

**Seminar-8Hrs**

**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 Syke- 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

# M.Sc. CHEMISTRY SEMESTER – II

## PAPER -III

### PHYSICAL CHEMISTRY

68HRS

#### 1 Quantum Chemistry

15 Hrs

A. **Angular Momentum** :- Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum.

B. **Electronic Structure of Atoms** :- Electronic configuration, Russell - Saunders term and coupling schemes, term separation energies of  $P^n$  &  $d^n$  configurations, magnetic effects :- spin-orbit coupling and zeeman splitting.

C. **Molecular Orbital Theory** :- The Born Oppenheimer Approximation, LCAO approximation & its application to hydrogen molecule ion .

#### 2. Thermodynamics

15 Hrs

##### A) Statistical Thermodynamics :-

1. Probability theorem in statistical thermodynamics, System Assembly and Ensemble, Statistical equilibrium, Thermodynamic

2. Partition function – Translational, rotational, vibrational and electronic partition function, calculation of thermodynamic properties in terms of partition function. Application of partition functions.

##### B) 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) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations.

#### 3. Chemical Dynamics

8Hrs

Homogeneous catalysis, kinetics of enzyme reaction (Michalis kinetics) study of fast reactions by flow method, relaxation method, flash photolysis and nuclear magnetic resonance method. Dynamics of unimolecular reactions (Lindemann- Hinshelwood and Rice-Ramsperger - Kassel theories)

#### 4. Surface Chemistry :-

12Hrs

A) **Micelles** :- Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC),

factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization - phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

**B) Macromolecules :-** Polymer - definition , types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerisation, number and mass average, molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering methods) sedimentation, chain configuration of macromolecules.

## **5. Electrochemistry**

**10Hrs**

**A.** Polarisation and decomposition potential - Demonstration of polarization, Elimination of polarisation decomposition potential, decomposition potential of aqueous solution and neutral solution.

**B. Over Voltage** - Hydrogen over voltage- its measurement, oxygen over voltage, Determination of factors affecting over voltage, importance of over voltage.

### **Seminar-8 Hrs**

#### **Book Suggested :-**

1. Physical Chemistry - P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry - A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry - Ira N.Levine, Prentice Hall.
4. Chemical Kinetics - K.J. Laidler, Mc Graw Hill.
5. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kuriacore, McMillan.
6. Modern Electrochemistry Vol.I and Vol.II J.O.M. Bockris and A.K.N. Reddy, plenum.
7. Introduction to Polymer Science - V.R. Gowariker N.V. Vishwanathan and J. Sridhar, Wiley Earthern.

# M.Sc. CHEMISTRY SEMESTER – II

## PAPER –IV

### SPECTROSCOPY, DIFFRACTION METHODS & COMPUTER FOR CHEMISTS

68 Hrs

#### 1. Electronic Spectroscopy :-

10 Hrs

**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-electic 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.

#### 2. Magnetic Resonance Spectroscopy :-

12 Hrs

**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.

### 3. X-ray Diffraction :-

8 Hrs

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.

## COMPUTER FOR CHEMISTS

30 Hrs

### 1. Introduction to Computer and Computer Programming in "C" 15 Hrs

**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.

### 2. Programming in Chemistry and use of Computer Programmes. 15 Hrs

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.

### SEMINAR 8 Hrs

#### 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.

### **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 Quantam Mechaniscs. J.P. Kilingbeck. Adam Hilger.
4. Computer Programming in fortran IV V. Rajaraman, Prentice Hall.
5. An Introduction to Digital Computer Design, V.Rajaraman and T. Radha Krishanan Prentice Hall.

## M.Sc. CHEMISTRY SEMESTER – II

### LABORATORY – COURSE III

#### INORGANIC-CHEMISTRY

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

Basic Radicals : - Ag, Pb, Hg, Cu, Cd, Bi, As, Sb, Sn, Fe, Al, Cr, Zn, Mn, Co, Ni, Ba, Sr, Ca, Mg, Na, K,  $\text{NH}_4$ , Ce, Th, Zr, W, Te, Ti, Mo, U, V, Be, Li, Au, Pt.

Acid Radicals :-  $\text{CO}_3$ ,  $\text{SO}_4$ ,  $\text{SO}_3$ ,  $\text{NO}_3$ , F, Cl, Br, I,  $\text{NO}_2$ ,  $\text{BO}_3$ ,  $\text{C}_2\text{O}_4$ ,  $\text{PO}_4$ ,  $\text{SiO}_4$ , Thiosulphate, Ferrocyanide, Ferricyanide, Chromate, Arsenite, Arsenate, Permanganate.

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, Ba, Ca, Mg, Chloride, Sulphate.

3. **Estimation of :-**

- (A) Phosphoric acid in Commercial orthophosphoric acid.
- (B) Boric Acid in Borax.
- (C) Ammonium Ion in Ammonium Salt.
- (D)  $\text{MnO}_2$  in pyrolusite
- (E) Available Chlorine in bleaching powder.
- (F)  $\text{H}_2\text{O}_2$  in commercial sample.

