

**HIMACHAL PRADESH UNIVERSITY, SHIMLA-171005**

**FACULTY OF PHYSICAL SCIENCES**



**SYLLABI**

**FOR M.Sc. CHEMISTRY**

**(SEMESTER SYSTEM)**

**(SESSION 2013-14 AND ONWARDS)**

**HIMACHAL PRADESH UNIVERSITY  
DEPARTMENT OF CHEMISTRY, SHIMLA-171005  
INDIA**

**HIMACHAL PRADESH UNIVERSITY  
DEPARTMENT OF CHEMISTRY**

**PROCEEDINGS OF THE MEETING OF THE BOPARD OF STUDIEIS IN (PG) IN THE SUBJECT OF CHEMISTRY**

A meeting of the Board of Studies in PG in the subject of Chemistry was held on 04-04-2012 at 11.00AM in the Departmental Library of the Chemistry Department. The following were present:

1. Prof. D. K. Sharma	Chairman & Convener
2. Prof. Pawan K. Sharma	Member & External Expert
3. Prof. Neelam Sharma	Member & External Expert
4. Prof. (Mrs.) Inderjeet Kaur	Member
5. Prof. M.S. Chauhan	Member
6. Prof. S.K. Lomesh	Member
7. Dr. (Mrs.) S.B. Kalia	Member
8. Dr. Baljit Singh	Member

The following decisions were taken:

1. The scheme as well as the course contents of the syllabi of M. Sc. Chemistry, spread over four semesters (I-IV) applicable w. e. f. the Academic Session 2013-2014 i.e. July, 2013 onwards, was discussed and recommended for the consideration of the Faculty of Physical Sciences (as per annexure "A") .
2. The scheme as well as the course contents of the syllabi of M. Phil, Chemistry (Organic, Inorganic and Physical Chemistry specialization), applicable w. e. f. the Academic Session 2013-2014 i.e. July, 2013 onwards, was discussed and recommended for the consideration of the Faculty of Physical Sciences (as per annexure "B").
3. BOS (PG) approved the syllabi for the Ph.D. course work for the students enrolled for Ph.D. without M. Phil degree as per H.P.U. rules and recommended the same for the consideration of the Faculty of Physical Sciences (as per annexure "C"). It was further resolved that the Ph.D. course work will run concurrently with the M. Phil Ist semester.
4. In order to maintain the academic standard in respect of research and teaching as well as to maintain the uniformity in PG Institutes of Chemistry affiliated to H.P. University, the BOS recommended that henceforth the concerned P. G. Institute will fix a suitable date for the P.G. practical examinations in consultation with the convener of BOS (PG) and the convener will draw a penal of examiners for final approval of the competent authorities.
5. It was resolved by the BOS (PG) that the pass percentage, as implemented from the Academic Session 2010-2011 i.e. 40% for the Undergraduate classes, shall also be applicable for M. Sc (Chemistry) from July 2013 in the light of the minutes of the meeting held on 24<sup>th</sup> August, 2011 in the office of the Controller of Examinations (as per annexure "D") to be incorporated in the relevant provisions of Ist Ordinances of H. P. University.

The detail of pass percentage effective from July, 2013 onwards will be as under:

A. In Theory	-	40% (32/80)
B. In I.A.	-	40% (08/20)
C. In Practical	-	40% (20/50)

However in case of M. Phil, the pass percentage will remain same as 50% as existing earlier ( as per annexure "D"). The same will also be applicable for Ph.D. course work.

The meeting ended with a vote of thanks to the chair.

Sd/- (Pawan K.Sharma) (Ext. Expert)	Sd/- (Neelam Sharma) (Ext. Expert)	Sd/- (Mrs. Inderjeet Kaur)	Sd/- (M.S. Chauhan)
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Sd/- (S.K. Lomesh)	Sd/- (Mrs. S.B. Kalia)	Sd/- (Baljit Singh)
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Sd/-

A Detailed Scheme and Course Contents of the Syllabi for M.Sc. Chemistry Spread Over Four Semesters (I-IV) For  
Session 2013-14 and Onwards

SEMESTER-I

Course No.	Title	Max. Marks
Course-I	Inorganic Chemistry	80
Course-II	Organic Chemistry	80
Course-III	Physical Chemistry	80
Course-IV	Mathematics for Chemists and Applications of computer in Chemistry	80

SEMESTER-II

Course-V	Inorganic Chemistry	80
Course-VI	Organic Chemistry	80
Course-VII	Physical Chemistry	80
Course-VIII	Chemistry of Life and Environmental Chemistry	80
Course-IX ( <i>Practical I and II Semesters Common to all</i> )	Inorganic Chemistry-A	50
	Organic Chemistry-B	50
	Physical Chemistry-C	50

SEMESTER-III

Course-X	Inorganic Chemistry	80
Course-XI	Organic Chemistry	80
Course-XII	Physical Chemistry	80
Course-XIII ( <i>Special Paper-I</i> )	Any one of the following: Inorganic Chemistry-A Organic Chemistry-B Physical Chemistry-C	80
Course-XIV ( <i>Practical Common to all</i> )	Inorganic Chemistry-A Organic Chemistry-B Physical Chemistry-C	50 50 50

SEMESTER-IV

**(A - Inorganic Chemistry specialization)**

Course-XV A ( <i>Special Paper-II</i> )	Advanced Organometallics	80
Course-XVI A ( <i>Special Paper-III</i> )	Modern Techniques of Chemical Analysis	80
Course-XVII A ( <i>Special Paper-IV</i> )	Inorganic Spectroscopy	80
Course-XVIII A ( <i>Special Paper-V</i> )	Bio-Inorganic Chemistry	80

SEMESTER-IV

**(B - Organic Chemistry specialization)**

Course-XV B ( <i>Special Paper-II</i> )	Synthetic Strategy	80
Course-XVI B ( <i>Special Paper-III</i> )	Natural products	80
Course-XVII B ( <i>Special Paper-IV</i> )	Medicinal Chemistry	80
Course-XVIII B ( <i>Special Paper-V</i> )	Polymer Chemistry	80

## SEMESTER-IV

### (C - Physical Chemistry specialization)

Course-XV C (Special Paper-II)	Advanced Quantum Chemistry	80
Course-XVI C (Special Paper-III)	Solid State Chemistry	80
Course-XVII C (Special Paper-IV)	Biophysical Chemistry	80
Course-XVIII C (Special Paper-V)	Chemistry of Macromolecules	80

### **Practicals**

Course-XIX A	Inorganic Chemistry Practicals	75
Course-XIX B	Organic Chemistry Practicals	75
Course-XIX C	Physical Chemistry Practicals	75
Course-XX	(SEMINARS For all three specializations)	25

Note : The following criteria will be implemented with regards to the award of internal assessment:

1. Internal Assessment (I.A.) of 20 Marks will be added to each theory paper.
2. These marks would , however be split as following: (a) 5 Marks for attendance in theory as well as in practical classes. The Weightage to attendance will be as follows: upto 75% with condonation from competent authority as per provision under ordinance-ZERO. Without condonation upto 75%- ONE MARK. 76-80%- TWO MARKS, 81-85% THREE MARKS, 86-90%- FOUR MARKS and above 91% FIVE MARKS.
3. The award of 15 Marks would be based on the performance of one Class Test of 15 Marks and this Test will be of objective / very short answer type .



**SEMESTER-I**  
**(COURSE – I)**  
**(INORGANIC CHEMISTRY)**

**Lectures-60**  
**Max. Marks-80**

*Note: i. Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*  
*ii. Students can ask for Character Tables (except for  $C_{2V}$  and  $C_{3V}$  point groups) if required.*

**UNIT-I**

**Group theory:** The concept of group, Symmetry elements and symmetry operations, Assignment of point groups to Inorganic molecules, Some general rules for multiplications of symmetry operations, Multiplication tables for water and ammonia, Representations (matrices, matrix representations for  $C_{2V}$  and  $C_{3V}$  point groups irreducible representations), Character and character tables for  $C_{2V}$  and  $C_{3V}$  point groups. Applications of group theory to chemical bonding (hybrid orbitals for  $\sigma$ -bonding in different geometries and hybrid orbitals for  $\pi$ -bonding. Symmetries of molecular orbitals in  $BF_3$ ,  $C_2H_4$  and  $B_2H_6$ .

**UNIT-II**

**Non-Aqueous Solvents:** Factors justifying the need of Non Aqueous solution Chemistry and failure of water as a Solvent. Solution chemistry of Sulphuric acid: Physical properties, Ionic self dehydration in  $H_2SO_4$ , high electrical conductance in spite of high viscosity, Chemistry of  $H_2SO_4$  as an acid, as an dehydrating agent, as an oxidizing agent, as an medium to carry out acid-base neutralization reaction and as a differentiating solvent. Liquid  $BrF_3$ : Physical properties, solubilities in  $BrF_3$ , self ionization, acid base neutralization reactions, solvolytic reactions and formation of transition metal fluorides.

**UNIT-III**

**Inorganic Hydrides:** Classification, preparation, bonding and their applications. Transition metal compounds with bonds to hydrogen, carbonyl hydrides and hydride anions. Classification, nomenclature, Wade's Rules, preparation, structure and bonding in boron hydrides

(boranes), carboranes, metalboranes and metallocarboranes.

**UNIT-IV**

**Organic Reagents in Inorganic Chemistry:** Chelation, factors determining the stability of chelates (effect of ring size, oxidation state of the metal, coordination number of the metal); Use of the following reagents in analysis:

- (a) Dimethylglyoxime (in analytical chemistry)
- (b) EDTA (in analytical chemistry and chemotherapy)
- (c) 8-Hydroxyquinoline (in analytical chemistry and chemotherapy)
- (d) 1,10-Phenanthroline (in analytical chemistry and chemotherapy)
- (e) Thiosemicarbazones (in analytical chemistry and chemotherapy)
- (f) Dithiazone (in analytical chemistry and chemotherapy)

**UNIT-V**

**Supramolecular Chemistry (Ref. Book 15):** Introduction, Some important concepts, Introduction to Recognition, information and complementarity, Principles of molecular receptor designs, Spherical recognition (cryptates of metal cations) Tetrahedral recognition by macrotricyclic cryptands, Recognition of ammonium ions, Recognition of neutral molecules and anionic substrates (anionic coordination)

**Books Recommended:**

1. Chemical applications of Group Theory – F.A.Cotton
2. Inorganic Chemistry – Durrant and Durrant
3. Symmetry in Chemistry- Jaffe and Orchin
4. Non-aqueous solvents – H.Sisler
5. Non-aqueous solvents – T.C.Waddington
6. Non-aqueous solvents – Logowsky
7. Concise course in Inorganic Chemistry- J.D.Lee
8. Chemistry of Elements – Greenwood and Earnshaw
9. Inorganic Chemistry – T. Moeller
10. Inorganic Chemistry – J.E.Huheey 3rd Edn.
11. Topics in Current Chemistry (Inorganic/Bio-Chemistry)–Vol. 64
12. A Text Book of Quantitative Inorganic Analysis- A.I. Vogel
13. Supramolecular Chemistry (Concepts and Perspectives) - Jean Marie Lehn(VCH-1995).
14. Introduction to ligand fields – B.N.Figgis

**SEMESTER-I**  
**(COURSE - II)**  
**(ORGANIC CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**Unit I**

**Supramolecular Chemistry:** Introduction, Bonding other than covalent bond. Addition compounds, Crown ether complexes and Cryptands, Inclusion compounds, Cyclodextrins, Catenanes and Rotaxenes and their applications.

**Unit II**

**Stereochemistry:** Introduction to Basic Concepts of Stereochemistry: Isomers and their properties, Threo and Erythro isomers, Chirality, Optical isomerism, Geometrical isomerism, Conventions for configurations- D,L and R,S systems, Racemic mixture and Racemization, Resolution of Racemic mixtures, Measurement of optical activity, optical purity, Stereoselective and Stereospecific reactions, epimerization, epimers, anomers and mutarotation, Axial Chirality (Allenes and Biphenyls), Planar chirality, Helicity, Chirality involving atoms other than carbon atoms, Prochirality: prostereoisomerism and Asymmetric synthesis. Conformational and Stereoisomerism of acyclic and cyclic systems, cyclohexane, decalins, effect of conformation on reactivity in acyclic and cyclohexane systems.

