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M.Sc (Chemistry)

# **SEMESTER-I**

#### (COURSE – I) (INORGANIC CHEMISTRY)

Lectures-60 Max. Marks-80

Note: i. Ten questions will be set by the examiner selecting <u>TWO</u> from each unit. As far as possible every question will be divided into <u>Two – Three Parts</u>. The students shall attempt <u>FIVE</u> questions selecting <u>ONE</u> from each unit.
ii. Students can ask for Character Tables (except for C<sub>2V</sub> and C<sub>3V</sub> 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 -bonding in different geometries and hybrid orbitals for -bonding. Symmetries of molecular orbitals in BF<sub>3</sub>,  $C_2H_4$  and  $B_2H_6$ .

#### UNIT-II

**Application of Group Theory in Vibrational Spectroscopy:** A brief idea about Infrared and Raman scattering spectroscopy. Vibrational modes as basis of group representations w.r.t.  $SO_2$ ,  $POCl_3$ ,  $PtCl_4^{2^2}$  and  $RuO_4$ . Mutual exclusion principle, Classification of vibrational modes (i.e. stretching and angle deformation vibrations w.r.t.  $SO_2$ ,  $POCl_3$  and  $PtCl_4^{2^2}$ .

#### UNIT-III

**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. Chemistry of Molten salts as Non-Aqueous Solvents: Solvent properties, solution of metals, complex formation, Unreactivity of molten salts, Low temperature molten salts.

#### <u>UNIT-IV</u>

**Inorganic Hydrides:** Classification, preparation, bonding and their applications. Transition metal compounds with bonds to hydrogen, carbonyl hydrides and hydride anions. Classification, nomenclature, Wadeøs Rules, preparation, structure and bonding in boron hydrides (boranes), carboranes, metalloboranes and metallocarboranes.

#### UNIT-V

**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)



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- 1. Chemical applications of Group Theory ó F.A.Cotton
- 2. Inorganic Chemistry ó Durrant and Durrant
- 3. Symmetry in Chemistry- Jaffe and Orchin
- 4. Non-aqueous solvents ó H.Sisler
- 5. Non-aqueous solvents ó T.C.Waddington
- 6. Non-aqueous solvents ó Logowsky
- 7. Advanced Inorganic Chemistry: Cotton & Wilkinson, Vth Edn.
- 8. Concise course in Inorganic Chemistry- J.D.Lee
- 9. Nature of Chemical Bond ó L. Pauling
- 10. Chemistry of Elements ó Greenwood and Earnshaw
- **11.** Inorganic Chemistry ó T. Moeller
- **12.** Inorganic Chemistry ó J.E.Huheey 3<sup>rd</sup> Edn.
- 13. Topics in Current Chemistry (Inorganic/Bio-Chemistry)óVol. 64
- 14. A Text Book of Quantitative Inorganic Analysis- A.I. Vogel



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# SEMESTER-I

#### (COURSE – II) RGANIC CHEMISTRY)

Lectures-60 Max. Marks-80

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

#### UNIT-I

**Nature of Bonding in Organic Molecules:** Delocalized Chemical Bonding: Kinds of molecules with delocalized bond, cross- conjugation, resonance, p -d bonding (ylides). aromaticity: other systems containing aromatic sextet, Aromatic systems with electron number other than six. Huckel rule, other aromatic compounds, hyperconjugation. **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:** Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity in acylic and cyclohexane systems. Steric strain due to unavoidable crowding. Elements of symmetry: chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, Optical activity due to chiral planes, Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Asymmetric Synthesis: Principle and categories with specific examples of asymmetric synthesis including newer methods involving enzymatic and catalytic reactions, enantio and diastereoselective synthesis. Stereoselective Reactions: Cyclopropanation, hydroboration, catalytic hydrogenation, and metal ammoni reduction, stereoselective synthesis of (-) ephedrine and (+) - ephedrine. Stereospecific Reactions at chiral carbon.

#### 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 mechanism.

#### UNIT-IV

Aliphatic Nucleophilic Substitution: The  $SN_2$ ,  $SN_1$ , mixed  $SN_1$  and  $SN_2$ , SET mechanisms & SNi mechanism. The neighboring group mechanism, neighboring group participation by and 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, transetherification and preparation of inorganic esters. Phase-transfer catalysis, and ultrasound, ambident nucleophile, regioselectivity.



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**bstitution:** Bimolecular mechanisms- SE2 and SEi. The SE1 ubstitution accompanied by double bond shifts, halogenation s and acyl halides. Effect of substrates, leaving group and the */*. Aliphatic diazonium coupling, Acylation at aliphatic carbon,

alkylation of alkene, Stork-enamine reactions

(B) Free radical reactions: 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, Sandmeyer reaction, Hoffmann -Loffler- Freytag reaction, Hunsdiecker reaction.

- 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.



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# <u>SEMESTER-I</u> (COURSE – III) HYSICAL CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT – I</u>

**Spectroscopy** – **I**: Theory of nuclear magnetic resonance NMR phenomenon, the chemical shift and its measurement. The fine structure (spin ó spin coupling). Factors influencing chemical ó shift and spin ó spin coupling. Non - first ó order spectra. Relaxation phenomena in NMR: spin ó spin and spin ó lattice relaxation processes. Line ówidth and rate processes. The nuclear Overhauser effect. An introduction to Fourier Transform NMR (FTNMR). Theory of Electron Spin Resonance (ESR) phenomenon. Fine and hyperfine structure of ESR. Zero ó field splitting of ESR signal. Mapping of charge density on molecule (McConnell relation). Mossbaur spectroscopy: a brief introduction ( isomer ó shift, quadrupole interaction and magnetic hyperfine interaction).

#### <u>UNIT - II</u>

**Spectroscopy** – **II**: Rotational and vibrational spectra. Moment of inertia and rotational spectra of rigid and non ó rigid diatomic molecules. Vibrational excitation effect.. Rotational spectra of symmetric - top molecules. Strak effect. Vibrational energy of diatomic molecules. Anharmonic oscillator, overtones and hot bands. Diatomic vibrator ó rotator (P, Q and R ó branches of diatomic vibrator ó rotator). Rotational ó vibrational spectra of symmetric ó top molecules. Raman Spectroscopy: qualitative quantum theory of Raman scattering. Rotational Raman spectra of linear and symmetric ó top molecules. Vibrational Raman spectra and mutual exclusion principle.