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)  $\text{VO}(\text{acac})_2$
- (ii)  $\text{Cis K} [\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ ,
- (iii)  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$
- trans  $\text{K} [\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$
- (iv)  $\text{Na} [\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
- (v)  $\text{Mn}(\text{acac})$
- (vi)  $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
- (vii) Prussian Blue Turnbells Blue.
- (viii)  $[\text{Co}(\text{NH}_3)_6] [\text{Co}(\text{NO}_2)_6]$
- (ix)  $\text{Hg} [\text{Co}(\text{SCN})_4]$
- (x)  $[\text{Ni}(\text{NH}_3)_4]\text{Cl}_2 \cdot [\text{Ni}(\text{NH}_3)_4]\text{Cl}_2$
- (xi)  $\text{Ni}(\text{DMG})_2$  (xii)  $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4$
- (xii)  $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3] \cdot 3\text{H}_2\text{O}$
- (xiii)  $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4$

## M.Sc. CHEMISTRY SEMESTER – II

### LABORATORY COURSE-IV

#### PHYSICAL CHEMISTRY

#### 1. Adsorption :-

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

#### 2. Phase Equilibria:

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

#### 3. Chemical Kinetics

- (i) Hydrolysis of an ester/ ionic reactions.
- (ii) 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.
- (iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide
- (iv) 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

- i. Determination of solubility of sparingly soluble salt (eg,  $\text{PbSO}_4$ ,  $\text{BaSO}_4$ ) Conductometrically.



ii. Determination of the strength of strong and weak acids in a given mixture conductometrically.

iii. Determination of dissociation constant of weak electrolyte by conductometer.

Iv Determination of velocity constant, Order of reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide.

## 5. pH Metry/Potentiometry

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

## 6. Colorimetry

1. Determination of wavelength of maximum absorption of a compound and concentration of unknown solution by spectrophotometer

2. Titration of a solution of HCl with NaOH spectrophotometrically.

## 7. Polarimetry:-

1. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter

2. Enzyme kinetic – inversion of sucrose.

## 8. Solutions:

(i) Determination of molecular weight of non-volatile and non-electrolyte/electrolytes by cryoscopy method and to determine the activity coefficient of an electrolyte.

(ii) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behavior that occurs with a strong electrolyte.

## 9. Educational Tour

## Instructions to Practical Examiners in Chemistry Semester - II

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.	Branch	Marks	Duration
(i). Lab Course-III	Inorganic Chemistry	100	10 hours
(ii) Lab Course-IV	Physical Chemistry	100	5 hours

2. Sessional marks will be awarded by External Examiner in consultation with the Internal Examiner.

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

### **For Lab. Course –III (Inorganic Chemistry):**

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

### **For Lab. Course –IV (Physical Chemistry):**

(a) One practical exercise	60 (80) marks
(b) Viva voce and manipulation	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.

# M.Sc. CHEMISTRY SEMESTER – III (2019-2020)

## Paper I

### APPLICATION OF SPECTROSCOPY

68 Hrs.

#### INORGANIC CHEMISTRY

##### 1. Vibrational Spectroscopy :

5Hrs

Symmetry and shape of  $AB_2$ ,  $AB_3$ ,  $AB_4$ ,  $AB_5$ ,  $AB_6$  mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly metallo-proteins.

##### 2. Electron Spin Resonance spectroscopy :

8Hrs

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 .

##### 3 Nuclear Magnetic Resonance of Paramagnetic substances in solution

7Hrs

Factors affecting nuclear relaxation, some applications including biological systems, an overview of NMR of metal nuclides with emphasis  $^{195}\text{Pt}$  and  $^{119}\text{Sn}$  NMR.

#### ORGANIC CHEMISTRY

##### 1. Ultraviolet and Visible Spectroscopy :

7Hrs

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.

##### 2. Infra-Red Spectroscopy :

8Hrs

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

### **3. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD) : 3Hrs**

Definition, deduction of absolute configuration, octant rule for ketone.

### **4. Nuclear Magnetic Resonance Spectroscopy : 10Hrs**

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).

### **5. Carbon-13 NMR Spectroscopy : 4Hrs**

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, Heteroaromatic and carbonyl carbon) coupling constants.

### **6. Mass Spectrometry : 8Hrs**

Introduction, ion production - EI, CI, 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.

### **Seminar – 8Hrs**

#### **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. MacLachlan  
Harper & Row
10. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H.  
Rankin and Cradock, ELBS.
11. Progress in Inorganic Chemistry, Vol. 8 Ed. F.A. Cotton Vol. 15 Ed. S.J.  
Lippard, Wiley

# M.Sc. CHEMISTRY SEMESTER – III

## PAPER – II

<b>BIO-INORGANIC &amp; BIO-PHYSICAL CHEMISTRY</b>	<b>68hrs</b>
<b>(A) BIO-INORGANIC CHEMISTRY</b>	<b>40HRS</b>
<b>1. Metal Ions in Biological systems. Essential and trace metals.</b>	<b>3Hrs</b>
<b>2. Na<sup>+</sup>/K<sup>+</sup> Pump :</b> Role of metal ions in biological processes	<b>4Hrs</b>
<b>3. Bioenergetics and ATP cycle :</b> DNA polymerisation, glucose storage, metal complexes in transmission of energy, photosystem I and Photosystem II in cleavage of water.	<b>8Hrs</b>
<b>4. Transport and storage of dioxygen :</b> Heme-proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanin and hemerythrin, model synthetic complexes of iron, cobalt and copper.	<b>8Hrs</b>
<b>5. Electron transfer in Biology :</b> Structure and function of metalloprotein in electron transport processes - cytochromes and Iron-Sulphur proteins.	<b>6Hrs</b>
<b>6. Nitrogenase :</b> Biological nitrogen fixation, Iron-sulphur proteins and nitrogen fixation, other nitrogenase model systems.	<b>5Hrs</b>
<b>7. Calcium in Biology :</b> Calcium in living cells, transport and regulation, sources of calcium, distribution of calcium in the body, Blood calcium and its regulation. Function of Calcium, Manifestation of altered calcium level in the plasma.	<b>6Hrs</b>

**(B) BIO-PHYSICAL CHEMISTRY** **20HRS**

- 1. Biological Cell and its constituents :** **4Hrs**  
Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems, Helix coil transition.
- 2. Bio-energetics :** **5Hrs**  
Standard free energy change in Biochemical reactions. Exergonic and Endergonic , Hydrolysis of A.T.P. Synthesis of ATP from ADP.
- 3. Statistical Mechanics in Biopolymers :** **6Hrs**  
Chain configuration of Macromolecules, Statistical distribution, end to end dimensions, calculation of average dimensions for various chain structure, Polypeptide and protein structure. Introduction to protein folding problem.
- 4. Biopolymer Interaction :** **5Hrs**  
Forces involved in Biopolymer interactions. Electrostatic charges and molecular expansion ,hydrophobic forces, dispersion force interaction.