**Unit III**

**Reaction Mechanism:** Structure and Reactivity: Thermodynamic and kinetic requirements, Kinetic and Thermodynamic control, Hammonds postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

**Effect of structure on reactivity:** resonance and field effects, steric effect. Quantitative treatment: Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation. Methods of determining Reaction mechanisms,

**Unit IV**

**Aliphatic Nucleophilic Substitution:** The  $SN_2$ ,  $SN_1$ , mixed  $SN_1$  and  $SN_2$ , SET mechanisms &  $SN_i$  mechanism. The neighboring group mechanism, neighboring group participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance. Non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements-Wagner-Meerwein, Pinacol-Pinacolone and Demjanov ring expansion and ring contraction. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Esterification of carboxylic acid, transesterification, Phase-transfer catalysis, and ultrasound, ambident nucleophile, regioselectivity.

**Unit V**

**Aliphatic Electrophilic substitution:** Bimolecular mechanisms-  $SE_2$  and  $SE_i$ . The  $SE_1$  mechanism, electrophilic substitution accompanied by double bond shifts, halogenation of aldehydes, ketones, acids and acyl halides. Effect of substrates, leaving group and the solvent system on reactivity. Aliphatic diazonium coupling, Acylation at aliphatic carbon, alkylation of alkanes, Stork-enamine reactions

**Free radical reactions:** Geometry of free radicals, Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate neighboring group assistance, Reactivity in aliphatic and aromatic substrates at a bridgehead and attacking radicals. 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 (Gomberg Bachmann reaction), Hoffmann -Löffler- Freytag reaction, Hunsdiecker reaction.

**Books Recommended:**

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

**SEMESTER-I  
(COURSE – III)  
(PHYSICAL CHEMISTRY)**

**Lectures-60  
Max. Marks-80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**UNIT – I**

**Resonance Spectroscopy:** Theory of nuclear magnetic resonance NMR, the chemical shift, spin – spin coupling. Factors influencing chemical – shift and spin – spin coupling. Spin – spin and spin – lattice relaxation processes. Line –width and rate processes. First and second order Spectra. Electron Spin Resonance (ESR). Fine and hyperfine structure of ESR. Zero – field splitting of ESR signal. McConnell relation. Mossbauer spectroscopy: isomer – shift, quadrupole interaction and magnetic hyperfine interaction.

**UNIT - II**

**Molecular Spectroscopy:** Rotational spectra of non – rigid diatomic molecules and symmetric - top molecules. Anharmonic oscillator, overtones and hot bands. Diatomic vibrator – rotator (P, Q and R – branches). Rotational – vibrational spectra of symmetric – top molecules. Raman Spectroscopy: Raman scattering (a qualitative treatment). Rotational and vibrational Raman spectra of linear molecules. Polarization of Raman scattered light. Mutual exclusion principle.

**UNIT - III**

**Kinetics of complex reactions:** Consecutive and competitive (parallel) first order reactions. Kinetic vs. thermodynamic control reaction. Chain / free radical reactions; thermal ( $H_2 - Br_2$ ) and photochemical ( $H_2 - Cl_2$ ) reactions. Rice – Herzfeld mechanism of dissociation of organic molecules viz. dissociation of ethane, decomposition of acetaldehyde as  $3/2$  or  $1/2$  order reactions. Reaction rates and chemical equilibrium, principle of microscopic reversibility, activation energy and activated complex.

**UNIT - IV**

Transition state theory and its kinetic thermodynamic formulation. Potential energy surfaces (basic idea). Kinetics in solutions: diffusion controlled reactions, their rates and influence of the solvent. Kinetics of polymerization: free radical polymerization and Step – Growth Polymerization. Comparison of collisions and transition state theories in simple gas reactions, Lindman and Hinshelwood treatment qualitative treatment of RRKM model.

**UNIT - V**

- 1) Catalytic activity at surfaces: adsorption and catalysis, the Langmuir – Hinshelwood mechanism, the Eley – Rideal mechanism. Examples of catalysis: hydrogenation, oxidation and cracking na drefprming (qualitative treatment only).
- 2) Study of fast reactions; Flash photolysis and Stopped flow method

**Books Recommended:**

1. Chemical Kinetics : K.J. Laidler
2. Kinetics and Mechanism of Reaction Rates: A.Frost and G. Pearson.
3. Modern Chemical Kinetics: H. Eyring
4. Theories of Reaction Rates: K.J. Laidler, H. Eyring and S. Glasston
5. Fast Reactions: J.N. Bradly
6. Fast Reaction:C. Kalidas
7. Fast Reactions in Solutions: Caldin
8. Basic Principles of Spectroscopy: R. Chang
9. NMR and Chemistry: J.W. Akit
10. Introduction to Molecular Spectroscopy: G.M. Barrow
11. Physical Chemistry: P.W. Atkins
12. Fundamentals of Molecular Spectroscopy: C.N. Banwell
13. Physical Chemistry: G.K. Vemulapalli



**SEMESTER-I**  
**(COURSE – IV)**  
**(MATHEMATICS FOR CHEMISTS & APPLICATION OF COMPUTER IN CHEMISTRY)**

**Lectures: 60**

**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be subdivided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**Mathematics for Chemists**

**UNIT - I**

Cartesian coordinates: plane polar coordinates, spherical representation of functions, the complex plane, polar coordinates in trigonometric functions. Differential calculus: functions of single and several variables, partial derivatives, the total derivative, maxima and minima theorem, and simple examples related to chemistry. Vectors: representation and simple properties of vectors (addition and subtraction) vector addition by method of triangles, resolution of vectors. Scalar product of vector. Concept of normalization, orthogonality and complete set of unit vectors.

**UNIT – II**

Integral calculus: general and special methods of integration, geometric interpretation of integral, evaluation of definite and some standard integrals related to chemistry. The significance of 'exponential' equations. Differential equations: simple differential equations, separable variables, homogeneous equations, exact equations, linear equations, and equations of first and second order. Application to simple chemistry problems.

**UNIT – III**

Matrices and Determinants: Definition of matrix, types of matrices (row, column, null, square, diagonal). Matrix algebra: addition, subtraction, and multiplication by a number, matrix multiplication. Transpose and adjoint of matrix, elementary transformation, representation and applications to solutions of linear equations. Definition of determinant, and its properties, evaluation of determinants. Application to simple chemistry problems.

**Application of Computer in Chemistry**

**UNIT – IV**

Chemistry and FORTRAN Programming: Introductory FORTRAN concepts, character set, constant variables, data types, subscripted variables, and FORTRAN functions. FORTRAN expressions and naming FORTRAN programme, assignment statements, FORTRAN commands. Data transfer and program execution control: Introduction, format specification for READ and WRITE statements, format commands, control commands and transfer commands.

**UNIT – V**

Arrays and repetitive computation; Introduction, arrays arrange storage, dimension statement, do control, Nested do – loop continue statement, implied do. Sub – programme (functions and sub –routines): Introduction, sub programme, functions in FORTRAN, function arguments, subroutines, save variable function vs. subroutine programme. Global variables and file manipulation: Introduction, common statement, equivalence declaration, data command, block data subprogramme, declaration external, character expression and assignment, the open and closed statement, internal file, file 'input' and 'output'. Developing Linear Least – Squares fit programs in FORTRAN, as well as for involving simple formulae in organic, inorganic and physical chemistry.

**Books Recommended:**

1. Mathematical Preparation for Physical Chemistry: F. Daniel
2. Mathematical Methods for Science Students: G. Stephemen
3. Applied Mathematics for Physical Chemistry: T.R. Barrante
4. Fortran 77 & 90: V. Rajaraman
5. Computer in Chemistry: K.V. Raman

**SEMESTER-II**  
**(COURSE –V)**  
**(INORGANIC CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT-I**

**Metal-Ligand Bonding:** Recapitulation of Crystal Field Theory including splitting of *d*-orbitals in different environments, Factors affecting the magnitude of crystal field splitting, structural effects (ionic radii, Jahn-Teller effect), Thermodynamic effects of crystal field theory (ligation, hydration and lattice energy), Limitations of crystal field theory, Adjusted Crystal Field Theory (ACFT), Evidences for Metal-Ligand overlap in complexes, *Molecular Orbital Theory* for octahedral, tetrahedral and square planar complexes (excluding mathematical treatment)

**UNIT-II**

**Atomic Spectroscopy:** Energy levels in an atom, Coupling of orbital angular momentum, Coupling of Spin angular momentum, Spin orbit coupling, spin orbit coupling *p2* case, Determining the Ground State Terms-Hund's Rule, Hole formulation, Derivation of the Term Symbol for a closed sub-shell, Derivation of the terms for a *d2* configuration, Calculation of the number of the microstates.

**UNIT-III**

**Electronic Spectra-I:** Splitting of spectroscopic terms (S,P,D,F and G,H,I),  $d^1$ - $d^9$  systems in weak fields (excluding mathematics), strong field configurations, transitions from weak to strong crystal fields.

**UNIT-IV**

**Electronic Spectra-II:** Correlation diagrams ( $d1$ - $d9$ ) in  $O_h$  and  $T_d$  environments, spin-cross over in coordination compounds. Tanabe Sugano diagrams, Orgel diagrams, evaluation of B,C and  $\beta$  parameters.

**UNIT-V**

**Magnetochemistry:** Origin of Magnetic moment, Magnetic susceptibility (diamagnetic, paramagnetic), spin only moment, Russell Saunder's coupling, quenching of orbital angular moment, orbital contribution to a magnetic moment, magnetic moments from magnetic susceptibilities, temperature dependence of magnetic susceptibility, Factors determining paramagnetism, application of magnetochemistry in co-ordination chemistry in spin free and spin paired octahedral and tetrahedral complexes, Van Vlecks formula for magnetic susceptibility.

**Books Recommended:**

- 1 Advanced Inorganic Chemistry – Cotton and Wilkinson
- 2 Coordination Chemistry- Experimental Methods – K.Burger
- 3 Theoretical Inorganic Chemistry – Day and Selbin
- 4 Magnetochemistry – R.L.Carlin
- 5 Inorganic Electronic Spectroscopy – A.B.P.Lever
- 6 Concise Inorganic Chemistry – J.D.Lee
- 7 Introduction to Ligand Fields – B.N.Figgis
- 8 Introduction to Magnetochemistry – A.Earnshaw, Academic Press.

**SEMESTER-II**  
**(COURSE - VI)**  
**(ORGANIC CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**Unit -I**

**(A) Aromatic Electrophilic Substitution:** Arenium ion mechanism, orientation and reactivity, The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeier - Haack reaction, Scholl reaction, Amination reaction, Fries rearrangement, Hofmann-Martius Reaction, Reversal of Friedel Craft alkylation.

**(B) Aromatic Nucleophilic Substitution:** S<sub>N</sub>Ar, S<sub>N</sub>1, benzyne and S<sub>RN</sub>1 mechanism. Reactivity, effect of substrate structure, leaving group and attacking nucleophile, Von Richter, Sommelet-Hauser, and Smiles rearrangements, Ullman reaction, Ziegler alkylation, Schiemann reaction.

**Unit -II**

**Common Organic Reactions and Their Mechanisms:** Perkin condensation, Michael reaction, Robinson annulation, Dieckmann reaction, Stobbe condensation, Mannich reaction, Knoevenagel condensation, Benzoin condensation, Wittig reaction, Hydroboration, Hydrocarboxylation, Ester hydrolysis, Epoxidation.

**Unit -III**

**Reagents in Organic Synthesis:** Synthesis and applications of BF<sub>3</sub>, NBS, Diazomethane, Lead tetra-acetate, Osmium tetroxide, Woodward Prevost hydroxylation reagent, LiAlH<sub>4</sub>, Grignard reagent, organozinc and organolithium reagent.