#### <u>UNIT - III</u>

**Kinetics of complex reactions:** Reversible / opposing reactions, consecutive / successive reactions, simultaneous side / parallel reactions, chain / free radical reactions viz. thermal ( $H_2$  ó  $Br_2$ ) and photochemical  $H_2$  ó  $Cl_2$ ) reactions. Rice ó Herzfeld mechanism of dissociation of organic molecules viz. dissociation of ethane, decomposition of acetaldehyde as 3/2 or ½ order reactions. Kinetics of polymerization (molecular and free radical mechanisms). Reaction rates and chemical equilibrium, principle of microscopic reversibility, activation energy and activated complex.

#### UNIT - IV

**Theories of reaction rates:** The kinetic theory of collisions, transition state theory, comparison of collisions and transition state theories in simple gas reactions, steric factor, transmission ó coefficient, steady ó state hypothesis / transient phase theory, Lindmans theory of unimolecular reaction, the thermodynamic formulation of reaction rates.

#### UNIT - V

- 1. Surface Reactions: Mechanism of surface reactions, unimolecular and bimolecular surface reactions, Langmuir ó Hinshelwood mechanism for gases only.
- **2. Fast Reaction in aqueous solutions:** Study of fast reactions by Stopped flow method (Principle and Theory). Absolute rate theory applied to fast reactions.

- 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 Reactions in Solutions: Caldin
- 7. Basic Principles of Spectroscopy: R. Chang
- 8. NMR and Chemistry: J.W. Akit
- 9. Introduction to Molecular Spectroscopy: G.M. Barrow
- **10.** Physical Chemistry: P.W. Atkins
- 11. Fundamentals of Molecular Spectroscopy: C.N. Banwell



#### <u>SEMESTER-I</u> (COURSE – IV) STS & APPLICATION OF COMPUTER IN CHEMISTRY)

Lectures: 60

Max. Marks: 80

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

# Mathematics for Chemists

# <u>UNIT - I</u>

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.

### <u>UNIT – II</u>

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 exponentialø 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.

### <u>UNIT – III</u>

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 propertie, evaluation of determinants. Application to simple chemistry problems.

# Application of Computer in Chemistry

#### <u>UNIT – IV</u>

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.

#### <u>UNIT – V</u>

Arrays and replitive computation; Introduction, arrays arrange storage, dimension statement, do comtruel, Nested do ó loop continue statement, implied do. Sub ó programme (functions and sub ó 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 -inputø and -outputø Developing Linear Least ó Squares fit programs in FORTRAN, as well as for involving simple formulae in organic, inorganic and physical chemistry.

- 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



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# **SEMESTER-II**

#### (COURSE –V) ORGANIC CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

# <u>UNIT-I</u>

**Metal-Ligand Bonding-I:** 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 momenta, coupling of spin angular momenta, spin orbit coupling, spin orbit coupling  $p^2$  case, Determining the Ground State Terms-Hundøs Rule, Hole formulation (derivation of the Term Symbol for a closed sub-shell, derivation of the terms for a  $d^2$  configuration), Calculation of the number of the microstates.

### <u>UNIT-III</u>

**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  $(d^1-d^9)$  in  $O_h$  and  $T_d$  environments, spin-cross over in coordination compounds. Tanabe Sugano diagrams, Orgel diagrams, evaluation of B,C and parameters.

# UNIT-V

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

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



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#### <u>SEMESTER-II</u> (COURSE –VI) )RGANIC CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT – I</u>

(A) Aromatic Electrophilic Substitution: Arenium ion mechanism, orientation and reactivity, energy profile diagrams, The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeir reaction, Scholl reaction, Amination reaction, Fries rearrangement, Reversal of Friedel Craft alkylation, Decarboxylation of aromatic acids.

**(B)** Aromatic Nucleophilic Substitution: SNAr, SN<sup>1</sup>, benzyne and SRN<sup>1</sup> 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, Diekmann reaction, Stobbe condensation, Mannich reaction, Knoevenagel condensation, Benzoin condensation, Witting reaction, Hydroboration, Hydrocarboxylation, Ester hydrolysis, Epoxidation.

#### <u>UNIT-III</u>

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

#### UNIT-IV

**Elimination Reactions:** Discussion of  $E_1$ ,  $E_2$ ,  $E_1cB$  and  $E_2C$  Mechanisms and orientation, Reactivity: Effects of substrate structures, attacking base, leaving group and medium. Cis elimination, elimination in cyclic systems, eclipsing effects, Pyrolytic eliminations, cleavage of quaternary ammonium hydroxides, Fragmentations: -Amino and -hydroxy halides, decarboxylation of -hydroxy carboxlic acid and -lactones.

#### 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.

- 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.



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# **SEMESTER-II**

#### (COURSE –VII) HYSICAL CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT – I</u>

Brief resume of law of thermodynamics. Gibbøs 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 (Gibbøs and Helmholtz ) change. Gibbøs 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.

#### <u>UNIT – II</u>

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 ó volatile solutes from colligative properties. Relationship between relative lowering of vapour pressure and osmotic pressure. Vanøt Hoff equation for dilute solutions and its application.

#### <u>UNIT – III</u>

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.

#### <u>UNIT – IV</u>

**Non–Equilibrium Thermodynamics:** Basic principles of non ó equilibrium thermodynamics: rate laws, second law of thermodynamics for open system, law of conservation of mass, charge and energy. Phenomenological equations for single and coupled flows. Onsager reciprocity relation. Theorm of minimum entropy production. Curie ó Prigogine principle. Applications of non ó equilibrium thermodynamic: thermoelectricity, electrokinetic phenomena and expressions for streaming potential, electro- osmotic pressure difference, streaming potential using the linear phenomenological equations, and to biological membrane system, a qualitative insight.

#### UNIT –V

**Electrochemistry:** Ionic conduction: non ó ideal behaviour of electrolytic solutions. Electrolytical potential. Derivation of Debye ó Huckel Limiting Law. Extended Debye ó Huckel Law. Structure of solutions. Detailed treatment of ion ó solvent interactions (ion solvation), solvation number. Energy conduction. Ion ó ion interactions (ion ó association). Bjerrumøs theory of ion ó association.