**Seminar-8Hrs**

***Books suggested :***

**Bio-Inorganic Chemistry**

1. Principles of Bio-Inorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bio-Inorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S.Valentine, University Science Books.
3. Inorganic Biochemistry Vols. I and II, Edi. G.L. Eichhorn, Elsevier.
4. Progress in Inorganic Chemistry, Vols. 18 & 38, Ed. J.J. Kipard, Wiley.

**Bio-Physical Chemistry**

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryes, W.H. Freeman
3. Biochemistry, J. David Rawn, Neil Patterson
4. Biochemsitry, Voet and Voet, John Wiley
5. Outline of Biochemsitry, E.E. Conn and P.K. Stumpf, John Wiley
6. Biophysical, Upadhyay, Upadhyay Nath, Himalaya Publishing House,
7. Macromolecules - Structure and Function, F. Wold, Prentice Hal



# M.Sc. CHEMISTRY SEMESTER –III

## GROUP -A PAPER – III

### ENVIRONMENTAL CHEMISTRY

68HRS

- 1. Environment :** **8Hrs**  
Introduction, Composition of atmosphere, Vertical temperature, Heat budget of the earth atmospheric system, Biogeochemical cycles of C, N, P, S and O, Biodistribution of elements.
- 2. Hydrosphere :** **12Hrs**  
Chemical composition of water bodies - lakes, streams, rivers and wetlands etc., Hydrological cycle.  
Aquatic pollution : Inorganic, Organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameter, dissolved oxygen, Biological Oxygen Demand, Solids, Metals, Contents of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards, analytical methods for measuring BOD, DO, COD, F, Oils, Metals (As, Cd, Cr, Hg, Sb, Se etc.). Residual chloride and chlorine demand. Purification and treatment of water.
- 3. Soils :** **6Hrs**  
Composition, Micro- and Macro-nutrients, Pollution, Fertilizers, Pesticides, Plastics and Metals. Waste treatment.
- 4. Atmosphere :** **8Hrs**  
Chemical composition of atmosphere - particles, ion and radicals and their formation. Chemical and photochemical reaction in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chloro-fluoro-hydrocarbons, Green house effect, Acid rain, Air pollution controls and their chemistry. Analytical methods for measuring air pollutants, Continuous monitoring instruments.
- 5. Industrial Pollution :** **12Hrs**  
Cement, Sugar, Distillery, Drug, Paper and pulp, Thermal power plants, Nuclear power plants, Metallurgy, Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.
- 6. Environmental Toxicology :** **14 Hrs**  
Chemical solution to environmental problems, Biodegradability, Principles of decomposition, better industrial processes, Biochemical effects of arsenic, cadmium, lead and mercury, Bhopal Gas Tragedy, Chernobyl, Three mile island, Sewozo and Minimata disasters.

## Seminar- 8Hrs

### Books suggested :

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.
3. Environmental Chemistry, A.K. De, Wiley Eastern.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern.
5. Standard Methods of Chemical Analysis, F.J. Welcher, Vol. III, Van Nostrand Reinhold Co.
6. Environmental Toxicology, Ed. J. Rose, Gordon & Breach Science Publication.
7. Elemental Analysis of Airborne particles, Ed. S. Landsberger & M. Creatchman, Gordon & Breach Science Publication.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern

## M.Sc. CHEMISTRY SEMESTER – III

### PAPER-IV

#### GROUP A -ORGANIC CHEMISTRY

#### CHEMISTRY OF HETEROCYCLIC COMPOUNDS

**68HRS**

1. Nomenclature of Heterocycles - **5 Hrs**  
Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles.
2. Aromatic Heterocycles - **8 Hrs**  
General chemical behaviour of aromatic heterocycles.  
Classification  
(structure type) criteria of aromaticity (bond lengths, ring current and chemical shift in  $^1\text{H}$ -NMR spectra, Empirical resonance energy, delocalisation energy and Dewar resonance energy, Heteroaromatic reactivity and tautomerism in aromatic heterocycles.

3. **Non aromatic Heterocycles** **8 Hrs**  
 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 interactions -hydrogen bonding and intermolecular nucleophilic-electrophilic interactions.
4. **Heterocyclic synthesis** **4Hrs**  
 Principle of heterocyclic synthesis involving cyclisation reactions and cyclo addition reactions.
5. **Small Ring Heterocycles** **7 Hrs**  
 Three membered and four membered Heterocycles - synthesis and reactions of Aziridines, oxirane, thirane, Azetidine, Oxetanes and Thietanes.
6. **Benzo-fused five membered Heterocycles** **7 Hrs**  
 Synthesis and reaction including medicinal applications of Benzo-pyrrole, Benzo-furans and Benzo-thiophenes.
7. **Six membered Heterocycles with one Hetero atom** **8 Hrs**  
 Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium and thiopyrylium salts and pyridones. synthesis and reactions of quinolizinium and Benzopyrilium salts, coumarins and chromones.
8. **Six membered Heterocycles with two or more Hetero atoms** **6 Hrs**  
 Synthesis and reactions of diazines, Triazines, Tetrazines and Thiazines.
9. **Seven and large membered Heterocycles** **7 Hrs**  
 Synthesis and reaction of azepines, oxepines, thiepines, diazepines, Thiazepines.