**Unit -IV**

**Elimination Reactions:** Discussion of E<sub>1</sub>, E<sub>2</sub>, E<sub>1</sub>cB and E<sub>2</sub>C Mechanisms and orientation, Reactivity: Effects of substrate structures, attacking base, leaving group and medium. Mechanism and Orientation in Pyrolytic eliminations, Cis elimination, elimination in cyclic systems, eclipsing effects, cleavage of quaternary ammonium hydroxides, Shapiro reaction, Conversion of Ketoxime to nitriles.

**Unit -V**

**Pericyclic Reaction:** Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5 hexatrienes and allyl system. Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions: conrotatory and disrotatory motions, 4n and 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and chelotropic reactions. Sigmatropic rearrangements-Suprafacial and Antarafacial shifts of H, sigmatropic shifts involving carbon moieties, Claisen, Cope and aza-Cope rearrangements, Ene reaction.

**Books recommended:**

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Pericyclic Reactions, S.M. Mukherji, Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.

**SEMESTER-II**  
**(COURSE -VII)**  
**(PHYSICAL CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT – I**

Brief resume of law of thermodynamics. Gibb's and Helmholtz free energy functions and their significance. Partial molal quantities. Partial molal free energy and its variation with temperature and pressure. Determination of partial molar volume. Thermodynamic criteria for the fugacity of the process in terms of entropy change, internal energy change, enthalpy and free energy (Gibb's and Helmholtz ) change. Gibb's and Helmholtz equation and its utility in thermodynamics of cell reaction. Thermodynamics of ideal solutions. Fugacity and activity and their variation with temperature and pressure. Graphical method for the determination of fugacity.

**UNIT – II**

Chemical potential in case of ideal gases. Chemical equilibrium constant and its temperature dependence. Law of chemical equilibrium and its application. Clausius and Clapeyron equation and its application for the determination of colligative properties (depression in freezing point, elevation in boiling point and relative lowering of vapour pressure). Determination of molecular weight of non – volatile solutes from colligative properties. Relationship between relative lowering of vapour pressure and osmotic pressure. Van't Hoff equation for dilute solutions and its application.

**UNIT – III**

Nernst heat theorem and third law of thermodynamics and its application. Thermodynamic derivation of phase rule and its application to two component systems. Distribution law, its thermodynamic derivation and application. Zeroth law of thermodynamics.

**UNIT – IV**

**Non-Equilibrium Thermodynamics:** Basic principles of non – equilibrium thermodynamics: rate laws, second law of thermodynamics for open system, law of conservation of mass, charge and energy flow. Electrokinetic phenomena and expressions for streaming potential, electro- osmotic pressure difference, streaming potential using the linear phenomenological equation.

**UNIT – V**

**Corrosion:** causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential). Corrosion measurements (weight loss, OCP measurement, and polarization methods), passivity and its breakdown. Corrosion prevention (electrochemical, inhibitor, and coating methods).

**Books Recommended:**

1. Thermodynamics for Chemists: S. Glasstone
2. Physical Chemistry: G.M. Barrow
3. Non – equilibrium Thermodynamics: C. Kalidas
4. Non – equilibrium Thermodynamics: I. Prigogene
5. Electrochemistry: S. Glasstone
6. Electrochemistry: P.H. Reiger
7. Thermodynamics; R.C. Srivastava, S.K. Saha and A.K. Jain
8. Modern Electrochemistry Vol. I: J.O'M Bockris and A.K.N. Reddy
9. Physical chemistry: P.W. Attkin.

**SEMESTER-II**  
**(COURSE –VIII)**  
**(CHEMISTRY OF LIFE & ENVIROMENTAL CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT-I**

**Cell structure and function:** Basic concepts, Overview of metabolic processes (catabolic and anabolic), energy transfer processes, role and significance of ATP (the biological energy currency). Introductory idea of metabolism of proteins and lipids, biosynthesis of proteins and glycerides.

**UNIT-II**

**Nucleic acids:** Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The Chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

**UNIT-III**

**Environmental Chemistry:** Atmosphere, environmental segments, composition of the atmosphere, earth's radiation balance, particulates, ions and radicals and their formation, chemical and photochemical reactions in the atmosphere, air pollution, oxides of C,N,S and their effects, acid-rain, smog formation, Green house effects (global warming and ozone depletion, air pollution controls and introduction to analytical methods for monitoring air pollution.

**UNIT-IV**

**Hydrosphere:** Chemical composition of water bodies-lakes, streams, rivers, sea etc, hydrological cycle, complexation in natural and waste water and microbially mediated redox reactions. Water pollution-inorganic, organic, pesticides, industrial and radioactive materials, oil spills and oil pollutants, eutrophication, acid-mine drainage, waste water treatment, domestic waste water (aerobic and anaerobic treatment), and industrial waste water treatment.

**UNIT-V**

**Water quality parameters and standards:** Analytical methods for measuring DO, BOD, COD, fluoride, oils and grease and metals (As, Cd, Hg, Pb, Zn,Cu,Cr), Biochemical effects of As, Cd, Hg, Pb, Cr, CN and pesticides. **Lithosphere:** Soil composition, micro and macro nutrients, soil pollution-fertilizers, pesticides.

**Books Recommend:**

1. Principles of Biochemistry –A.L.Lehringer
2. Introduction to Chemistry of Life-H.J.DeBay
3. Outlines of Biochemistry-Conn and Stumpf
4. Environmental Chemistry-A.K.De
5. Environmental Chemistry-Manaham
6. Environmental Pollution Analysis-Khopkar

**SEMESTER I AND II**  
**(COURSE – IX A)**  
**(INORGANIC CHEMISTRY PRACTICAL)**

**Time - 6 hr/week**  
**Max. Marks - 50**

**1. Volumetric Analysis:**

**(a) Potassium iodate titrations:** Determination of iodide, hydrazine, antimony(III) and arsenic (III)

**(b) Potassium bromate titrations**

- i) Determination of antimony (III) and arsenic (III) Direct Method
- ii) Determination of aluminium, cobalt and zinc (by oxine method)

**(c) EDTA titrations**

- i) Determination of copper, nickel, magnesium
- ii) Back titration
- iii) Alkalimetric titration
- iv) Titration of mixtures using masking and demasking agents
- v) Determination of hardness of water

**2. Commercial Analysis:**

- i) Determination of available chlorine in bleaching powder
- ii) Determination of Oxygen in hydrogen peroxide.
- iii) Determination of Phosphoric acid in commercial phosphoric acid.
- iv) Determination of Boric acid in borax.
- iv) Analysis of Ores (Dolomite, Pyrolusite) and alloys (Coin, Brass, Bronze).

**3. Analysis of mixtures by gravimetric and volumetric methods from the mixture solutions:**

- 1. Copper- Nickel
- 2. Copper -Magnesium
- 3. Copper-Zinc
- 4. Iron-Magnesium
- 5. Silver-Zinc
- 6. Copper-Nickel-Zinc
- 7. Fe(II)-Fe(III)

**4. Green methods of Preparation of the following:**

- (i) Bis(acetylacetonato)copper(II)
- (ii) Tris(acetylacetonato)iron(III)
- (iii) Tris(acetylacetonato)manganese(III)

**Books Recommended:**

- 1. A text Book of Quantitative Inorganic Analysis: A.I.Vogal.
- 2. Applied Analytical Chemistry: Vermani.
- 3. Commercial Methods of Analysis: Shell & Biffen

**SEMESTER I AND II**  
**(COURSE – IX B)**  
**(ORGANIC CHEMISTRY PRACTICAL)**

**Time - 6 hr/week**

**Max. Marks - 50**

**Qualitative Analysis:** Separation, purification and identification of binary mixture of organic compounds by chemical tests, TLC, column chromatography and IR spectroscopy.

**Organic Synthesis:** Acetylation: - Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography. Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol. Grignard reaction: Synthesis of triphenyl methanol from benzoic acid. Aldol condensation: Dibenzal acetone from benzaldehyde. Sandmeyer reaction: p-chlorotoluene from p-toluidine. Acetoacetic ester condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E condensation. Preparation of iodoform from acetone (Haloform reaction). Preparation of polystyrene, anthranilic acid, fluoresceine-eosin, and methyl orange

**Books Recommended:**

1. Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.
2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.
3. Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.
4. Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark, Adward Arnold.
5. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.

COURSE – IXC  
(COURSE – IX B)  
**(ORGANIC CHEMISTRY PRACTICAL)**

**Time - 6 hr/week**  
**Max. Marks - 50**

1. **Refractive Index (RI) Measurements:** Refractive index measurements of pure solvents and analysis of solvent mixtures in terms of composition from the calibration plot..
2. **Conductometric Measurements:** Determination of cell constant, limiting molar conductance of simple electrolytes in water, verification of Ostwald, dilution law for weak acetic acid.
3. **Surface Tension Measurements:** Surface tension of pure solvents, analysis of mixtures of two miscible solvents, verification of Gibb's Thomson Rule of surface tension.
4. **Partition – Coefficient:** Determination of partition – coefficient for I<sub>2</sub> and benzoic acid between two immiscible solvents.
5. **Adsorption Measurements:** Verification of Freundlich adsorption isotherm for I<sub>2</sub>, and acetic acid on charcoal.
6. **Colloidal Solution:** Preparation of sol solution of arsenic sulphide and estimation of flocculation value for NaCl, KCl, BaCl<sub>2</sub>, AlCl<sub>3</sub>.
7. **Thermochemistry:** Determination of water equivalent of thermos flask, and estimation of heat of neutralization for strong acid strong base, weak acid strong base or vice – versa, heat of hydration and solution of salts.

**Books Recommended:**

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu



### SEMESTER-III

### (COURSE –X) (INORGANIC CHEMISTRY)

Lectures: 60  
Max. Marks: 80

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

#### UNIT-I

**Metal  $\pi$  Complexes:** Preparation, reactions, structures and bonding in carbonyl, nitrosyl and phosphine complexes, structural evidences from vibrational spectra. Structure and bonding in metal cyanides, stabilization of unusual oxidation states of transition metals.

#### UNIT-II

**Introductory Analytical Chemistry: Data Analysis**– Types and sources of errors, propagation of errors, detection and minimization of various types of errors. Accuracy and precision, average and standard deviation, variance, its analysis and confidence interval, tests of significance (*F*-test, *t*-test and paired *t*-test), criteria for the rejection of analytical data (4d rule, 2.5d rule, *Q*-test, average deviation and standard deviation), least-square analysis.

**Food and Drug Analysis**- General methods for the analysis in food (moisture, ash, crude fiber and nitrogen (proteins). Discussion of official (pharmacopoeia) methods for the determination of following drugs as such: (i) Analgin (ii) oxyphenbutazone, (iii) phenyl butazone, (iv) sulphonamides.

#### UNIT-III

**Photoelectron Spectroscopy:** Basic principle, photoionization process, ionization energies, Koopman's theorem, ESCA, photoelectron spectra of simple molecules, ( $N_2$ ,  $O_2$  and  $F_2$ ) Photoelectron spectra for the isoelectronic sequence Ne, HF,  $H_2O$ ,  $NH_3$  and  $CH_4$ , chemical information from ESCA, Auger electron spectroscopy – basic idea.

#### UNIT-IV

Lanthanides and Actinides:- Spectral and magnetic properties, comparison of Inner transition and transition metals, Transuranium elements (formation and colour of ions in aqueous solution), uses of lanthanide compounds as shift reagents, periodicity of transactinoid elements.

#### UNIT-V

**Nuclear Chemistry:** Nuclear binding energy and stability, nuclear models (nuclear shell model and collective model). Nuclear reactions: types of reactions, nuclear cross-sections, *Q*-value. Natural and artificial radioactivity, radioactive decay and equilibrium, Nuclear fission-fissionproduct and fission yields, Nuclear fusion.

**Radioactive techniques:** Tracer technique, (neutron activation analysis), Counting techniques such as G.M. Ionization and proportional counters.