- 1. Thermodynamics for Chemists: S. Glasstone
- 2. Physical Chemistry: G.M. Barrow
- 3. Non ó equilibrium Thermodynamics: C. Kalidas
- 4. Non ó 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.OoM Bockris and A.K.N. Reddy



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# SEMESTER-II

# (COURSE –VIII) LIFE & ENVIROMENTAL CHEMISTRY

Lectures: 60 Max. Marks: 80

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

# <u>UNIT-I</u>

**Cell structure and function:** 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.

- 1. Principles of Biochemistry óA.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



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# SEMESTER I AND II

(COURSE – IX A) NIC CHEMISTRY PRACTICAL)

Time - 6 hr 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.

v) Determination of metals: copper in copper oxychloride and zinc in zineb fungicides.

# 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)

- 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) IC CHEMISTRY PRACTICAL)

Time - 6 hr Max. Marks - 50

**<u>Qualitative Analysis:</u>** 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, fluorosceine-eosin, and methyl orange

- 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. Vogeløs Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.



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# SEMESTER I AND II

(COURSE – IXC) AL CHEMISTRY PRACTICAL)

Time - 6 hr Max. Marks - 50

- 1. <u>Refractive Index (RI) Measurements:</u> Refractive index (RI) measurements of pure solvents, analysis of mixtures of two miscible solvents, molar and atomic refraction determination, polarizability of liquids.
- 2. <u>Conductometric Measurements:</u> Determination of cell constant, limiting molar conductance of simple electrolytes in water, verification of Ostwald, dilution law for week acetic acid.
- **3.** <u>Surface Tension Measurements:</u> Surface tension of pure solvents, analysis of mixtures of two miscible solvents, verification of Gibbøs Thomson Rule of surface tension.
- **4.** <u>**Partition** Coefficient</u>: Determination of partition ó coefficient for I<sub>2</sub> between water and CCl<sub>4</sub> and for benzoic acid between water and benzene.
- 5. <u>Adsorption Measurements</u>: Verification of Freundlich adsorption isotherm for I<sub>2</sub>, acetic acid and oxalic acid on charcoal.
- 6. <u>Colloidal Solution</u>: Preparation of sol solution of arsenic sulphide and estimation of flocculation value for NaCl, KCl, BaCl<sub>2</sub>, AlCl<sub>3</sub>.
- 7. <u>Thermochemistry:</u> Determination of water equivalent of thermos flask, and estimation of heat of neutralization for strong acid strong base, weak acid strong base or vice ó versa, heat of hydration and solution of salts.
- 8. <u>Kinetic Measurement:</u> Kinetics of Hydrolysis of methylacetate and ethylacetate in the presence of HCl.

- 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



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# <u>SEMESTER-III</u> (COURSE –X) ORGANIC CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT-I</u>

Metal  $\pi$  Complexes: Preparation, reactions, structures and bonding in carbonyl, nitrosyl, phosphine and related complexes, structural evidences from vibrational spectra, bonding and important reactions of metal carbonyls. 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 proximate and mineral analysis in food (moisture, ash, crude fiber, nitrogen (proteins) and minerals (iron, calcium, potassium, sodium and phosphorus). Discussion of official (pharmacopea) methods for the determination of following drugs as such: (i) Analgin/oxyphenbutazone, (ii) chloramphenicol and related nitro compounds, (iii) chloroquinine, (iv) phenyl butazone, (v) salicylic acid and (vi) sulphonamides.

#### <u>UNIT-III</u>

**Photoelectron Spectroscopy:** Basic principle, photoionization process, ionization energies, Koopmanøs theorem, ESCA, photoelectron spectra of simple molecules,  $(N_2, O_2 \text{ and } F_2)$  Photoelectron spectra for the isoelectronic sequence Ne, HF, H<sub>2</sub>O, NH<sub>3</sub> and CH<sub>4</sub>, chemical information from ESCA, Auger electron spectroscopy ó 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 translawrencium 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-fission product and fission yields, Nuclear fusion.

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

- 1. Advanced Inorganic Chemistry ó Cotton and Wilkinson
- 2. Fundamentals of Analytical Chemistry ó Skoog and West
- 3. Quantitative Inorganic Analysis ó Vogel
- 4. Chemistry of the Elements ó Greenwood and Earnshaw
- 5. Nuclear Chemistry-U.C.Dash
- 6. Nuclear Chemistry ó B.G.Harvey
- 7. Nuclear Chemistry ó Arnikar
- 8. Techniques in Inorganic Chemistry Vol. II (Nuclear Chemistry-Johnson and Others).
- 9. Modern Aspects of Inorganic Chemistry-H.J.Emeleus and A.G.Sharpe
- 10. Inorganic Chemistry, 4<sup>th</sup> Edition, J.E.Huheey, E.A.Keiter and R.L.Keiter.
- 11. Analytical Chemistry-G.D.Christian
- 12. Chemical Structure and Bonding- Dekock and Gray
- 13. The Organometallic Chemistry of Transition metals: R.H. Crabtree.
- 14. Electronic absorption spectroscopy and related techniques: D.N. Sathyanarayan



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# SEMESTER-III

#### (COURSE –XI) )RGANIC CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT-1</u>

#### Spectroscopy:

(A) 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. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Ultra- Violet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls. Applications of UV- visible spectroscopy in organic chemistry.

**(B) Infrared Spectroscopy:** 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-II

**Nuclear Magnetic Resonance (NMR) Spectroscopy:** General introduction, chemical shift, spinspin interaction, shielding mechanism, chemical shift values and correlation of protons present in different groups in organic compounds. chemical exchange, effect of deuteration, complex spinspin interaction between two, three, four and five nuclei, virtual coupling. Stereochemistry, hindered rotation, Karplus- relationship of coupling constant with dihedral angle. 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 óF, P, Principle and introduction to C<sup>13</sup> NMR, 2-D and 3-D NMR, Applications of NMR in organic chemistry.

#### UNIT-III

**Mass Spectrometry:** Introduction, ion productionô 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. High-resolution mass spectrometry. 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 spectroscopy.

#### UNIT-IV

**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

#### <u>UNIT-V</u>

**Photochemistry** – **II:** Photochemistry of Carbonyl compounds: Norrish Type I and II, Intermolecular and Intramolecular hydrogen abstraction, Paterno-Buchi reaction, and - cleavage reactions of cyclic and acyclic carbonyl compounds, Formation of oxetane and cyclobutane from



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ction of carbonyl compounds, Photo-rearrangement of enones, rearrangement.

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*I.L.* Martin, J.J. Delpeuch 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.