**Seminar-** 8Hrs

**Books 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
5. Rodds Chemistry of Carbon Compounds Ed. S. Coffery, Elsevier
6. Natural Products chemistry and Biological Significance by J. Mann, 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, and W.W. Pandler, Wiley Interscience

# M.Sc. CHEMISTRY SEMESTER – III

## Paper IV

### Group B -PHYSICAL CHEMISTRY CHEMICAL DYNAMICS

68Hrs

- 1. The Rate of chemical reactions** 4Hrs  
Empirical chemical kinetics  
Elementary reaction'  
Consecutive elementary reaction.
- 2. The Kinetics of Complex reactions** 8Hrs  
Complex reaction or reaction of higher order,  
polymerisation kinetics, condensation or stepwise  
polymerisation, Addition or Chain Polymerisation, Kinetics of  
fractional order reactions, characteristics of fractional order  
reaction.
- 3. The Kinetic study in Liquid solution** 8Hrs  
Solvent effect on reaction rate  
Linear Free Energy Relationship (LFER) and its thermodynamic  
implication.
- 4. Diffusion controlled reaction** 6Hrs  
Hammett equation and its derivation, Weakness of Hammett  
equation and development of Taft equation, significance of sigma  
( $\sigma$ ) and rho ( $\rho$ ).
- 5. Reaction on surface and in the solid state** 6Hrs  
Bimolecular surface reaction, absolute rate of surface reaction,  
kinetics of fast reaction, Absolute role theory applied to fast  
reaction.
- 6. Disturbing factors in determining order of reactions** 4Hrs  
Side reactions, parallel reaction, opposing reaction, consecutive  
reaction.
- 7. Dynamics of electron transfer reactions** 8Hrs  
Electron transfer in Homogeneous system, theory of electron transfer  
process, experimental results, electron transfer in heterogenous  
system, the rate of charge transfer reactions.
- 8. Reaction in solid state heterogeneous system** 8Hrs  
Reactions in solid state, surface heterogeneity, electronic theory of  
chemisorptions, heterogeneous catalysis of reaction by solid,

oxidation of metal surface.

**9. Measurement of rate of a chemical Reaction** 8Hrs

Static and flow method, static method for slow reaction, static method for fast reaction (stopped flow, flash photolysis) Flow method for slow reaction.

**Seminar –8Hrs**

***Books suggested -***

1. Physical Chemistry by P.W. Atkins, ELBS
2. Chemical Kinetics by K.J. Laidler, McGraw Hill.
3. Kinetics and Mechanism of chemical Transformation by J. Rajaraman and J. Kuriacose, McMillan.
4. Mechanism and Theory in Organic Chemistry by T.H. Lowry and K.C. Richardson, Harper and Row
5. Physical Organic Chemistry by N.S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry, concepts and Perspectives by J.M. Lehn, VCH
7. Physical Organic Chemistry, by Neil
8. Physical Organic Chemistry by Ritchie
9. Organic Chemistry by Morrison Boyd, Prentis Hall
10. Advanced Organic Chemistry - Reaction Mechanism and Structure by Jerry March, John Wiley
11. A Guide Book to Mechanism in Organic Chemistry by Peter Syke, Longman

# M.Sc. CHEMISTRY SEMESTER – III

## LABORATORY COURSE V-( 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

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

#### B. Colorimetry

- i. Determine the composition of  $\text{K}_2\text{Cr}_2\text{O}_7$  and  $\text{KMnO}_4$  using spectrophotometer
- ii. Determine the dissociation constant of methyl red by spectrophotometric method.
- iii. to verify additivity 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

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

#### D. Potentiometry

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

#### E. Distribution coefficient

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

#### F. Partial molar volume:

- i. Determine the partial molar volume of  $\text{NaCl}$  in aq. Solution at room temperature.

## **INORGANIC CHEMISTRY**

### **A. Instrumental methods and Analytical Technique**

#### Spectrophotometric determination

- i. Manganese/Chromium/Vanadium in steel sample.
  - ii. Iron-salicylic acid complex by Job's method of continuous variation of concentration
  - iii. Zirconium-Alizarin red-s-complex; Mole ratio method.
  - iv. 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**

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

### **E. Quantitative & Qualitative Analysis :**

- i. Paper chromatography - Cadmium and Zinc, Zinc and Magnesium
- ii. Thin layer chromatography - separation of Nickel, Manganese, Cobalt and Zinc. Determination of  $R_f$  values.
- iii. Ion Exchange
- iv. Solvent Extraction
- vi. Electrophoretic separation.

### **F.(i) Analysis of Dolomite.**

- (ii) Estimation of available oxygen in  $H_2O_2$  by Iodometry .