#### **Books Recommended:**

1. Advanced Inorganic Chemistry – Cotton and Wilkinson
2. Fundamentals of Analytical Chemistry – Skoog, West, Holler and Crouch.
3. Chemistry of the Elements – Greenwood and Earnshaw
4. Nuclear Chemistry-U.C.Dash
5. Nuclear Chemistry – B.G.Harvey
6. Nuclear Chemistry – Arnikar
7. Techniques in Inorganic Chemistry Vol. II (Nuclear Chemistry-Johnson and Others).
8. Modern Aspects of Inorganic Chemistry-H.J.Emeleus and A.G.Sharpe
9. Analytical Chemistry-G.D.Christian
10. Chemical Structure and Bonding- DeKock and Gray
11. The Organometallic Chemistry of Transition metals: R.H. Crabtree.
12. Electronic absorption spectroscopy and related techniques: D.N. Sathyanarayan
13. Pharmacopoeia of India, Volume I and II.

**SEMESTER-III**  
**(COURSE - XI)**  
**(ORGANIC CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**Unit -I**

**Ultra Violet and Visible Spectroscopy:** Electronic transitions (185-800 nm), Beer- Lambert Law, Effect of solvent on electronic transitions, Ultra Violet bands of carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Steric effect in biphenyls, Fieser- Woodward rules for conjugated dienes and carbonyl compounds, ultra violet spectra of aromatic and heterocyclic compounds.. Applications of UV- visible spectroscopy in organic chemistry.

**Unit -II**

**Infrared Spectroscopy:** Principle, Instrumentation and sample handling, Characteristic vibrational frequencies of common organic compounds, Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Introduction to Raman spectroscopy. Applications of IR and Raman Spectroscopy in organic chemistry.

**Unit -III**

**Nuclear Magnetic Resonance (NMR) Spectroscopy:** General introduction, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation of protons present in different groups in organic compounds. chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei, virtual coupling. Stereochemistry, hindered rotation, Karplus- relationship of coupling constant with dihedral angle. First and second order spectra, Simplification of complex spectra-nuclear magnetic double resonance, spin tickling, INDOR, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Introduction to resonance of other nuclei –<sup>19</sup>F, <sup>31</sup>P, <sup>13</sup>C, NMR, 2-D and 3-D NMR, Applications of NMR in organic chemistry.

**Unit -V**

**Mass Spectrometry:** Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta-stable peak, McLafferty rearrangement. Nitrogen Rule. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Introduction to negative ion Mass spectrometry, TOF-MALDI.

Problems based upon IR, UV, NMR and mass spectrometry.

**Unit -V**

**Photochemistry – I:** Introduction and Basic principles of photochemistry. Interaction of electromagnetic radiations with matter, Types of excitations, fate of excited molecules, quantum yield, transfer of excitation energy, actinometry. Photochemistry of alkenes: cis-trans isomerization, dimerization of alkenes, photochemistry of conjugated olefins, photo-oxidation of alkenes and polyenes Photochemistry of Aromatic compounds: Isomerization, addition and substitution, photo-reduction of aromatic hydrocarbons

**Photochemistry – II:** Photochemistry of Carbonyl compounds: Norrish Type I and II, Intermolecular and Intramolecular hydrogen abstraction, Paterno -Buchi reaction,  $\alpha$  and  $\beta$ - cleavage reactions of cyclic and acyclic carbonyl compounds, Formation of oxetane and cyclobutane from  $\alpha,\beta$  unsaturated ketones, Photo-reduction of carbonyl compounds, Photo-rearrangement of enones, dienones, epoxyketones, Photo Fries rearrangement.

**Books Recommended:**

1. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpuch and G.J. Martin, Heyden.
2. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
3. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
6. Organic spectroscopy by Jagmohan
7. Organic spectroscopy by W. Kemp.
8. Fundamentals of Photochemistry, K.K. Rohtagi - Mukherji, Wiley-Eastern.
9. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggot, Blackwell Scientific Publication.
10. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
11. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill.
12. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
13. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
14. Organic Photochemistry Vol. I, II, III. Ed. Orville L. Chapman.
15. Organic Photochemistry, Ed. Robert O. Kan.
16. Spectroscopy by Pavia

**SEMESTER-III**  
**(COURSE –XII)**  
**(PHYSICAL CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**Statistical Thermodynamics**

**UNIT – I**

Basic Terminology: probability, phase space, micro and macro states, thermodynamic probability, statistical weight, assembly, ensemble, The most probable distribution: Maxwell-Boltzmann distribution, quantum statistics: The Bose- Einstein statistics and Fermi- Dirac Statistics. Thermodynamic probability (W) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance.

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions.

**UNIT – II**

Thermodynamic properties of molecules from partition function: Total energy, entropy, Helmholtz free energy, pressure, heat content, heat capacity and Gibb's free energy, equilibrium constant and partition function, Heat capacity of crystals and statistical thermodynamics, Third law of thermodynamics and entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, Einstein theory and Debye theory of heat capacities of monatomic solids.

**Basic Quantum Chemistry**

**UNIT – III**

Operators in quantum mechanics. Introduction to angular momentum. Eigenvalues and eigenfunctions. Hermitian operator. Postulates of quantum mechanics. Time dependent and time independent Schrodinger wave equations.

**UNIT – IV**

Some analytically soluble problems (complete solutions) of particle in a one and three dimensional box, harmonic – oscillator, the rigid rotor, the hydrogen atom and the quantum mechanical tunnelling.

**UNIT – V**

**Photochemistry:** Photophysical processes of electronically excited molecules (Jablonski Diagram). Franck-Condon principle. Kinetics of Excimer and exciplex formation. Energy transfer from electronically excited molecules (Stern – Volmer mechanism). E- type and P- type delayed fluorescence.

**Suggested Reading:**

1. Physical Chemistry: P.W. Atkins
2. Theoretical Chemistry by S. Glasston
3. Statistical Chemistry by I. Prigogine
4. Quantum Chemistry An Introduction: H.L. Strauss
5. Introductory Quantum Chemistry: A.K. Chandra
6. Quantum Chemistry: A. Mcquarrie
7. Quantum Chemistry: I.N. Levine

**SEMESTER-III**  
**(COURSE –XIII (A))**  
**(INORGANIC CHEMISTRY SPECIAL THEORY - I)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**UNIT-I**

Basic principles, absorption, excitation, kasha rule, electronically excited state, its life-time and energy dissipation process. Thaxi state, Photochemical behaviour of transition metal complexes, charge transfer spectra of crystalline and gaseous alkali halides. Photochemistry of chromium(III) octahedral complexes,  $[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$  and  $[\text{Cr}(\text{NH}_3)_6]^{3+}$ . Photolysis/Adamson rules, photochemistry of cobalt(III) complexes,  $[\text{Co}(\text{NH}_3)_5\text{X}]^{2+}$  and  $[\text{Co}(\text{en})_3]^{3+}$ .

**UNIT-II**

**Inorganic Reactions and Mechanism:** Substitution reactions in octahedral complexes, acid hydrolysis reactions, base hydrolysis and anation reactions, reactions occurring without rupture of metal-ligand bond. Substitution reactions of square planar complexes. Theories of trans-effect, labile and inert complexes. Mechanism of redox reactions.

**UNIT-III**

**Polymeric Inorganic Compounds:** General chemical aspects (synthesis, properties and structure) of phosphazenes, borazines, silicones, sulphur- nitrogen cyclic compounds and condensed phosphates.

**UNIT-IV**

**Stability of Coordination Compounds** – Stability constants, stepwise formation constants, overall formation constants, relationship between stepwise and overall formation constants, factors affecting the stability constants (with special reference to metal and ligand ions), Difference between thermodynamic and kinetic stability.

Determination of stability constants by:

- (i) Spectrophotometric methods (Job's method, Mole ratio and slope ratio method).
- (ii) Bjerrum's method
- (iii) Polarographic method

**UNIT-V**

**Electronic Spectra – III (Electronic spectra of complex ions):** Selection rules (Laporte, orbital and spin selection rules), band intensities, band widths, spectra in solids, spectra of aqueous solutions of d1-d9 ions in Oh and Td environments, Evaluation of 10 Dq, spectrochemical and nephelauxetic series, charge- transfer spectra.

**Books Recommended:**

1. Instability Constants- Yttermiskii
2. Advanced Inorganic Chemistry- Cotton and Wilkinson
3. Inorganic Chemistry- T.Moeller
4. Concise Inorganic Chemistry- J.D.Lee
5. Introduction to Ligand Fields- B.N.Figgis
6. Modern Aspects of Inorganic Chemistry-H.J.Emeleus and A.G.Sharpe
7. Inorganic chemistry: A Unified Approach- W.W.Porterfield
8. Inorganic Reaction Mechanism – Edberg
9. Inorganic Reaction Mechanism – Basolo and Pearson
10. Inorganic Photochemistry -- Adamson

### **SEMESTER-III**

#### **(COURSE – XIII (B)) (BIO-ORGANIC CHEMISTRY SPECIAL THEORY - I)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

#### **Unit-I**

Carbohydrates: Types of naturally occurring sugars: Deoxy-sugars, amino sugars, branched chain sugars. General methods of structure and ring size determination with particular reference to maltose, lactose, sucrose, pectin, starch and cellulose, photosynthesis of carbohydrates, metabolism of glucose, Glycoside- (amygdalin).

#### **Unit-II**

Amino acid, peptides and proteins: General methods of peptide synthesis, sequence determination. Chemistry of insulin and oxytocin. Purines and nucleic acid. Chemistry of uric acid, adenine, protein synthesis.

#### **Unit-III**

Vitamins: A general study, detailed study of chemistry of thiamine (Vitamin B1), Ascorbic acid (Vitamin C), Pantothenic acid, biotin (Vitamin H),  $\alpha$ -tocopherol (Vitamin E), Biological importance of vitamins.

#### **Unit-IV**

Enzymes: Remarkable properties of enzymes like catalytic power, specificity and regulation, Mechanism of enzyme action: Proximity effects and molecular adaptation, Chemical and biological catalysis, Transition state theory, orientation and steric effects, acid base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms (chymotrypsin, ribo nuclease, lysozyme and carboxypeptidase A). Fischer's lock and key and Koshland's induced fit hypothesis, Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

#### **Unit-V**

**Coenzyme Chemistry:** Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate,  $\text{NAD}^+$ ,  $\text{NADP}^+$ , FMN, FAD, Lipoic acid, vitamin  $\text{B}_{12}$ . Mechanisms of reactions catalyzed by the above coenzymes.

#### **Books recommended:**

1. Bioinorganic Chemistry: A Chemical Approach to Enzyme Action, Herman Duags and C. Penny, and Springer-Verlag.
2. Understanding Enzymes, Trevor Palmer, Prentice Hall.
3. Enzyme Chemistry; Impact and Applications, Ed. Collin J Suckling, Chapman and Hall.
4. Enzyme Mechanisms Ed, M.I. Page and A. Williams, Royal Society Of Chemistry.
5. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford Univ. Press.
6. Immobilized Enzymes: An Introduction and Applications In Biotechnology, Michael D. Trevan, John Wiley.
7. Enzymatic Reaction Mechanisms. 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.
10. Carbohydrates by N. Sharon.
11. Carbohydrates by Guthrie.
12. Carbohydrates by Pigman and Wolfrom.
13. The Nucleic Acids (Vol I-III) by Chargoff and Davidson.
14. Protein Structures and Functions by A. Light.
15. Chemistry of Natural Products Vol. I by K. Nakanishi.
16. Peptides and Amino Acids by R.H. Thomson.
17. The chemistry of Natural Products by P.S. Kalsi.

**SEMESTER-III**  
**(COURSE –XIII C)**  
**(Physical Chemistry Special Theory - I)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT –I**

Adsorption at solid – gas interface: Concept of ideal and non – ideal adsorption. Heat of adsorption. Types of adsorption isotherms. Single – layer adsorption – Langmuir adsorption isotherm and its derivation. Multilayer adsorption – B.E.T. theory and its kinetic derivation. Application of BET theory in its determination of surface area of the solid. Catalytic activities at surfaces: adsorption and catalysis.