# SEMESTER-III

#### (COURSE –XII) HYSICAL CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

#### **Statistical Thermodynamics**

#### <u>UNIT – I</u>

Basic Terminology: probability, phase space, micro and macro states, thermodynamic probability, statistical weight, assembly, ensemble, probability considerations and chemistry. The most probable distribution: Maxwell-Boltzmann distribution, Thermodynamic properties from statistical Thermodynamics, The Partition Function for monoatomic gas, State functions in terms of partition function, separating partition function: the nuclear and electronic partition function, for molecules, electronic and vibrational partition function,

#### <u>UNIT – II</u>

Diatomic molecules: Rotations, Polyatomic molecules: Rotations, The partition function of a system, Thermodynamic properties of molecules from partition function: Total energy, entropy, Helmholtz free energy, pressure, heat content, heat capacity and Gibbøs free energy, equilibrium constant and partition function, Heat capacity of crystals and statistical thermodynamics, quantum statistics: The Bose- Einstein statistics and Fermi- Dirac Statistics.

#### **Basic Quantum Chemistry**

#### UNIT – III

Operators in quantum mechanics. Eignvalues and eignfunctions. Hermitian operator and its application. Postulates of quantum mechanics. Angularmomentum of a one ó particle system, and its commutative relations. Schreodinger wave equatuion and its formulation as an eignvalue problem. The uncertainty principle.

#### <u>UNIT – IV</u>

Quantum mechanical treatment of translational motion of a particle, particle in one and three dimensional boxes, harmonic ó oscillator, rotational motion of a particle: particle on a ring, particle on a sphere, rigid rotator and hydrogen atom. Graphical presentation of orbitals (s, p and d), radial and angular probability distribution plots.

#### UNIT – V

**Photochemistry:** Photophysical processes of electronically excited molecules. Intensity distribution in the electronic vibrational species. Franck ó Condon principle a quantum ó mechanical treatment. Excited state dipole moment and acidity constant. Dissociation and pre ó dissociation of diatomic molecules. Energy transfer from electronically excited molecules: Stern ó Volmer mechanism only. Photophysical pathways: fluorescence, phosphorescence, E-type and P- type delayed fluorescence. Kinetic treatment of excimer and exciplex formation.

- 1. Physical Chemistry: D.W. Ball
- 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



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#### <u>SEMESTER-III</u> (COURSE –XIII (A)) CHEMISTRY SPECIAL THEORY - I)

Lectures: 60 Max. Marks: 80

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

# <u>UNIT-I</u>

**Inorganic Photochemistry :** Basic principles, Basic photochemical processes, Kashia¢s rule, Thexi state, Photochemical behaviour of transition metal complexes, charge transfer spectra of crystalline and gaseous alkali halides, photochemical reactions of coordination compounds, oxidation-reduction reactions, Photo substitution reactions, Adamson¢s rules and photo-substitution reactions of cobalt(III) complexes i.e.  $[Co(NH_3)_5X]^{2+}$ ,  $[Co(en)_3]^{3+}$ , and chromium(III) complexes i.e.  $[Cr(H_2O)_6]^{3+}$  and  $[Cr(NH_3)_6]^{3+}$  and ruthenium (II) polypyridyl complexes.

# <u>UNIT-II</u>

**Inorganic Reactions and Mechanism:** Substitution reactions in octahedral complexes, acid hydrolysis reactions, base hydrolysis and anation reactions, substitution reaction, 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.

### <u>UNIT-III</u>

**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, difference between thermodynamic and kinetic stability.

Determination of stability constants by:

- (i) Spectrophotometric methods (Jobøs method, Mole ratio and slope ratio method).
- (ii) Bjerrumøs method
- (iii) Ledenøs method
- (iv) Polarographic method

Factors affecting the stability constants (with special reference to metal and ligand ions).

#### 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  $d^1$ - $d^9$  ions in O<sub>h</sub> and T<sub>d</sub> environments, Evaluation of 10 D<sub>q</sub>, Spectrochemical and Nephelauxetic series, charge- transfer spectra.

- 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 ó Edberg
- 9. Inorganic Reaction Mechanism ó Basoloavd Pearsor



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# SEMESTER-III

#### (COURSE –XIII (B)) C CHEMISTRY SPECIAL THEORY - I)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT-I</u>

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 B<sub>1</sub>), Ascorbic acid (Vitamin C), Pantothenic acid, biotin (Vitamin H), -tocopherol (Vitamin E), Biological importance of vitamins.

#### UNIT-IV

Enzymes: Nomenclature and classification, extraction and purification, Remarkable properties of enzymes like catalytic power, specificity and regulation, Proximity effects and molecular adaptation, Chemical and biological catalysis. Mechanism of enzyme action: Transition state theory, orientation and steric effect, acid base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms (chymotrypsin, ribo nuclease, lysozyme and carboxypetidase A). Fischerøs lock and key and Koshlandøs induced fit hypothesis, concept and identification of active site by the use of inhibitors affinity labeling and enzyme modification by site directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

#### UNIT-V

(A) Kinds of reactions catalyzed by Enzymes: Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate addition and elimination reactions, enolic intermediates in isomerization reactions, - cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation reactions.

(B) Coenzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate pyridoxal phosphate,  $NAD^+$ ,  $NADP^+$ , FMN, FAD, Lipoic acid, vitamin B<sub>12</sub>. Mechanisms of reactions catalyzed by the above cofactors.

- 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.



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roduction and Applications In Biotechnology, Michael D. Trevan,

ctions of Living Cells, D.E. Metzler, Academic Press.

ns. C. Walsh, W. H, Freeman. sm, A. Fersht, W.H. Freeman.

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10. Carbonydrates by N. Snaron.

- 11. Carbohydrates by Gutherie.
- 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.

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- 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.



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#### <u>SEMESTER-III</u> (COURSE –XIII (C)) CHEMISTRY SPECIAL THEORY - I)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT –I</u>

Adsorption at solid ó gas interface: Concept of ideal and non ó ideal adsorption. Heat of adsorption. Types of adsorption isotherms. Single ó layer adsorption ó Langmuir adsorption isotherm and its derivation. Multilayer adsorption ó 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.

#### <u>UNIT –II</u>

Adsorption at solid ó 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.