## **ORGANIC CHEMISTRY**

### **A. Instrumental methods and Analytical Techniques**

- i. Estimation of Sulphur by Messengers method.
- ii. Estimation of Nitrogen by Kjeldahl method
- iii. Estimation of Halogen by Fusion method

### **B. Functional Group Estimation -**

- i. Estimation of Aniline
- ii. Estimation of Amino group by Acetylation method
- iii. Estimation of Hydroxyl group by Acetylation method



- iv. Estimation of Carboxyl group by Hydrazone formation method.
- v. Estimation of Glucose
- vi. Estimation of Sucrose

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  $P_{ka}$  of weak acids by pH metric and spectrophotometric methods.
3. Purification of water by using natural materials, i.e. silica, alumina, iron oxide and ziedite, 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, Electrophoresis.
7. Analysis of carbohydrates, amino acids, protein, alkaloid etc.
8. Analysis of vitamins, enzymes, harmones etc.
9. Analysis of pharmaceutical materials
10. Analysis of surfactants, detergents, soap, oil etc.
11. Analysis of ore ,minerals, alloy,soil, sediment
12. Application of Redox titration for analysis of Sn(iv), Fe(iii), Cr(VI) ,Mn(vii).
13. Analysis of water.
14. Collection sampling digestion and extraction of volatile materials.
15. Determination of equilibrium constant and composition of complexes.
16. Determination of dimerization /polymerization constant.

**M.Sc. CHEMISTRY SEMESTER – IV**  
**PAPER-I**  
**PHOTOCHEMISTRY & SOLID STATE CHEMISTRY**

**68Hrs**

**A- PHOTOCHEMISTRY**

**30HRS**

- 1. Photochemical Reaction :** **4Hrs**  
Interaction of electromagnetic radiation with matter, Types of excitation, Fate of excited molecule. Quantum yield. Transfer of excitation energy.
- 2. Determination of reaction mechanism :** **4Hrs**  
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.
- 3. Photochemistry of Alkenes :** **6Hrs**  
Intermolecular reactions of olefinic bond, geometrical isomerism. Cyclisation reaction, Rearrangement of 1,4 and 1,5-dienes.
- 4. Photochemistry of Carbonyl compounds :** **8Hrs**  
Intra-molecular reaction of Carbonyl compounds, saturated cyclic and acyclic,  $\beta,\gamma$ -unsaturated and  $\alpha,\beta$ -unsaturated compounds, cyclohexadienone. Inter-molecular cyclo addition reactions. Dimerisation and Oxetane formation.
- 5. Photochemistry of Aromatic compounds :** **4Hrs**  
Isomerisation, Addition, Substitution.
- 6. Miscellaneous photochemical reactions :** **4Hrs**  
Photo fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog.

**B - SOLID STATE CHEMISTRY**

**30HRS**

- 1. Solid State Reactions :** **4Hrs**  
General principles, experimental procedures, precursor methods, kinetics of solid state reactions.

**2. Crystal Defects and Non-stoichiometry : 6Hrs**

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.

**3. Electronic properties and Band Theory : 15Hrs**

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.

**4. Superconductivity and organic solids, Occurrence, Principle and uses of conventional ,organic and New super conductors. 5Hrs**

**Seminar – 8Hrs**

**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. Rohtagi Mukherji, Wiley Eastern.
6. Essentials of molecular photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication.
7. Molecular photochemistry, N.J. Turro, W.A. Benjamin.
8. Introductory photochemistry, A. Cox and T. Camp, McGraw-Hill.
9. Photochemistry, R.P. Kundall and Gilbert, Thomson Nelson.
10. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.

# M.Sc. CHEMISTRY SEMESTER -- IV

## PAPER -II

### BIO-ORGANIC & BIO-PHYSICAL CHEMISTRY

**68HRS**

#### BIO-ORGANIC CHEMISTRY

**40HRS**

- 1. Introduction :** **2Hrs**  
Basic consideration, Proximity effects and molecular adaptation.
- 2. Enzyme :** **10 Hrs**  
Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzyme like catalytic power specificity and regulation. Nomenclature and classification. Extraction and purification. Fisher's Lock and Key and Koshland's Induced Fit hypothesis, concept and identification of active sites by the use of inhibitors, affinity labelling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibitor.
- 3. Mechanism of Enzyme Action :** **6 Hrs**  
Transition state theory, Orientation and steric effect, Acid-base catalysis, covalent catalysis , strain or distortion. Example of some typical enzyme mechanism for chymotrypsin, Ribonuclease, Lysozyme and Carboxypeptidase A
- 4. Co-enzyme Chemistry :** **6 Hrs**  
Cofactors as derived from vitamins, coenzyme, prosthetic groups, Apo-enzymes, structure and biological function of coenzyme A, Thiamine, Pyrophosphate, Pyridoxal, Phosphate  $\text{NAD}^+$ ,  $\text{NADP}^+$ , FMN, FAD, Lipoic Acid, Vitamin  $\text{B}_{12}$ , Mechanism of reactions catalyzed by above co-factors.
- 5. Metalloenzyme :** **10 Hrs**  
Carboxypeptidase and carbonic anhydrase, Iron enzyme - Catalase, peroxidase and cytochrome P-450, Copper enzymes - Superoxide dismutase, Enzyme Xanthin oxidase, Coenzyme Vitamin  $\text{B}_{12}$ .

- 6. Biotechnical application of Enzyme :** **6 Hrs**  
Application of enzymes, Large scale production and purification of enzyme, Techniques and methods of immobilisation of enzymes . Effect of immobilisation of enzyme activity. Use of enzyme in food and drink industry - brewing and cheese-making, syrup from corn starch enzyme as target for drug design clinical use of enzyme, Enzyme therapy.