**UNIT –II**

Adsorption at solid – liquid interface: Gibbs adsorption equation. Isotherms of concentration and temperature change for the adsorption in solutions. Chromatographic adsorption: column chromatography and its theory. Theory of chromatography involving one solute and several solutes.

**UNIT –III**

Solution and Interfacial Behaviour of Surfactants: Definition and classification of surfactants. Solution properties of surfactants: micelle formation, critical micelle concentration (CMC), dependence of CMC on chain length of the surfactant, micelle shape and size. Thermodynamics of micelle formation, hydrophobic effect (a qualitative view only). Aggregation at high surfactant concentration (a qualitative aspect). to micelles. Surface tension and detergent., Practical application of surfactants.

**UNIT –IV**

**Electrochemistry:** Quantitative treatment of Debye - Hückel and Debye-Hückel-Onsagar (D-H-O) theory of conductance of electrolyte solution their limitations and modifications. Pair-wise association of ions (Bjerrum and Fuoss treatment). Determination of association constant (KA) from Debye – Huckel Limiting Law. Extended Debye – Huckel Law. Qualitative treatment of ion – solvent interactions (ion solvation).

**UNIT –V**

Chemistry of nano – materials: Definition and historical perspective. Effect of nanoscience and nanotechnology in various fields. Synthesis of nanoparticles by chemical routes and their characterization techniques. Properties of nanostructured material: optical, magnetic and chemical properties. An overview of applied chemistry of nanomaterials.

**Books Recommended:**

1. Physical Chemistry of Surfaces: A.W. Admson
2. Adsorption from Solutions: J.J. Kipling
3. Micelles (Theoretical and Applied Aspects): Y. Moroi
4. Foundation of Colloid Science Vol. I and II: R.J. Hunter
5. Physical Chemistry: P.W. Atkins
6. Frontiers in Applied Chemistry: A.K. Biswas

**SEMESTER III**  
**(COURSE – XIV A)**  
**(INORGANIC CHEMISTRY PRACTICAL)**

**Time - 6 hr/week**  
**Max. Marks - 50**

**Preparation of following compounds:**

1. Tetrapyridine copper(II)persulphate
2. Dinitritotetrapyridine nickel(II)
3. Mercury (tetraisoithiocyanato)cobaltate(II).
4. Potassium tris(oxalato)aluminate(III)
5. Sodium hexa(nitro)cobaltate(III)
6. Potassium tris(oxalato)cobaltate(III)
7. Hexa(ammine)cobalt (III)chloride

**Characterization of above compounds by the following techniques:**

- i) Elemental analysis
- ii) Molar conductance values
- iii) I.R. Spectral interpretation
- iv) Thermal analysis
- v) UV-Visible Spectra

**Books Recommended:**

1. A Text Book of Qualitative Inorganic Analysis – A.I. Vogel
2. Synthetic Coordination Chemistry: Principles and Practice- J.A. Davies, C.M. Hockensmith, V.Y.Kukushkin and Y.N. Kukushkin.

**SEMESTER III**  
**(COURSE – XIV B)**  
**(ORGANIC CHEMISTRY PRACTICAL)**

**Time - 6 hr/week**  
**Max. Marks - 50**

**A. Quantitative Analysis:** Determination of the percentage/ number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/ phenols using bromate – bromide solution/ acetylation method. Determination of iodine and saponification values of an oil sample. Determination of DO, COD and BOD of water sample.

**B. Multistep Synthesis:** Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.

Benzilic Acid Rearrangement: Benzaldehyde → Benzoin → Benzil → Benzilic acid.

Hofmann bromamide Rearrangement: Phthalic anhydride → Phthalimide → Anthranilic acid

Beckmann Rearrangement: Benzene → Benzophenone → Benzophenone oxime → Benzanilide.

Skraup Synthesis: Preparation of quinoline from aniline.

Synthesis using Phase Transfer Catalysis: Alkylation of diethyl malonate or ethyl acetoacetate and an alkyl halide.

**Books Recommended:**

1. Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.
2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.
3. Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.
4. Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark, Adward Arnold.
5. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.



**SEMESTER III**  
**(COURSE – XIV C)**  
**(Physical Chemistry Practical)**

**Time - 6 hr/week**  
**Max. Marks - 50**

1. **Solubility Measurements:** Heat of solution of electrolytes by solubility measurements.
2. **Heat of transfer Measurements:** Heat of transfer for benzoic acid and I<sub>2</sub> between two immiscible solvents.
3. **Conductometric Measurements:** Precipitation, and acid base titration. Determination of relative strength of acids in the given mixtures of acids. Solubility of sparingly soluble salt.
4. **Construction of Phase Diagram:** Phase diagram for liquids, (benzene and methanol) and phase diagram for solids, (benzoic acid and cinnamic acid, benzoic acid and naphthalene and acetamide and salicylic acid).
5. **Colorimetric Measurements:** Verification of Beer – Lambert's law for aqueous solutions of KMnO<sub>4</sub>, K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and CuSO<sub>4</sub> and construction of calibration plot to estimate the unknown concentration.
6. **Kinetic Measurement:** Acid hydrolysis of ethylacetate and Saponification of ethylacetate.

**Books Recommended:**

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu

**SEMESTER-IV**  
**(COURSE –XV A)**  
**(INORGANIC CHEMISTRY SPECIAL THEORY - II)**  
**(ADVANCED ORGANOMETALLICS)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT-I**

**Organometallic Compounds of transition elements:** Types of ligands and their classifications in organometallic compounds, 16 and 18 electron rule and its limitations. Hapto-nomenclature, synthesis, structure and bonding aspects of following organometallic compounds with carbon-  $\pi$  donor ligands: (a) Two electron donor (olefin and acetylenic complexes of transition metals): (b) Three electron donor ( $\pi$ -allyl complexes of transition metals): (c) Four electron donor (butadiene and cyclobutadiene complexes of transition metals): (d) Five electron donor cyclopentadienyl complexes of transition metals – metallocenes with special emphasis to ferrocenes): (e) Six electron donor [Benzene (arene) complex]. Fluxional Organometallic compounds (classification)

**UNIT-II**

**Homogeneous Transition metal catalysis:** General considerations, Reason for selecting transition metals in catalysis (bonding ability, ligand effects, variability of oxidation state and coordination number), basic concept of catalysis (molecular activation by coordination and addition), proximity interaction (insertion/inter-ligand migration and elimination, rearrangement). Phase transfer catalysis. Homogeneous hydrogenation of unsaturated compounds (alkenes, alkynes, aldehydes and ketones). Asymmetric hydrogenation (Olefins).

**UNIT-III**

**Some important homogeneous catalytic reactions:-** Ziegler Natta polymerization of ethylene and propylene, oligomerisation of alkenes by aluminumalkyl, Wackers acetaldehyde synthesis, hydroformylation of unsaturated compounds using cobalt and rhodium complexes, Monsanto acetic acid synthesis, carbonylation of alkenes and alkynes using nickel carbonyl and palladium complexes.

**UNIT-IV**

**Metal-metal bonding in carbonyl and halide clusters:-** Polyhedral model of metal clusters, effect of electronic configuration and coordination number, Structures of metal carbonyl clusters of three atoms  $M_3(CO)_4$  (M=Fe, Ru & Os), Four metal atoms (tetrahedra)  $[M_4(CO)_6]$  {M= Co, Rh & Ir} and octahedron of type  $M_6(CO)_8$  [M= Co & Rh], and halide derivatives of Rhenium (III) triangles, metal carbonyls involving bridged-terminal exchange and scrambling of CO group.

**UNIT-V**

**Transition Metal-Carbon multiple bonded compounds:-** Metal carbenes and carbenes (preparation, reactions, structure and bonding considerations). Biological and industrial applications, and environmental aspects of organometallic compounds.

**Books Recommended:**

1. Principles of organometallic compounds – Powell

2. Organometallic chemistry (an Introduction) – Perkin and Pollar
3. Advanced Inorganic Chemistry – Cotton and Wilkinson
4. Organometallic Chemistry-R.C.Mehrotra
5. Organometallic compounds of Transition Metal-Crabbtree
6. Chemistry of the Elements – Greenwood and Earnshaw
7. Homogeneous transition metal catalysis – Christopher Masters
8. Homogeneous Catalysis – Parshall
9. Principles and Application of Homogeneous Catalysis – Nakamura and Tsutsui
10. Progress in Inorganic Chemistry Vol. 15 – Lipard. (Transition metal clusters – R.B.King)
11. Organotransition metal chemistry by S.G.Davis, Pergamon press 1982.
12. Principles and applications of organotransition metal chemistry by Ccollmen and Hegden

**SEMESTER-IV**  
**(COURSE –XVI A)**  
**(INORGANIC CHEMISTRY SPECIAL THEORY - III)**  
**(MODERN TECHNIQUES OF CHEMICAL ANALYSIS)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT-I**

**Spectrophotometry:** i) Introduction, fundamental laws of photometry, the electromagnetic spectrum and spectrochemical methods, UV/Visible instrumentation, absorption spectra, Beer-Lambert's Law, deviation from Beer-Lambert's Beer's Law. ii) *Photometric Titrations:-* Simultaneous spectrophotometric determination, differential spectrophotometry, titration curves and applications to quantitative analysis. iii) *Molecular Fluorescence Spectroscopy:-* Theory, relaxation processes, relationship between excitation spectra and fluorescence spectra, fluorescent species, effect of concentration on fluorescence intensity, instrumentation and application of fluorescence methods.

**UNIT-II**

**Atomic Spectroscopy:** Theory of flame photometer, intensities of spectral lines, selection of optimal working conditions, applications of flame photometry to quantitative analysis. The Theory of Atomic Absorption Spectroscopy (AAS), Origin of atomic spectra, line width effects in atomic absorption, instrumentation and its application, Atomic emission spectroscopy (AES) and the detailed description of the techniques of inductively coupled plasma AES (ICP-AES) and its instrumentation. Chemical and spectral interferences encountered in both techniques and how to overcome them.

**UNIT-III**

**Electroanalytical Methods :** a) *Electrogravimetric methods:-* i) Current-voltage relationship during electrolysis, operation of a cell at a fixed applied potential, constant current electrolysis, physical properties of electrolytic precipitates, chemical factors of importance in electrodeposition, anodic deposition. ii) Spontaneous electrogravimetric analysis (internal electrolysis), apparatus and applications. iii) Electrolytic method with and without potential control, apparatus and applications.

b) *Coulometric Methods:* i) Controlled potential Coulometry, instrumentation and applications. ii) Coulometric titrations, cell for coulometric titrations, applications of coulometric titrations (neutralization, precipitation, and complex formation titrations), comparison of coulometric and volumetric titrations.

**UNIT-IV**

**Polarographic Methods:** General introduction: Theoretical measurements of classical polarography, polarographic measurements, polarograms, interpretation of polarographic waves, equation for polarographic waves, half-wave potential, effect of complex formation on polarographic waves, dropping mercury electrode (advantages and limitations), current variation with a dropping electrode, polarographic diffusion current, the ilkovic equation, effect of capillary characterization on diffusion current, diffusion coefficient temperature, kinetic and catalytic current, polarograms for mixtures of reactants, anodic waves and mixed anodic and cathodic waves, current maxima and its suppression, residual current, supporting electrolytes, oxygen waves, instrumentation and applications to inorganic and organic analysis.

**UNIT-V**

**Thermoanalytical methods:** (a) **Thermogravimetric analysis:** Introduction, Factors affecting thermogravimetric curves, Instrumentation, Applications to inorganic compounds (analysis of Ca and Mg in binary mixture, calcium oxalate, determination of Ca, Sr & Ba in the mixture, drying of sodium carbonate) and analysis of clays and soils, and determination of titanium content of non-stoichiometric sample of titanium carbide).

(b) **Differential thermal analysis:** Introduction, Factors affecting DTA curves, Instrumentation, Applications to inorganic compounds : Mixtures of lanthanum-cerium and praseodymium oxalate,  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ , detection of organic contamination in ammonium nitrate, different magnesium carbonate samples and determination of uncalcined gypsum in plaster of paris.