#### <u>UNIT –III</u>

Solution and Interfacial Behaviour of Surfactants: Definition and classification of surfactants. Solution properties of surfactants: micelle and reverse 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: Mechanism of electrolytic conductance, relaxation and electrophoretic effects, Debye ó Huckel ó Onsager (DHO) equation and its validity in aqueous and non aqueous solutions. Deviations from the Onsager equation, conductance ratio and Onsager equation. Dispersion of conductance at high frequencies (Debye ó Falkenhagen effect). Conductance with high potential gradients (Wien effect). Activity and activity coefficient, forms of activity coefficients, activities of electrolytes and mean ion activity coefficient. The Debye ó Huckel Limiting law. Electrokinetic phenomena: Electrical double layer and its structure (Sternøs theory), Electroosmosis, Streaming potential, Electrophoresis, Influence of ions on electrokinetic phenomena (Qualitative insight).

#### UNIT –V

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

- 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
- 7. Introduction to nanotechnology: Charles P.Poole, Jr. Frank, J. Owens: Wiley India



# SEMESTER III

# es (COURSE – XIV A) (inokgaNIC CHEMISTRY PRACTICAL)

Time - 6 hr Max. Marks - 50

- 1. Analysis of the given sample (Ores)/Both Qualitative and Quantitative Dolomite, Pyrolusite, Galena.
- 2. Analysis of the given alloys: Coin, Gunmetal, Brass and Bronze.
- 3. To prepare a pure and dry sample of the following compounds:
  - 1. Potassium tris(oxalato)aluminate(III)
  - 2. Sodium hexa(nitro)cobaltate(III)
  - 3. Potassium tris(oxalato)cobaltate(III)
  - 4. Hexa(ammine)cobalt (III)chloride
  - 5. Tetrapyridine copper(II)persulphate
  - 6. Dinitrotetrapyridine nickel(II)
  - 7. Lead tetraacetate
  - 8. Mercury (tetraisothiocyanato)cobaltate(II).

and characterize them 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 ó A.I. Vogel



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# SEMESTER III

# (COURSE – XIV B) IC CHEMISTRY PRACTICAL)

Time - 6 hr Max. Marks - 50

- A. <u>Quantitative Analysis:</u> Determination of the percentage/ number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/ phenols using bromate ó bromide solution/ acetylation method. Determination of iodine and sponification values of an oil sample. Determination of DO, COD and BOD of water sample.
- B. <u>Multistep Synthesis:</u> 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.

- 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. Vogeløs Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.



# <u>SEMESTER III</u>

# (COURSE – XIV C) AL CHEMISTRY PRACTICAL)

Time - 6 hr Max. Marks - 50

- 1. Solubility Measurements: Heat of solution of electrolytes by solubility measurements.
- 2. <u>Heat of transfer Measurements:</u> Heat of transfer for benzoic acid between benzene and water and  $I_2$  between CCl<sub>4</sub> and water.
- 3. <u>Conductometric Measurements:</u> Precipitation titration (AgNO<sub>3</sub> ó KCl), acid ó base neutralization titration, determination of relative strength of acids in the given mixtures, solubility of sparingly soluble salt.
- 4. <u>Construction of Phase Diagram:</u> 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. <u>Colorimetric Measurements</u>: Verification of Beer ó Lambertøs 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. <u>Kinetic Measurement:</u> Saponification of ethylacetate by NaOH solution.

- 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



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#### **SEMESTER-IV**

#### eatures (COURSE –XV A) (INORGAINC CHEMISTRY SPECIAL THEORY - II) (ADVANCED ORGANOMETALLICS)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT-I</u>

**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-donor ligands

- a) Two electron donor (olefin and acetylenic complexes of transition metals)
- b) Three electron donor ( -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 ó metallocenes with special emphasis to ferrocenes)
- e) Six electron donor [Benzene (arene) complex]

Fluxional and dynamic equillibria in compounds such as  $^2$ -olefin,  $^3$ - allyl and dienyl complexes.

### 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.

#### <u>UNIT-III</u>

**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, carboxylation reactions of alkenes and alkynes using nickel carbonyl and palladium complexes. Carbonylation of alkynes (acetylene) using nickel carbonyls or 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  $M_3(CO)_{12}$  (M=Fe, Ru & Os), Four metal atoms (tetrahedra) [ $M_4(CO)_{12}$  {M= Co, Rh &Ir}] and octahedron of type  $M_6(CO)_{16}$  [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 carbynes (preparation, reactions, structure and bonding considerations). Biological applications and environmental aspects of organometallic compounds, Organometallic compounds in medicine, agriculture and industry.



mpounds ó Powell ntroduction) ó Perkin and Pollar

- rison 4. Advanced Inorganic Chemistry ó Cotton and Wilkinson
- 5. Organometallic Chemistry-R.C.Mehrotra
- Organometallic compounds of Transition Metal-Crabtree 6.
- 7. Chemistry of the Elements ó Greenwood and Earnshaw
- 8. Inorganic Chemistry ó J.E.Huheey
- 9. Homogeneous transition metal catalysis ó Christopher Masters
- 10. Homogeneous Catalysis ó Parshall
- 11. Principles and Application of HomogeneousCatalysis ó Nakamura and Tsutsui
- 12. Progress in Inorganic Chemistry Vol. 15 ó Lipard. (Transition metal clusters ó R.B.King)
- 13. Organotransition metal chemistry by S.G.Davis, Pergamon press 1982.
- 14. Principles and applications of organotransition metal chemistry by Ccollmen and Hegden



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# SEMESTER-IV

#### ded Features (COURSE –XVI A) CHEMISTRY SPECIAL THEORY - III) (MODERN FECHNIQUES OF CHEMICAL ANALYSIS)

Lectures: 60 Max. Marks: 80

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

# UNIT-I

**Spectrophotometry: i)** Introduction, fundamental laws of photometry, the electromagnetic spectrum and spectrochemical methods, UV/Visible instrumentation, absorption spectra, Beer-Lambertøs Law, deviation from Beer-Lambertøs Beerøs 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 florescence spectra, florescence species, effect of concentration on florescence intensity, instrumentation and application of florescence 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, costant 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 analysis.



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- and provide analysis: Introduction, Factors affecting thermogravimetric curves, instrumentation, applications to inorganic compounds (analysis of binary mixtures i.e. Ca and Mg, TG curves of calcium oxalate, determination of Ca, Sr & Ba ions in the mixture, drying of sodium carbonate, analysis of clays and soils, decomposition of potassium hydrogen phthalate, oxidation of nickel sulphide, determination of titanium content of non-stoichiometric sample of titanium carbide).
- (b) Differential thermal analysis: Introduction, Factors effecting DTA curves, instrumentation, applications, to inorganic compounds (thermal decomposition of mixtures of lanthanum-cerium and praseodymium oxalate, DTA curves for CuSO<sub>4</sub>.5H<sub>2</sub>O, sulphur, detection of organic contamination in ammonium nitrate, thermal decomposition for different magnesium carbonate samples, determination of uncalcined gypsum in plaster of paris.