**BIO-PHYSICAL CHEMISTRY** **20HRS**

1. Thermodynamics of Biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy of generation in mechano-chemical system. **5Hrs**
2. Cell membrane and transport of ions, structure and functions of cell membrane, Ion transport through cell membrane, Irreversible thermodynamic treatment of membrane transport, Nerve conduction. **5Hrs**
- 3. Biopolymers and their molecular weights :**  
Evaluation of size, shape, molecular weight and extent of hydration of Biopolymers by various experimental techniques, Sedimentation equilibrium, Hydrodynamic methods, diffusion, sedimentation, velocity, viscosity, electrophoresis and rotational motions. **6Hrs**
- 4. Diffraction Methods :**  
Light scattering, Low angle X-ray scattering, X-ray diffractions and Photo-correlation. Spectroscopy, ORD. **4Hrs**

**Seminar-8 Hrs**

## **Reference Books**

### **Bio-Organic Chemistry**

1. Bio-organic Chemistry : A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.
2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
3. Enzyme Chemistry : Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall.
4. Enzyme Mechanism Ed. M.I. Page and A. Williams, Royal Society of Chemistry.
5. Fundamentals of Enzymology, N.C. Price and L. Stenens, Oxford University Press.
6. Immobilized Enzymes : An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley
7. Enzymatic Reaction Mechanism, C. Walsh, W.H. Freeman
8. Enzyme Structure and Mechanism, A. Fersht, W.H. Freeman
9. Biochemistry : The Chemical Reactions of Living Cells, D.E. Metzler, Academic Press.

### **Bio-Physical Chemistry**

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 and Voet, John Wiley
5. Outline of Biochemistry, E.E. Conn and P.K. Stumpf, John Wiley
6. Biophysical, Upadhyay, Upadhyay Nath, Himalaya Publishing House,
7. Macromolecules - Structure and Function, F. Wold, Prentice H

## **M Sc .CHEMISTRY**

### **SEMESTER-IV**

#### **PAPER- III Group-A**

##### **MEDICINAL CHEMISTRY**

68Hrs.

##### **1. Pharmacokinetics**

10 Hrs.

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

##### **2. Antineoplastic Agents**

10 Hrs.

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, mustard, and 6-mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

##### **3. Cardiovascular Drugs**

10 Hrs.

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, methyl dopa, atenolol oxyprenolol.

##### **4. Local Anti-infective Drugs**

10 Hrs.

Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin,

norfloxacin, dapson, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econazole, griseofulvin, chloroquin and primaquin.

**5. Psychoactive Drugs the chemotherapy of mind** 12Hrs.

Introduction, neurotransmitters, CNS depressants, general anaesthetics, 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 barbitrates, thiopental sodium, glutethimide,

**6. Antibiotics** 10 Hrs.

Structure and Synthesis of penicillin G. penicillin V, ampicillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

**7. Seminar – 8 Hrs.**

**Reference book**

1. Insecticides of natural origin, such derv, Harwood, academic publishers.
2. Introduction to medicinal chemistry, A gringuage, wiley-vch
3. Wilson and Gisold's text book of organic medicinal and Pharmaceutical Chemistry Ed Robert F. Dorge.



4. An Introduction to Drug Design, S.S. Pandeya and J.R. Dim mock, New Age International.
5. Burger's Medicinal Chemistry and Drug Discovery, vol-1 (chapter – 9 and ch-14) Ed. M.E. Wolff, John Wiley.
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw Hill.
7. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, academic press.
8. Strategies for Organic Drug Synthesis and Design, D. lednicer, John Wiley.
9. BioPharmaceutics & Pharmacokinetics, G. R. Chhatwal Himalaya Prakashan
10. Medicinal Chemistry - Dr. J. P. Mishra & Sarika Bajpai – Anusandhan Prakashan Kanpur
11. Clinical Pharmacology - Laurence , P. N. Benet, Longman – Singapur Publication
12. Medicinal Chemistry - Alka k. Gupta , Pragati Prakashan
- 13 Medicinal Chemistry –Ashutosh Kar, New Age International.

**M. Sc .CHEMISTRY**  
**SEMESTER-IV**  
**PAPER- IV**  
**GROUP A-ORGANIC CHEMISTRY**

**Chemistry of Natural Product**

68 HRS

1. Terpenoids and Carotenoids 16 Hrs  
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, Zingiberene, Phytol ,abietic acid , $\beta$ -carotene and its relation with Vitamin A.
2. Alkaloids 17 Hrs  
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.
3. Steroids and Hormones 17Hrs  
Occurrence, Nomenclature, Basic skeleton, Diels-Hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of cholesterol , bile acids, Androsterone, Testosterone, Ergosterol, Sigmasterol, Oestrone, Progesterone, Aldosterone. Non steroid Harmones Thyroxine, Adrenaline.
4. Plant pigment 7Hrs  
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.
5. Porphyrins 3 Hrs  
Structure and synthesis of Haemoglobin and chlorophyll.
6. Seminar 8 Hrs

### **Books 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
5. Rodds Chemistry of Carbon Compounds Ed. S. Coffery, Elsevier
6. Natural Products chemistry and Biological Significance by J. Mann, 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, and W.W. Pandler, Wiley Interscience.
10. Comprehensive Heterocyclic Chemistry by A.R. Katritzky & C.W. Rees Eds. Pergamon Press.

**M Sc .CHEMISTRY**  
**SEMESTER-IV**  
**PAPER- III Group-B**  
**ANALYTICAL CHEMISTRY**

**68HRS**

**1. Introduction :**

**12Hrs**

Role of Analytical Chemistry, Classification of analytical methods, classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness, Laboratory operations and practices, analytical volumetric glassware, Cleaning and calibration of glassware, sample preparations, dissolution and decompositions, Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory.