**Books Recommended:**

1. Instrumental methods of analysis.-H.H.Willard, LL.Marritt and J.A.Dean
2. Fundamentals of Analytical Chemistry – Skoog , West, Holler and Crouch.
3. Instrumental Methods of Chemical Analysis-G.K.Ewing
4. Modern Polarographic Methods in Analytical Chemistry -A.M.Bond
5. Thermal Methods of Analysis-W.W. Wendlandt.

**SEMESTER-IV**  
**(COURSE –XVII A)**  
**(INORGANIC CHEMISTRY SPECIAL THEORY - IV)**  
**(INORGANIC SPECTROSCOPY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**UNIT-I**

**Infrared Spectroscopy:** Theory of IR absorption, Types of vibrations, Observed number of modes of vibrations, Intensity of absorption bands, Theoretical group frequencies, Factors affecting group frequencies and band shapes (Physical state, Vibrational Coupling, Electrical effects, Resonance, Inductive effects, Ring strain) Vibrational-rotational fine-structure. Experimental method.

Applications of IR to the following:

- i) Distinction between
  - a) Ionic and coordinate anions such as  $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$  and  $\text{SCN}^-$
  - b) Lattice and coordinated water.
- ii) Modes of bonding of ligands such as urea and dimethylsulphoxide.

**UNIT-II**

**Nuclear Magnetic Resonance Spectroscopy:** Introduction, Chemical shift, Mechanism of electron shielding and factors contributing to the magnitude of chemical shift, Nuclear overhauser effect, Double resonance, Chemical exchange, Lanthanide shift reagents and NMR spectra of paramagnetic complexes. Experimental techniques (CW and FT).

**Stereochemical non-rigidity and fluxionality:** Introduction, use of NMR in its detection in  $\text{PF}_5$ ,  $\text{Ti}(\text{acac})_2\text{Cl}_2$ ,  $\text{Ti}(\text{acac})_2\text{Br}_2$ ,  $\text{Ta}_2(\text{OMe})_{10}$ .

**UNIT-III**

**Nuclear Quadrupole Resonance Spectroscopy:** Basic concepts of NQR (Nuclear electric quadrupole moment, Electric field gradient, Energy levels and NQR frequencies), Effect of magnetic field on spectra, Factors affecting the resonance signal (Line shape, position of resonance signal) Relationship between electric field gradient and molecular structure. Structural information of the following:  $\text{PCl}_5$ ,  $\text{TeCl}_4$ ,  $\text{Na}^+\text{GaCl}_4^-$ ,  $\text{BrCN}$ , and Hexahalometallates

**UNIT-IV**

**Mössbauer Spectroscopy:** Introduction, Principle, Conditions for Mössbauer Spectroscopy, Parameters from Mössbauer Spectra- Isomer shift, Electric Quadrupole Interactions, Magnetic Interactions, MB instrumentation, Applications of MB spectroscopy in structural determination of the following:

- i) High spin Fe (II) and Fe (III) halides-  $\text{FeF}_2$ ,  $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$ ,  $\text{FeF}_3$ ,  $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ .
- ii) Low spin Fe(II) and Fe(III) Complexes- Ferrocyanides, Ferricyanides, Prussian Blue.
- iii) Iron carbonyls.  $\text{Fe}(\text{CO})_5$ ,  $\text{Fe}_2(\text{CO})_9$  and  $\text{Fe}_3(\text{CO})_{12}$
- iv) Inorganic Sn(II) and Sn(IV) halides.

## **UNIT-V**

**Electron Spin Resonance Spectroscopy:-** Introduction, Similarities between ESR and NMR, Behaviour of a free electron in an external Magnetic Field, Basic Principle of an Electron Spin Resonance Spectrometer, Presentation of the spectrum, Hyperfine coupling in Isotropic Systems (methyl, benzene and Naphthalene radicals). Factors affecting the magnitude of g-values. Zero field splitting and Kramer's Degeneracy, Line width in solid state ESR, Double resonance technique in e.s.r. (ENDOR) Experimental method. Applications of ESR to the following:

1. Bis-Salicylaldimine - Copper(II)
2.  $\text{CuSiF}_6 \cdot 6\text{H}_2\text{O}$  &  $(\text{NH}_3)_5\text{Co}-\text{O}-\text{Co}(\text{NH}_3)_5$

### **Books Recommended:**

1. Physical methods in Inorganic Chemistry - R.S.Drago.
2. Modern Optical methods of Analysis - Eugens D.Olsen
3. Infrared spectra of Inorganic and coordination compounds - Kazuo Nakamoto
4. Introduction to Chemistry - Donald L.Pavia and G.M.Lampman.
5. Fundamentals of Molecular Spectroscopy-C.N.Banwel
6. Spectroscopy in Inorganic Chemistry - Rao & Ferraro Vol I & II
7. Advances in Inorganic and Radiation Chemistry Vol 6 & 8.
8. Quarterly reviews Vol 11 (1957)
9. Progress in Inorganic Chemistry Vol 8
10. Organic Spectroscopy-W. Kemp

## SEMESTER-IV

### (COURSE –XVIII A) (INORGANIC CHEMISTRY SPECIAL THEORY - IV) (BIO-INORGANIC CHEMISTRY)

Lectures: 60  
Max. Marks: 80

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

#### UNIT-I

**(a) Metalloporphyrins:** Porphyrins and their salient features, characteristic absorption spectrum of porphyrins, chlorophyll (structure and its role in photosynthesis). Transport of Iron in microorganisms (siderophores), types of siderophores (catecholates and Hydroxamate siderophores).

**(b) Metalloenzymes:** Definitions: Apoenzyme, Coenzyme, Metalloenzyme, structure and functions of Carboxy peptidases and Carbonic anhydrase.

#### UNIT-II

**Oxygen Carriers:** a) *Natural oxygen carriers:* Structure of hemoglobin and myoglobin, Bohr effect, Models for cooperative interaction in hemoglobin, oxygen Transport in human body (-perutz mechanism), Cyanide poisoning and its remedy. Non-heme proteins (Hemerythrin & Hemocyanin).

b) *Synthetic oxygen carriers:* Oxygen molecule and its reduction products, model compounds for oxygen carrier (Vaska's Iridium complex, cobalt complexes with dimethyl glyoxime and Schiff base ligands).

#### UNIT-III

**Transport and storage of metals:** The transport mechanism, transport of alkali and alkaline earth metals, ionophores, transport by neutral macrocycles and anionic carriers, sodium/potassium pump, transport and storage of Iron (Transferrin & Ferritin).

#### UNIT-IV

**Inorganic compounds as therapeutic Agents :-** Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (Platinum complexes), Lithium and mental health.

#### UNIT-V

**Nitrogen fixation :** A. Nitrogen molecule (MO picture) and its transition metal complexes, reactivity of coordinated dinitrogen, *in-vivo* and *in-vitro* nitrogen fixation, symbiotic and asymbiotic nitrogen fixation.

B. Nitrogen metabolism : Introduction, elementary idea about nitrogen nutrition in various forms (nitrate and ammonia nitrogen).

#### **Books Recommended:**

1. The Inorganic Chemistry of Biological processes - M.N.Hughes.
2. Bio Inorganic Chemistry - Robert Hay
3. Advanced Inorganic Chemistry (4th Edn) - Cotton and Wilkinson.
4. Topics in current chemistry (Inorganic Biochemistry) vol. 64 (1976) – Davison and Coworkers.
5. General Biochemistry - Fruton J.S. and Simmonds S.
6. Plant Physiology - Robert N.Devlin.
7. Inorganic chemistry – James E. Huheey.

**SEMESTER-IV**  
**(COURSE – XV B)**  
**(ORGANIC CHEMISTRY SPECIAL THEORY - II)**  
**(SYNTHETIC STRATEGY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**Unit- I**

**Organic Reagents:** Reagents in organic synthesis: Wilkinson catalyst, Lithium dialkyl cuprates (Gilman's reagents), Lithium diisopropylamide (LDA), 1,3-Dithiane (Umpolung) Dicyclohexylcarbodiimide (DCC), and Trimethylsilyliodide, DDQ, SeO<sub>2</sub>, Baker yeast, Tri-n-butyltinhydride, Nickel tetracarbonyl, Trimethylchlorosilane. Grubbs Catalysts.

**Unit- II**

**Oxidations:** Introduction, Different oxidative process. Aromatization of six membered ring, dehydrogenation yielding C-C double bond, Oxidation of alcohols, Oxidation involving C-C double bond, Oxidative cleavage of ketones, aldehydes and alcohols, double bonds and aromatic rings, Ozonolysis, Oxidative decarboxylation, Bisdecarboxylation, Oxidation of methylene to carbonyl, Oxidation of olefins to aldehydes and ketones

**Unit- III**

**Reductions:** Introduction, Different reductive processes. Reduction of carbonyl to methylene in aldehydes and ketones, Reduction of nitro compounds and oximes, Reductive coupling, Bimolecular reduction of aldehydes or ketones to alkenes, metal hydride reduction, Acyloin ester condensation, Cannizzaro reaction, Tishchenko reaction, Willgerodt reaction .

**Unit- IV**

**Rearrangements:** General mechanistic considerations-nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Backmann, Hofmann, Curtius, Schmidt, Benzidine, Baeyer-Villiger, Shapiro reaction, Wittig rearrangement and Stevens rearrangement.

**Unit- V**

**Disconnection Approach:** An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity cyclisation reactions, amine synthesis. Protecting Groups: Principle of protection of alcohol, amine, carbonyl and carboxyl groups. One Group C-C Disconnection: Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes in organic synthesis.

**Books Recommended:**

1. Designing Organic Synthesis, S. Warren, Wiley.
2. Organic Synthesis- Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlage VCH.
3. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
4. Modern Synthetic Reactions, H.O. House, W. A. Benjamin.
5. Advanced Organic Chemistry-Reactions Mechanisms and Structure, J. March, Wiley.
6. Principles of Organic Synthesis, R. Norman and J.M. Coxon, Blakie Academic and Professional.
7. Advanced Organic Chemistry Part-B, F.A. Carey and R. J. Sundburg, Plenum Press.
8. Organometallic Chemistry-A Unified Approach, R.C. Mehrotra, A. Singh.

**SEMESTER-IV**  
**(COURSE – XVI B)**  
**(ORGANIC CHEMISTRY SPECIAL THEORY - II)**  
**(NATURAL PRODUCTS)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**Unit- I**

**Terpenoids:** Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, biosynthesis and synthesis of the following representative molecules: Monoterpenoids: Citral, geraniol (acyclic),  $\alpha$ -terpeneol, menthol (monocyclic). Sesquiterpenoids: Farnesol (acyclic), zingiberene (monocyclic), santonin (bicyclic), Diterpenoids: Phytol and abietic acid.

**Unit- II**

**Carotenoids and Xanthophylls:** General methods of structure determination of Carotenes:  $\beta$ -carotene,  $\alpha$ - carotene,  $\gamma$ - carotene, lycopene and vitamin A. Xanthophylls: Spirilloxanthin, Capsorubin, Fucoxanthin. Carotenoid acids (Apocarotenoids): Bixin and Crocetin. Bio synthesis of carotenoids

**Unit- III**

**Alkaloids:** Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, synthesis and biosynthesis of the following: Ephedrine, Coniine, Nicotine, Atropine, Quinine and Morphine.

**Unit- IV**

**Steroids:** Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Androsterone, Testosterone, Estrone, Progesterone. Biosynthesis of steroids

**Unit- V**

**Plant Pigments:** Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Anthocyanins (Cyanin and pelargonidin), polyphenols: Flavones (chrysin), Flavonols (quercetin) and isoflavones (daidzein) coumarin, Quinones (lapachol), Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

**Books Recommended:**

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. II, I.L. Finar, ELBS.
3. Stereo selective 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-ur-Rahman M. I. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.