- 1. Instrumental methods of analysis.-H.H.Willard, LL.Marritt and J.A.Dean
- 2. Fundamental of analytical Chemistry -D.A.Skoog & D.M.West
- 3. Basic concepts of analytical Chemistry-S.M.Khopkar
- 4. Instrumental Methods of Chemcial Analysis-G.K.Ewring
- 5. Quantitative Inorganic Analysis-A.I.Vogel
- 6. Ion Exchange-AellFerish
- 7. Modern Polarographic Methods in Analytical Chemistry -A.M.Bond
- 8. Thermal Methods of Analysis-W.W. Wandlandt.
- 9. D.A.Skoog, F.J.Holler and T.E.Nieman, Principles of Instrumental analysis, 5<sup>th</sup> Edition, Saunderøs college Pub. 1998.



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# SEMESTER-IV

# (COURSE –XVII A) CHEMISTRY SPECIAL THEORY - IV) (HVORGANIC SPECTROSCOPY)

Lectures: 60 Max. Marks: 80

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

# 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. Application of IR to the following:

- i) Distinction between
  - a) Ionic and coordinate anions such as  $NO_3^-$ ,  $SO_4^{-2-}$  and  $SCN^-$
  - b) Lattice and coordinated water.
- ii) Mode of bonding of ligands such as urea, dimethylsulphoxide and hexamethylphosphoramide.

### <u>UNIT-II</u>

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

*Stereochemical non-rigidity and fluxionality:* Introduction, use of NMR in its detection, its presence in trigonal bipyramidal molecules ( $PF_5$ ), Systems with coordination number six ( $Ti(acac)_2Cl_2$ ,  $Ti(acac)_2Br_2$ ,  $Ta_2(OMe)_{10}$ ,).

# <u>UNIT-III</u>

**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. Interpretation of NQR data, Structural information of the following: PCl<sub>5</sub> TeCl<sub>4</sub>, Na<sup>+</sup>GaCl<sub>4</sub>, BrCN, HIO<sub>3</sub> and Hexahalometallates

# <u>UNIT-IV</u>

**Mössbauer Spectroscopy:** Introduction, Principle, Conditions for Mössbauer Spectroscopy, parameters from Mössbauer Spectra, Isomer shift, Electric Quadrupole Interactions, Magnetic Interactions MB experiment, Application of MB spectroscopy in structural determination of the following:

- i) High spin Fe (II) and Fe (III) halides FeF<sub>2</sub>, FeCl<sub>2</sub>.2H<sub>2</sub>O, FeF<sub>3</sub>, FeCl<sub>3</sub>.6H<sub>2</sub>O. Low spin Fe(II) and Fe(III) Complexes-Ferrocyanides, Ferricyanides, Prussian Blue.
- ii) Iron carbonyls. Fe(CO)<sub>5</sub>, Fe<sub>2</sub>(CO)<sub>9</sub> and Fe<sub>3</sub> (CO)<sub>12</sub>
- iii) 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



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on of the spectrum, Hyperfine coupling in Isotropic Systems radicals). Factors affecting the magnitude of g-values. Zero neracy, Line width in solid state ESR, Double resonance nental method. Applications of ESR to the following: : -

Copper óII

#### 2. CuSiF<sub>6</sub>.6H<sub>2</sub>O & (NH<sub>3</sub>)<sub>5</sub>Co-O.Co(NH<sub>3</sub>)<sub>5</sub>

- Physical methods in Inorganic Chemistry R.S.Drago. 1.
- 2. Modern Optical methods of Analysis - Eugens D.Olsen
- 3. Infrared spectra of Inorganic and coordination compounds - Kazuo Nakamoto
- 4. Introduction to Chemistry óDonald 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



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# <u>SEMESTER-IV</u> (COURSE –XVIII A) CHEMISTRY SPECIAL THEORY - IV) <u>ND SUPRAMOLECULAR CHEMISTRY</u>)

Lectures: 60 Max. Marks: 80

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

# **UNIT-I**

(a) Metalloporphyrins: (ref. Books No. 1,5,6): Porphyrins and their salient features, characteristic absorption spectrum of porphyrins, chlorophyll (structure and its role in photosynthesis). Transport of Iron in microorganisms (sidrophores), types of siderophores (catecholate and Hydroxamato siderophores).

(b) Metalloenzymes: (Ref. Book No. 1,2): Definitions: Apoenzyme, Coenzyme, Metalloenzyme, structure and functions of carbonic anhydrase A & B, carboxy peptidases.

### <u>UNIT-II</u>

#### Oxygen Carriers: (Ref. Book No. 1,8):

- a) *Natural oxygen carriers:* Structure of hemoglobin and myoglobin, Bohr effect, Models for cooperative interaction in hemoglobin, oxygen Transport in human body (-perutz machanism), Cyanide poisoning and its remedy. Non-heme protiens (Hemerythrin & Hemocyanin).
- **b)** *Synthetic oxygen carriers:* Oxygen molecule and its reduction products, model compounds for oxygen carrier (Vaskaøs Iridium cjomplex, cobalt complexes with dimethyl glyoxime and schiff base ligands).

#### <u>UNIT-III</u>

Transport and storage of metals: (Ref. Books No. 1,2) 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 (Ref. Books N. 1,4,8):-** Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (Platinum complexes), Lithium and mental health.

#### UNIT-V

**Supramolecular Chemistry (Ref. Book 9):** 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)

- 1. The Inorganic Chemistry of Biological processes M.N.Hughes.
- 2. Bio Inorganic Chemistry Robert Wittay
- 3. Advanced Inorganic Chemistry (4<sup>th</sup> Edn) Cotton and Wilkinson.
- 4. Topics in current chemistry (Inorganic Biochemistry) vol. 64 (1976) ó Davison and Coworkers.
- 5. An Introduction to Biochemcial Reaction Mechanism James N.Lowe and Lloyalt Ingraham.
- 6. General Biochemistry Fruton J.S. and Simmonds S.
- 7. Plant Physiology Robeert N.Devtin.
- 8. Inorganic chemistry ó James E. Huheey.
- 9. Supramolecular Chemistry (Concepts and Perspectives) Jean Marie Lehn(VCH-1995).