- 2. Errors and Evaluation : 7Hrs**  
 Definition of terms in mean and median precision - standard deviation, relative standard deviation, Accuracy - absolute error, relative error. Types of error in experimental data . Determinate (Systematic), Indeterminate (or random) and gross sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data indeterminate errors. The uses of statistics.
- 3. Food Analysis : 12Hrs**  
 Moisture, ash, crude protein, fat, crude fiber, carbohydrates, calcium, potassium, sodium and phosphate, food adulteration, common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC Gas chromatography for organophosphates. Thin layer chromatography for chlorinated pesticides in food products.
- 4. Analysis of water pollution : 12Hrs**  
 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. Objectives of analysis parameter for analysis, colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness , choride, 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 metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.
- 5. Analysis of Soil, Fuel, Body fluids and Drugs : 17Hrs**
- a) Analysis of soil : Moisture, pH, Total nitrogen, Phosphorus, Silica, Lime, Magnesia, Manganese, Sulphur and Alkali salts.
  - b) Fuel analysis : Solid, liquid and 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 value.
  - (c) Clinical chemistry : Composition of blood collection and preservation of samples, clinical analysis, blood glucose, blood urea, nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphates.
  - (d) Drug analysis : Narcotics and dangerous drugs, classification of drugs, Screening by gas and thin layer chromatography and spectrophotometric measurements.

**Seminars : 8Hrs**

Book Suggested:

1. Analytical Chemistry, G.D. Christian, J. Wiley
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West & F.J. Holler, W.B. Saunders.
3. Analytical Chemistry Principles, J.J. Kennedy, W.B. Saunders.
4. Analytical Chemistry : Principles & Techniques, L.G. Hargis, Prentice Hall.
5. Principles of Instrumental Analysis, D.A. Skoog & J.L. Loary, W.B. Saunders.
6. Principles of Instrumental Analysis, D.A. Skoog, W.B. Saunders.
7. Quantitative Analysis, R.A. Day Jr. and A.L. Underwood, Prentice Hall.
8. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern.
- 9 Basic Concepts of Analytical Chemistry, S.M. Khopkar, Wiley Eastern.
10. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.

**M. Sc. CHEMISTRY**  
**SEMESTER-IV**

**PAPER- IV**  
**GROUP B - PHYSICAL CHEMISTRY**  
**PHYSICAL ORGANIC CHEMISTRY**

**68HRS**

- 1 Concepts in molecular orbital (MO) and Valence bond (VB) 10Hrs**  
Molecular orbitals for polyatomic orbitals, Huckel approximation.  
The Born Oppenheimer Approximation, LCAO approximation. The matrix formulation of the Huckel method. Quantitative M.O. theory, Huckel Molecular Orbital method as applied to ethane, and butadiene, Qualitative M.O. Theory, Application of LCAO approximation to hydrogen molecule ion and hydrogen molecule. Valence Bond Theory and its application. Potential Energy Profile and diagrams.
- 2. Principles of Reactivity 6Hrs**  
Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory, Uses of activation parameters, Hammond's postulates, Bell-Evans Polanyi principle, Potential energy surface models, Marcus theory of electron transfer. Reactivity and selectivity principles.
- 3. Kinetic Isotope effect 5Hrs**  
Theory of isotope effects, primary and secondary isotope effects, Heavy atom isotope effects. Tunneling effect. Solvent effects.
- 4. Structural Effects on Reactivity 5Hrs**  
Linear Free Energy Relationship (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of  $\rho$  values. Reaction constant  $\rho$ . Deviations from Hammett equation. Dual parameter correlations, The Taft model.
- 5. Solvation and solvent effects 8Hrs**  
Qualitative understanding of solvent-solute effects on reactivity,  
Effects of solvation on reaction rates and equilibria. Thermo-dynamic measure of solvation, Thermodynamic formulation of conventional transition state theory, Assumption and limitations of CTST. Multiple crossing and the equilibrium hypothesis. Solvent effect from curve crossing model.
- 6. Acids, Bases, Electrophiles, Nucleophiles and Catalysis 8Hrs**

Acid-Base dissociation, interpretation of  $K_A$ , theories of proton transfer, highly acidic and highly basic solution, acidity function and its uses. Nucleophilicity and Electrophilicity, Hard and soft acids and bases, Frontier orbital interactions, Nucleophilicity scales, Relationship between nucleophilicity and Nucleofugacity,  $\alpha$ -effect.

### **7. Nucleophilic and Electrophilic Reactivity**

**8Hrs**

Structural and electronic effects on  $S_N1$  and  $S_N2$  reactivity, Potential energy diagrams for  $S_N1$  and  $S_N2$  reaction. Nucleophilic aromatic substitution bimolecular displacement, Reactivity in nucleophilic aromatic substitution, Electron withdrawal by resonance, Evidence for the two steps in bimolecular displacement. Structural effects on rates and selectivity.

### **8. Supramolecular chemistry**

**10Hrs**

Properties of covalent bonds-bond length, inter-bond angles, force constant, bond and molecular dipole moments, molecular and bond polarisability, bond dissociation, enthalpy, entropy, intermolecular forces, hydrophobic effects, Electrostatic, induction, dispersion and resonance energy, magnetic interactions, forces between macro-scopic bodies, medium effects, Hydrogen bond. Principles of molecular association and organisation as exemplified in biological macromolecules like enzymes, nucleic acids, membranes and model systems like micelles and vesicles.