**SEMESTER-IV**  
**(COURSE – XVII (B))**  
**(ORGANIC CHEMISTRY SPECIAL THEORY - II)**  
**(MEDICINAL CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**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 relationships (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. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-Chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Free-Wilson analysis, Hansch analysis relationships between Free-Wilson and Hansch analysis. Naming of drugs-Trade names and Generic names

**Unit- II**

**Pharmacokinetics and Pharmacodynamics:** Pharmacokinetics: Introduction to drug absorption, distribution, metabolism, elimination using pharmacokinetics. Importance of pharmacokinetic parameters in defining drug distribution and in therapeutics. Importance of pharmacokinetics in drug development process.

**Pharmacodynamics:** Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, membrane active drugs, drug metabolism, xenobiotics, biotransformation, Significance of drug metabolism in medicinal chemistry.

**Unit- III**

**Antibiotics and Antiinfective Drugs: Antibiotics:** Historic development in the structural modifications of Penicillin antibiotics. Structure, SAR and biological action of antibiotics. Examples: penicillin: penicillin-G, penicillin-V, ampicillin, amoxicillin, chloramphenicol, cephalosporin, tetracycline and streptomycin. Sulfonamides: Structure, SAR and mode of action of sulfonamides, sulfonamide inhibition and probable mechanisms of bacterial resistance to sulfonamides. Examples: sulfadiazine, sulfafurazole, Acetyl Sulfafurazole, Sulfaguanidine, Phthalylsulfacetamide, Mafenide, Sulphonamide related compounds Dapsone.: Introduction and general mode of action of Local antiinfective drugs, Examples: sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, chloroquin and primaquin

**Unit- IV**

**Psychoactive Drugs:** Introduction, neurotransmitters-receptor interaction, CNS depressants and stimulants. SAR and Mode of action, Central Nervous System Depressant: **General anaesthetics, Sedatives & Hypnotics:** Barbiturates and Benzodiazepines. **Anticonvulsants:** Barbiturates, Oxazolidinediones, Succinimides, Phenacemide and Benzodiazepines. **Psychotropic Drugs:** The neuroleptics (Phenothiazines and butyrophenones), **antidepressants** (Monoamine oxidases inhibitors and Tricyclic antidepressants) and anti-anxiety agents (Benzodiazepines). Central Nervous System Stimulants: Strychnine, Purines, Phenylethylamine, analeptics, Indole ethylamine derivatives,

**Unit- V**

**Therapeutic Agents, SAR and Their mode of Action: Antineoplastic Agents:** Cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Biological action of mechlorethamine, cyclophosphamide, melphalan, uracil, and 6-mercaptopurine.

**Cardiovascular Drugs:** Antihypertensive and hypotensive drugs, antiarrhythmic agents, vasopressor drug, Direct acting arteriolar dilators. Biological action of methyldopa, propranolol hydrochloride, amyl nitrate, sorbitrate, verapamil, Atenolol.

**Antihistaminic agents:** Ethylene diamine derivatives, amino alkyl ether analogues, cyclic basic chain analogues. **Antifertility agents:** General antifertility agents. HIV and anti AIDS drugs, **Diuretics:** Mercurial diuretic, Non mercurial diuretics (Thiazides, carbonic-anhydrase inhibitors, xanthine derivatives, pyrimidine diuretics and osmotic diuretics

**Books Recommended:**

1. An Introduction to Medicinal Chemistry, Graham L. Patrick.
2. Medicinal Chemistry: Principles and Practice Edited by F.D. King.
3. Textbook of Organic Medicinal and Pharmaceutical Chemistry, Edited by Charles O. Wilson, et al.
4. Introduction to Medicinal Chemistry, Alex Gringuage.
5. Principles of Medicinal Chemistry, William O. Foye, Thomas L. Lemice and David A. Williams.
6. Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.
7. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 Ed. M.E. Wolff, John Wiley.
8. Goodman and Gilman's Pharmacological Basis of Therapeutics, Mc Graw-Hill.
9. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.
10. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

**SEMESTER-IV**  
**(COURSE – XVIII (B))**  
**(ORGANIC CHEMISTRY SPECIAL THEORY - II)**  
**(POLYMER CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**UNIT -I**

**Chemistry of Polymerization:** Macromolecular Concept, Chain polymerization – Radical, Cationic and Anionic polymerization, Step Growth polymerization, Electrochemical-initiated polymerization, Metathetical polymerization, Group transfer polymerization, Co-ordination polymerization, Kinetics of chain and step growth polymerization. Concept of chain transfer, Concept of copolymerization, Graft and Block copolymers, Copolymer equation, Monomer reactivity ratio, Alfrey-price scheme.

**UNIT- II**

**Polymer synthesis:** Bulk, solution, suspension, polycondensation, interfacial condensation and emulsion techniques of polymer synthesis

**Polymer Characterization:** Average molecular weight concept. Number, weight and viscosity, average molecular weights, Polydispersity and molecular weight distribution, The practical significance of molecular weight. Measurement of molecular weights - End group, viscosity, light scattering, osmotic and ultra centrifugation methods. Analysis and testing of polymers - Chemical analysis, Spectroscopic methods, Thermal Analysis, XRD and SEM.

**Unit III**

**Stereoisomerism in polymers:** Types of stereoisomerism in polymers, Monosubstituted ethylenes (Site of steric isomerism, Tacticity), Disubstituted ethylenes (1,1-disubstituted ethylenes, 1,2- disubstituted ethylenes), Stereoregular polymers: Significance of stereoregularity (isotactic, syndiotactic, and atactic polypropenes), Cis- and trans-1,4-poly-1,3- dienes, Cellulose and amylose.

**Morphology and order in crystalline polymers:** Configuration of polymer chains. Crystal structures of polymers, Strain-induced morphology, Crystallization and melting, Polymer structures and physical properties - crystalline melting point, T<sub>m</sub>, Effect of chain flexibility and other steric factors, entropy and heat of fusion, Glass transition temperature, T<sub>g</sub>, Relationship between T<sub>m</sub> and T<sub>g</sub>, Effect of molecular weight, diluents, chemical structure, chain topology, branching and crosslinking. Property requirement and polymer utilization.

**UNIT- IV**

**Polymer Reactions:** General introduction to the polymer reactions, Vulcanization, Chemical and radiation crosslinking, Derivatization of Cellulose: etherification and esterification, Graft co-polymerization, Methods of Graft Copolymerization.

Polymer as carriers or supports, polymeric reagents, polymeric substrates, Merrifield resins, polymeric supports as catalysts and drug carrier.

**UNIT-V**

**Commercial and Specialty Polymers:** Polyethylene, Polyvinyl chloride, Polyamides, Polyesters, Polyurethanes, Phenolic and epoxy resins and Silicone polymers. Applications of starch, gelatin, pectin and Chitosan in polymer industry. Fire retarding polymers, Conducting polymers, Biodegradable polymers (lactic and glycolic acid based). biomedical applications of polymers, Fundamentals of Supramolecular chemistry of polymers.

**Books Recommended:**

1. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemist's Book of Orbitals. 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,
5. Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry; Concepts and Perspectives, J.M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H.Maskill, Oxford Univ. Press.
8. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
9. Polymer Science, V.R. Gowarikar, N.V. Visvanathan and J. Sreedhar, Wiley Eastern.
10. Functional Monomers & Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
11. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
12. Physics & Chemistry of Polymers, J.M.G. Cowie, Blakie Academic and Professional.

**SEMESTER-IV**  
**(COURSE -XV C)**  
**(PHYSICAL CHEMISTRY SPECIAL THEORY - II)**  
**(ADVANCED QUANTUM CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT - I**

Time – independent perturbation theory for non – degenerate and degenerate states. The first - order correction to the energy and wavefunction. Perturbation treatment of particle in a one – dimensional box, ground state helium atom and harmonic – oscillator. First order perturbation of degenerate states.

**UNIT - II**

Variational method. Linear and non – linear variation functions. Variational treatment of the particle in a one dimensional box, ground state hydrogen atom, helium atom and one – dimensional harmonic oscillator. Concept of spin and Pauli's Exclusion principle.

**UNIT - III**

Multielectron atoms: Hartree's and Hartree – Fock self – consistent – field theory. Slater type orbitals and Slater rules. Roothan's method. Qualitative treatment of Density functional theory (DFT); Hohenberg – Kohn theorem, Kohn – Sham formulation.

**UNIT – VI**

Theory of chemical bonding (diatomic molecules) Born-Oppenheimer approximation. Linear combination of atomic orbitals (LCAO) approximation Variational treatment of hydrogen molecule ion (ground state). Valence bond and MO (LCAO) treatment of hydrogen molecule. Comparison of the MO and VB treatments. Configuration Interaction.

**UNIT – V**

Quantum – mechanical treatment of conjugated  $\pi$ - electron systems: The  $\pi$ - electron approximation. The Huckel – Molecular Orbital Theory for conjugated hydrocarbon systems. Application to ethylene, butadiene, cyclobutadiene and benzene.

**Books Recommended:**

1. Quantum Chemistry An Introduction: H.L. Strauss
2. Introductory Quantum Chemistry: A.K. Chandra
3. Quantum Chemistry: D.A. McQuarri
4. Quantum Chemistry: I.N. Levine
5. Molecular Quantum Mechanics: P.W. Atkins
6. Elementary Quantum Chemistry: F.L. Pilar
7. Introductory Quantum Chemistry: S.R. LaPaglia
8. Fundamental Quantum Chemistry: T.E. Peacock

**SEMESTER-IV**  
**(COURSE –XVI C)**  
**(PHYSICAL CHEMISTRY SPECIAL THEORY - III)**  
**(SOLID STATE CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT - I**

**X-ray Diffraction & Crystal Structure:** X-rays Diffraction by crystals. The Laue equations and Bragg's law. Definitions related to crystal structure. Crystallographic direction and crystallographic phases. X-ray diffraction experiments: The powder method and the single crystal method. Reciprocal lattice. Structure factor and its relation to intensity and Electron density.

**UNIT - II**

Bonding in crystals: Ionic crystals, lattice energy of ionic crystals, metallic crystals. Band theory. Imperfections: Point defects (Schottky and Frankel defects). Thermodynamic derivation of these defects. Theories of Bonding: Free electro theory (a qualitative treatment) Zone theory; allowed energy zones , Brillouin zones, k – space, Fermi surfaces and density states.

**UNIT - III**

Properties of crystals: Electrical properties of metals; conductors and non – conductors, conductivity in pure metals. Hall effect. Thermal properties: Theories of specific heat. Electrical properties of semiconductors: Band theory, intrinsic and extrinsic semiconductors. Electrons and holes. Temperature dependence and mobility of charge carriers. Optical properties: Dielectric properties: Piezoelectricity, Ferro electricity, Ionic conductivity and electric breakdown.

**UNIT – IV**

Superconductivity: occurrence of superconductivity, destruction of superconductivity by magnetic fields (Meissner effect). Thermodynamic effects of superconducting species (entropy, thermal conductivity and energy gap). Theoretical survey (thermodynamics of superconducting transition, London equation, coherence length). BCS theory of superconductivity.

**UNIT - V**

Solid State Reactions: General principles: experimental procedures, kinetics of solid state reactions, vapour phase transport methods, interaction or ion exchange reaction, electrochemical reduction methods, preparation of thin films, growth of single crystal.

**Books Recommended:**

1. Introduction to Solids: Azaroff
2. Solid State Chemistry and its applications: West
3. Solid State Chemistry: Chakrabarty
4. Solid State Chemistry: N.B. Hannay
5. Solid State Physics: Kittel

**SEMESTER-IV**  
**(COURSE –XVII C)**  
**(PHYSICAL CHEMISTRY SPECIAL THEORY - IV)**  
**(BIOPHYSICAL CHEMISTRY)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting TWO from each unit. As far as possible, every question will be divided into Two – Three Parts. The students shall attempt FIVE questions selecting ONE from each unit.*

**UNIT – I**

Cell membrane and its structure: The Cell Membrane, lipids in biological membranes, phospholipids, sphingolipids, glycolipids, cholesterol, gangliosides, lipoproteins, types and arrangements of proteins in membranes. Danielli and Davson model, Fluid Mosaic Model, permeability of cell membrane. Bio-Energetics: Thermodynamic Considerations: standard free energy change in bio-chemical reactions, exergonic, endergonic reactions, High energy molecules, hydrolysis of ATP and its synthesis from ADP.