# SEMESTER-IV

#### (COURSE –XV B) HEMISTRY SPECIAL THEORY - II) (5-7'NTHETIC STRATEGIES)

Lectures: 60 Max. Marks: 80

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

#### UNIT-I

**Organic Reagents:** Reagents in organic synthesis: Willkinson catalyst, Lithium dialkyl cuprates (Gilmanøs reagents), Lithium diisopropylamide (LDA), 1,3-Dithiane (Umpolung) Dicyclohexylcarbobiimide (DCC), and Trimethylsilyliodide, DDQ, SeO<sub>2</sub>, Baker yeast, Tri-nbutyltinhydride, Nickel tetracarbonyl, Trimethylchlorosilane.

### <u>UNIT-II</u>

**Oxidations:** Introduction, Different oxidative process. Aromatiztion 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 olefines to aldehydes and ketones.

#### <u>UNIT –III</u>

**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, Witting 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.

- 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. Organomettalic Chemistry-A Unified Approach, R.C. Mehrotra, A. Singh.



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# SEMESTER-IV

#### (COURSE –XVI B) HEMISTRY SPECIAL THEORY - III) URAL PRODUCTS)

Lectures: 60 Max. Marks: 80

**Note:** Ten questions will be set by the examiner selecting <u>**TWO**</u> from each unit. As far as possible, every question will be divided into <u>**Two – Three Parts**</u>. The students shall attempt <u>**FIVE**</u> questions selecting <u>**ONE**</u> 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), -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: - carotene, - carotene, - carotene, lycopene and vitamin A. Xanthophylls: Spirilloxanthin, Capsorubin, Fucoxanthin. Carotenoid acids (Apocarotenoids): Bixin and Crocetin. Bio synthesis of carotenoids

#### <u>UNIT-III</u>

**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, Dieløs hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Androsterone, Testosterone, Estrone, Progestrone. 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 (quercitin) and isoflavones (daidzein) coumarin, Quinones (lapachol), Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

- 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. Roddøs 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.



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# <u>SEMESTER-IV</u> (COURSE –XVII B) HEMISTRY SPECIAL THEORY - IV) ICINAL CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

# <u>UNIT-I</u>

**Drug Design:** Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism bioisosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-Chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Free-Wilson analysis, Hansch analysis relationships between Free-Wilson and Hansch analysis.

#### UNIT-II

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

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

#### UNIT-III

Antibiotics and Antiinfective Drugs: Antibiotics: Structure, SAR and biological action of antibiotics. Examples: penicillin: penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Sufonanmides: Structure, SAR and mode of action of sulfonamides, sulfonamide inhibition and probable mechanisms of bacterial resistance to sulfonamides. Examples: sulfodiazine, sulfofurazole, acetyl sulfafurazole, Sulfagnanidine, Phthalylsulfo acetamide, Mafenide. Sulphonamide related compounds Dapsone. Local antiinfective drugs: Introduction and general mode of action. Examples: sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, chloroquin and primaquin

#### UNIT-IV

**Psychoactive Drugs:** Introduction, neurotransmitters, CNS depressants and stimulants. SAR and Mode of actions. Central Nervous System Depressant: General anaesthetics.

Sedatives & Hypnotics: Barbiturates and Benzodiazepines.

Anticonvulsants: Barbiturates, Oxazolidinediones, Succinimides, Phenacemide and Benzodiazepines.

Psycotropic 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 Actions:** Antineoplastic Agents: Cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antiobiotics and mitotic inhibitors. Biological action of mechlorethamine, cyclophosphamide, melphalan, uracil, and 6-mercaptopurine.



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mine derivatives, amino alkyl ether analogues, cyclic basic

#### Antifertility agents: General antifertility agents.

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Diuretics: Mercurial diuretic, Non mercurial diuretics (Thiazides, carbonic-anhydrase inhibitors, xanthine derivatives, pyrimidine diuretics and osmotic diureteics

- 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, Ole Gisvold, Robert F. Doerge.
- 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. Burgerøs Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch-14), Ed. M.E. Wolff, John Wiley.
- 8. Goodman and Gilmanøs 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) HEMISTRY SPECIAL THEORY - V) OLYMER CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

# <u>UNIT -I</u>

**Polymers:** Macromolecular Concepts, Importance of polymers, Chemical and geometrical structure of polymers, Polymerization: Chain polymerization, step growth polymerization, electrochemical, metathetical polymerization, group transfer polymerization, co-ordination. Concept of copolymerization, copolymer equation, reactivity ratio, Alfrey-price scheme, Polymerization techniques, Kinetics of chain and step growth polymerization.

### <u>UNIT-II</u>

**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), 1,3- Butadiene and 2-Substituted 1,3-Butadienes (1,2- and 3,4-Polymerizations, 1,4-Polymerizations), 1-Substituted and 1,4-Disubstituted 1,3-Butadienes (1,2- and 3,4-Polymerizations, and 1,4-Polymerizations). Stereoregular polymers: Significance of stereoregularity (isotactic, syndiotactic, and atactic polypropenes), Cis- and trans-1,4-poly-1,3-dienes, Cellulose and amylose. Coordination polymerization: Ziegler Natta catalyst.

#### <u>UNIT-III</u>

**Structure and Properties of Polymers:** Morphology and order in crystalline polymersconfigurations of polymer chains. Crystal structures of polymers. Strain-induced morphology, crystallization and melting. Polymer structures and physical properties- crystalline melting point,  $T_m$ - melting points of homogeneous series, effect of chain flexibility and other steric factor, entropy and heat of fusion. The glass transition temperature,  $T_g$  relationship between  $T_m$  and  $T_g$ , Effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirement and polymer utilization.

#### <u>UNIT-IV</u>

**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-V

(A) Commercial Polymers: Polyethylene, Polyvinyl chloride, Polyamides, Polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers-Fire retarding polymers and electrically conducting polymers.

**(B) Supramolecular polymer chemistry:** Supramolecular polymer chemistry: Generation of hydrogen bonded supramolecular molecules polymers and liquid crystals, Basic features of supramolecular polymers, Supramolecular polymers as supramolecular materials. Supramolecular low molecular weight complexes (Liquid-crystalline complexes and nonliquid -crystallne complexes. Supramolecular side chain polymers (Liquid-crystalline polymeric complexes and nonliquid -crystallne polymeric complexes). Functionalization of complexes. Nanochemistry: Basic concepts and Applications.