### **Seminar- 8Hrs**

#### ***Books suggested -***

1. Physical Chemistry by P.W. Atkins, ELBS
2. Chemical Kinetics by K.J. Laidler, McGraw Hill.
3. Kinetics and Mechanism of chemical Transformation by J. Rajaraman and J. Kuriacose, McMillan.
4. Mechanism and Theory in Organic Chemistry by T.H. Lowry and K.C. Richardson, Harper and Row
5. Physical Organic Chemistry by N.S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry, concepts and Perspectives by J.M. Lehn, VCH
7. Physical Organic Chemistry, by Neil
8. Physical Organic Chemistry by Ritchie
9. Organic Chemistry by Morrison Boyd, Prentis Hall
10. Advanced Organic Chemistry - Reaction Mechanism and Structure by Jerry

March, John Wiley

11. A Guide Book to Mechanism in Organic Chemistry by Peter Syke, Longman

**M.Sc CHEMISTRY**  
**SEMESTER-IV**  
**LABORATORY COURSE –VI**  
**GROUP-A Organic Chemistry**

**MM-200 ;Duration-12 hrs .**

**NOTE: laboratory course with Group ‘A’ 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 -**

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 → Benzophemone → Benzophenone oxime → Benzunilide
3. Benzilic acid rearrangement : Benzilic acid from benzoin  
Benzoin → Benzil → Benzilic acid
4. Synthesis of heterocyclic compounds  
Skraup synthesis : Preparation of quinoline from aniline  
Fisher-Indol synthesis : Preparation of 2 phenyl-indole from phenyl hydrazine.
5. Sandmeyer Reaction: Preparation of o chlorobenzoic acid from anthranilic acid.



- Ullman reaction- Preparation of N-Phenyl anthranilic acid from o-chlorobenzoic acid.
- Preparation of Acridone from N-Phenyl anthranilic acid .
- Preparation of p nitro aniline
- Preparation of p bromo aniline
- Preparation of methyl orange from aniline via sulphanilic acid.

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

- Isolation of caffeine from tea leaves
- Isolation of casein from milk
- Isolation of lactose from milk
- Isolation of nicotine dipicrate from tobacco
- Isolation of piperine from black pepper
- Isolation of lycopene from tomatoes
- 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

- Amino acids
- Proteins,
- Carbohydrates
- Aspirin

### **Educational Tour**

### **Laboratory Course –Group-B**

### **Special (PHYSICAL CHEMISTRY)**

- Study of kinetics of exchange between ethyl iodide and the iodide ion.
- Determination of the solubility product of lead iodide.
- Determination of the dissociation constant of barium nitrate.
- 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 the inversion of can-sugar in presence of HCl and  $\text{H}_2\text{SO}_4$  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  $\text{H}_2\text{O}_2$  and HI.
11. Study the kinetics of decomposition of benzene diazonium chloride at different temperatures.
12. Study the kinetics of reaction between  $\text{K}_2\text{S}_2\text{O}_8$  and KI.
  - (a) Determine the rate constant and order of reaction.
  - (b) Study of influence of ionic strength on the rate constant.
13. Investigate the kinetics of autocatalytic reaction between  $\text{KMnO}_4$  and Oxalic acid.
14. Determination of order of reaction between bromic acid and hydrobromic acids.
15. Determination of concentration of 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 per-

- sulphate ion).
18. Investigate the adsorption of oxalic acid from aqueous solution by activated charcoal and verify Freundlich and Langmuir's adsorption isotherms.
  19. Determine adsorption isotherms of acetic acid from aqueous solution by charcoal.

## **COURSE STRUCTURE FOR M. Sc. CHEMISTRY SEMESTER SYSTEM**

(Two Years Course 2019-2020)

**Candidate will be required 36% of marks to pass external and internal examination separately**

Total No. of Semester-4

### **SEMESTER-I**

S.No.	Paper	Hours	Marks		
			Theory	Int. Assessment	
			Two unit test	One Seminar	
I.	Inorganic Chemistry	68	80	10	10
II.	Organic Chemistry	68	80	10	10
III.	Physical Chemistry	68	80	10	10
IV.	Spectroscopy & Maths/Bio	68	80	10	10

### **Laboratory Course-**

I - Organic Chemistry 100

II- Analytical Chemistry 100

### **SEMESTER-II**

S.No.	Paper	Hours	Marks		
			Theory	Int. Assessment	
			Two unit test	One Seminar	
V.	Inorganic Chemistry	68	80	10	10
VI.	Organic Chemistry	68	80	10	10

VII.	Physical Chemistry	68	80	10	10
VIII.	Spectroscopy & Maths/Bio	68	80	10	10

**Laboratory Course-**

III-	Inorganic Chemistry	.100
IV-	Physical Chemistry	100

**SEMESTER-III**

S.No.	Paper	Hours	Marks		
			Theory	Int. Assessment Two unit test	One Seminar
IX	Application of Spectroscopy	68	80	10	10
X	Bio-Inorganic & Bio-Physical Chemistry	68	80	10	10
XI.	Env. Chemistry	68	80	10	10
XII	Gr-A Chemistry of Heterocyclic Compounds Gr- B Chemical Dynamics	68	80	10	10

**Laboratory Course-V**

General Chemistry	200
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**SEMESTER-IV**

S.No.	Paper	Hours	Marks		
			Theory	Int. Assessment Two unit test	One Seminar
XIII .	Photochemistry & Solid State Chemistry	68	80	10	10
XIV	Bio- Organic & Bio- Physical Chemistry	68	80	10	10
XV	Gr-A Medicinal Chemistry	68	80	10	10

	Gr-B Analytical Chemistry				
XVI	Gr-A Chemistry of Natural Product/ Gr- B Physical Organic Chemistry	68	80	10	10
	<b>Laboratory Course – VI</b>				
	Group A Organic Chemistry	200			
	Group B- Physical Chemistry	200			