**UNIT – II**

Statistical mechanics in biopolymers chain configuration of macromolecules, statistical distribution end – to - end dimensions, Polypeptide and protein structures and protein folding. calculation of average dimensions for various chain structures. Neurobiophysics: neurons, synapse, physics of membrane potential, neurotransmitters: Serotonin, GABA.

**UNIT – III**

Mechanism of Membrane Transport: Transport through cell membrane, active and passive transport (chemi-osmotic theory) systems, Irreversible thermodynamic treatment of membrane transport, Donnan effect in Osmosis, its dependence on pH difference across the membrane, Bio-mechanics: striated muscles, contractile proteins, mechanical properties of muscles and role of calcium.

**UNIT – IV**

Biomolecular Interactions: Interactions between biomolecules (proteins), Interaction of biomolecules with small ligands, independent ligand binding sites, the Scatchard plot, forces involved in the stability of proteins, hydrophobic interactions, hydrogen bonding, electrostatic interactions, electron delocalization, van der Waal's forces weak interactions crucial to macromolecular structure and function, blood –the buffering system

**UNIT – V**

Protein molecules: Protein sequence and structure (primary structure), secondary structure: Ramachandran plot, ( $\alpha$ -helix,  $\beta$ -strand,  $\beta$ -sheet, turns and loops), torsion angles, tertiary structure (ion-ion, ion-dipole and dipole-dipole interactions), quaternary structure, globular and fibrous proteins, structure of hemoglobin and myoglobin. Protein folding and refolding, Protein misfolding, Chaperones and chemical factors (Intra and intermolecular interactions) leading to folding/refolding/misfolding. Brain diseases associated with it, structure of virus.

**Books Recommended:**

1. Physical Chemistry of Macromolecules: S.F.Sun
2. The Enzyme Molecules: W. Ferdinand
3. Outlines of Biochemistry: E.E. Conn and P.K. Stumph
4. Biochemistry: Zubay
5. Principles of Biochemistry: A.I. Leninger
6. Physical Biochemistry: D. Friefelder
7. Biophysics: Volkenstein
8. Biophysical Chemistry (Vol. I-III): Schimell and Cantour
9. Biophysics : Vasantha Patabhi, N.Gautam
10. Biophysical Chemistry: Gurtu &Gurtu

**SEMESTER-IV**  
**(COURSE –XVIII C)**  
**(PHYSICAL CHEMISTRY SPECIAL THEORY - V)**  
**(CHEMISTRY OF MACROMOLECULES)**

**Lectures: 60**  
**Max. Marks: 80**

*Note: Ten questions will be set by the examiner selecting **TWO** from each unit. As far as possible, every question will be divided into **Two – Three Parts**. The students shall attempt **FIVE** questions selecting **ONE** from each unit.*

**UNIT – I**

Introduction to Macromolecules, (classification and importance). Synthetic and natural polymer. Polymerization (condensation and addition reactions). Molecular forces and chemical bonding in macromolecules and their effects on the physical properties. Polymer solutions, criteria for polymer solubility, conformations of dissolved polymer chains. The Amorphous, Semicrystalline and Crystalline States of Polymers.

**UNIT – II**

Thermodynamics of polymer solutions, ideal solutions, regular solutions, lattice model of solutions (Flory – Huggins Theory), Flory – Krigbaum theory for dilute polymer solutions. Fractionation of polymers by different techniques, theory of swelling of cross – linked / network polymers. Structure determination techniques: X-ray crystallography, NMR, Microscopy: TEM, SEM, STEM, AFM (qualitative treatment only)

**UNIT – III**

Chain conformation of macromolecules: statistical thermodynamics of interpenetrating random coiling polymers in solution with application to phase separations, swelling of networks, depression of melting point. The isolated chain molecule in dilute solutions analyzed for mass or size by static methods (osmometry, light scattering, neutron scattering) and by dynamic methods (intrinsic viscosity, size exclusion chromatography, sedimentation).

**UNIT – VI**

Rheology and Mechanical Properties of Polymers: Brief introduction to rheology and mechanical properties of polymers, phenomena of viscous flow, kinetic theory of rubber elasticity, amorphous polymers and practical importance of their aggregation states, viscoelasticity (experimental and dynamic method), The glassy state and glass transition temperature. Applications of polymers in Structural Polymers and Composites, Packaging Materials and Coatings, Transparent and Optical Materials, Biological and Medical Materials, Fluid Modifiers and Suspension Stabilizers

**UNIT – V**

- 1. Mechanical strength of polymers:** Mechanical strength and life time of polymer mechanism of polymer fracture, effect of various factors on the mechanical properties of polymers (effect of size and shape, effect of fillers, effect of cross – linked density).
- 2. Polyelectrolytes:** The water soluble charged polymers and their applications. Ionomers (ion containing polymers) conducting polymers solid polymer electrolytes, mechanism of conductivity. Polymers in combating environmental pollution and as chemical reagents.

**Books Recommended:**

1. Text Book of Physical Chemistry: G.M. Barrow
2. Text Book of Polymer Chemistry: Billmeyer
3. Polymer Chemistry: P.J. Flory
4. Physical Chemistry of Polymers: A Tagger
5. Physical Chemistry of Macromolecules: C. Tanford
6. Introduction to Polymer Science: V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar
7. Principles of Polymer Science: P. Bhadur and N.V. Sastry

**SEMESTER - IV**  
**COURSE – XIX (A)**  
**(INORGANIC CHEMISTRY PRACTICAL - SPECIAL)**

**Time: 12 hrs/week**

**Max. Marks: 75**

Preparation of the following compounds and a study of the important properties viz. Molar conductance, magnetic susceptibility, electronic and infrared spectra.

1. Stannic iodide
2. Bis(acetylacetonato) oxovanadium (IV)
3. Mercuration of phenol.
4. Hexa ammine nickel (II) chloride.
5. Lead tetraacetate
6. Cis- and trans-  $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$

**INSTRUMENTAL ANALYSIS:**

**A) Conductometric Titrations:**

- i) Differential behaviour of acetic acid to determine the relative acid strength of various acids.
- ii) Strong acid-strong base titration in acetic acid.
- iii) Potassium acetate- pyridine titration in acetic acid.

**B) Potentiometric Titrations.**

1. *Neutralisation reactions:*

- i) Sodium hydroxide-hydrochloric acid.
- ii) Sodium hydroxide-Boric acid
- iii) Acetic acid and hydrochloric acid-sodium hydroxide.

2. *Oxidation-Reduction Reactions.*

- i) Ferrous-dichromate
- ii) Ferrous-Ceric
- iii) Iodine-Thiosulphate

3. *Precipitation Reactions:*

- i) Silver nitrate-sodium halides.
- ii) Chloride-Iodide mixture.

**C) Colorimetric Analysis:**

- 1) Verification of Beer's law for  $\text{KMnO}_4$ ,  $\text{K}_2\text{Cr}_2\text{O}_7$  solutions and determination of the conc. of  $\text{KMnO}_4$ ,  $\text{K}_2\text{Cr}_2\text{O}_7$ .
- 2) Colorimetric determination of Iron (II) with o-Phenanthroline method.
- 3) Determination of traces of manganese (in steel samples) colorimetrically by oxidation to permanganic acid with potassium periodate.
- 4) Spectrophotometric determination of pK value of an indicator (acid dissociation constt. of methyl red)
- 5) Simultaneous determination of chromium (as  $\text{Cr}_2\text{O}_7^{2-}$ ) and manganese (as  $\text{MnO}_4^-$ ) in mixture.
- 6) Simultaneous determination of Fe(II) and Fe(III).
- 7) Photometric titration (simple illustrations)
- 8) Determination of stability constant of a complex by spectrophotometric method.

**(D) pH metric –titrations**

- 1) Acid base titrations.
- 2) Mixtures of acids with a base.

**E) Polarography/Pulse polarography:**

- 1) Determination of half wave potentials of cadmium, zinc and manganous ions in potassium chloride solution.
- 2) Investigation of the influence of dissolved oxygen.
- 3) Differential pulse polarographic determination of copper and zinc.
- 4) Determination of formation constant of a complex metal ion by polarography/pulse polarography.

**(F) Cyclic voltammetry:**

1. Determination of  $E^{\circ}$  and  $n$  values of  $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$  couple.
2. Study of electrode mechanism of cyclic voltammetry.

**(G) Flame Photometry:** Determination of sodium, potassium and calcium

**Books Recommended:**

1. A Text Book of Quantitative Inorganic Analysis- A.I. Vogel
2. Chemistry Experiments for Instrumental Methods: D.T. Sawyer, W.R. Heineman and J.M. Beebe.
3. Inorganic Synthesis- R.A. Rowe and M.M. Jones (1957)5, 113 – 116.

**SEMESTER - IV**

**COURSE – XIX (B)**

**(ORGANIC CHEMISTRY PRACTICAL - SPECIAL)**

**Time: 12 hrs/week**

**Max. Marks: 75**

**(A) Extraction of Organic Compounds from Natural Sources:** Isolation of Caffeine from tea leaves, casein from milk (the students are required to try some typical color reactions of proteins), lactose from milk (purity of sugar should be checked by TLC and PC and  $R_f$  value reported). lycopene from tomatoes and  $\beta$ - carotene from carrots.

**(B) Paper Chromatography:** Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of  $R_f$  values.

**(C) Spectroscopy:**

Identification of some organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR and MS)

Multistep Synthesis

Synthesis of Vacor

Synthesis of Indigo

Synthesis of p- nitro aniline

**Books Recommended:**

1. Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.
2. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.
3. Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.
4. Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark, Adward Arnold.
5. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.



**SEMESTER - IV**  
**COURSE – XIX (C)**  
**(Physical Chemistry Practical - SPECIAL)**

**Time: 12 hrs/week**  
**Max. Marks: 75**

1. **Viscosity Measurements:** Verification of the Jones – Dole equation for simple electrolytes in water and in aqueous mixtures of organic solvents.
2. **Conductometric Measurements:** Determination of Walden's product in case of simple electrolytes.
3. **Potentiometric Titration:** Titration of HCl with NaOH, determination of dissociation constant of acetic acid and phosphoric acid. Oxidation – reduction titration.
4. **Flamephotometric Measurements:** Estimation of concentration of  $\text{Ca}^{+2}$ ,  $\text{Na}^+$  and  $\text{K}^+$  ions and in the given aqueous solution at ppm level.
5. **Determination of Molar Mass:** (i) Cryoscopic and Rast's methods.
6. Determination of molar mass of polymer by viscosity measurement.
7. **Colometry Measurements:** Determination of composition and free energy of formation of ferric ions – salicylic acid complex using Job's continuous method.
8. **Polarimetry Measurements:** Determination of specific and molecular rotation, percentage of two optically active substances, kinetics of acid catalysed inversion of cane sugar and comparison of strengths of two acids.

**Books Recommended:**

1. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla
2. Experimental Physical Chemistry: V. Athawale and P. Mathur.
3. Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.
4. Practical in Physical Chemistry: P.S. Sindhu
5. Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla

**SEMESTER - IV**

**(COURSE – XX)**

**(SEMINARS FOR ALL THREE SPECIALIZATIONS)**

**Time: ½ hr**  
**Max. Marks: 25**

Every candidate will have to deliver a seminar of 30 minutes duration on a topic (not from the syllabus) which will be chosen by him / her in consultation with the teacher of the department. The seminar will be delivered before the students and teachers of the department. A three member committee (one coordinator and two teachers of the department of different branches) duly approved by the departmental council will be constituted to evaluate the seminar. The following factors will be taken into consideration while evaluating the candidate.

- (i) Expression
- (ii) Presentation
- (iii) Depth of the subject matter and answers to the questions.