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ert and N.L. Allinger, ACS Monograph 177, 1982. Ditals. L. Salem and W.L. Jorgensen, Academic press. unic Chemistry, T.H.Lowry and K.C. Richardson, Harper and Row.

- 4. Introduction to Theoretical Organic Chemistry and Molecular Modeling, W.B. Smith, VCH, Weinheim.
- 5. Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman.
- 6. Supramolecular Chemistry; Concepts and Perspectives, J.M. 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.



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# <u>SEMESTER-IV</u> (COURSE –XV C) HEMISTRY SPECIAL THEORY - II) ED QUANTUM CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

# UNIT - I

Time ó independent perturbation theory for non ó degenerate states (first order correction to energy and wave function), and its application to particle in a one ó dimensional box, ground state helium atom (without spin consideration) and perturbed harmonic ó oscillator. Variational method: theory and application to ground state hydrogen and helium atoms and one ó dimensional oscillator.

### <u>UNIT - II</u>

Theory of time ó dependent quantum approximation technique. Fermi Golden Rule. Radiation ó Matter interaction (induced emission and absorption of radiation). Einsteinøs transition probabilities. Determination of selection rules in respect of rigid rotation and harmonic ó oscillator approximation.

#### <u>UNIT - III</u>

Quantum ó mechanical of multielectron atoms: Hartree self ó consistent method. Hartree ó Fock self ó Consistent (HFSCF) method. Roothamøs method. Correlation energy (CE) and configuration interaction (CI). Koopmannøs theorm. Basic idea of Density Functional Theory (DFT): Kohn ó Sham equation.

#### <u>UNIT – VI</u>

Quantum ó mechanical treatment of diatomic molecules: The Born Oppenheimer approximation and its formulation. The valence ó bond treatment of a hydrogen molecule. Heitler ó London treatment and ionic contribution. Molecular Orbital Theory (MOT) of  $H_2^+$ . MOT with configuration interaction (CI). Hybridization (sp, sp<sup>2</sup> and sp<sup>3</sup>) from a quantum ó mechnical view ó point.

#### <u>UNIT – V</u>

Quantum ó mechanical treatment of  $\ddot{U}$  - electron systems. The  $\ddot{U}$  - electron approximation . Free electron molecular orbital (FEMO) method and its application to polyenes. The Huckel ó Molecular Orbital Theory (HMOT) for conjugated hydrocarbons and cyclic conjugated systems. Huckel calculations for ethylene, allyl systems, cyclobutadiene and benzene. Calculation of electron density, charge distribution and bond orders.

- 1. Quantum Chemistry An Introduction: H.L. Strauss
- 2. ntroductory 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



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# <u>SEMESTER-IV</u> (COURSE –XVI C) HEMISTRY SPECIAL THEORY - III) TATE CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT - I</u>

X- ray diffraction: Indexing of powder and crystal photographs. Determination of Bravais lattice, point group and space group. Determination of space group with examples. Electron diffraction: The scattering of electron by gases (Wierl equation), visual method, radial distribution method and applications. Neutron diffraction: Introduction, differences between neutron and X- ray diffraction. Application to structure modification and magnetic compounds.

### <u>UNIT - II</u>

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; quantum approach, Fermi ó Dirac statistics. Zone theory: quantum approach, allowed energy zones, Brillioun zones, k ó space, Fermi surfaces and density states.

### <u>UNIT - III</u>

Properties of crystals: Electrical properties of metals; conductors and non ó 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: Absorption spectrum, photoconductivity, photovoltaic effect and luminescence. Refraction Birefringence and color centre. Dielectric properties: Piezoelectricity, Rerro electricity, Ionic conductivity and electric breakdown.

#### <u>UNIT – IV</u>

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

#### <u>UNIT - V</u>

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 t5his films, growth of single crystal, high pressure and hypothetical method.

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



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# <u>SEMESTER-IV</u> (COURSE –XVII C) HEMISTRY SPECIAL THEORY - IV) YSICAL CHEMISTRY)

Lectures: 60 Max. Marks: 80

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

### <u>UNIT – I</u>

Cell membrane and its structure: The Cell Membrane, lipids in biological membranes, types and arrangements of proteins in membranes, lipo proteins. 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, hydrolysis of ATP and its synthesis from ADP.

#### <u>UNIT – II</u>

Thermodynamics of Biopolymers Solutions: osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system. Statistical mechanics in biopolymers chain configuration of macromolecules, statistical distribution end ó to - end dimensions, calculation of average dimensions for various chain structures. Polypeptide and protein structures and protein folding.

### UNIT – III

Mechanism of Membrane Transport: Transport through cell membrane, active and passive transport systems, Ping - pong mechanism for transport of diffusion, Macromolecules across the Plasma Membrane, Role of Intercellular spaces in transport process, Homocellular, Transcellular, Intracellular transport, Irreversible thermodynamic treatment of membrane transport. Nerve conduction, Donnan effect in Osmosis, its dependence on pH difference across the membrane. Semipermeable membrane and Donnan membrane equilibrium.

#### <u>UNIT – IV</u>

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 Waaløs forces Scope of Genomics, proteomics and bioinformatics, ribosomes: Site and Function of protein synthesis.

#### <u>UNIT –V</u>

Protein molecules: Protein sequence and structure (primary structure), secondary structure: - Helix, - Sheet, classification of proteins, torsion angles, tertiary structure, quarternary structure, Protein folding and refolding, computer simulation: thermodynamic-kinetic approach, statistical mechanics approach, Homolog Modelling, De Novo prediction, Protein misfolding, Biological factors (Chaperones) and chemical factors(Intra and intermolecular interactions) leading tfolding/refolding/misfolding. Brain diseases associated with it.

- 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. iophysics: Volkenstein
- 8. Biophysical Chemistry (Vol. I-III): Schimell and Cantour



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# <u>SEMESTER-IV</u> (COURSE –XVIII C) HEMISTRY SPECIAL THEORY – V) Y OF MACROMOLECULES)

Lectures: 60 Max. Marks: 80

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

#### <u>UNIT – I</u>

The science of macromolecules, Importance of macromolecules / polymers, basic concepts of polymers viz. monomers, repeat units, degree of polymerization, classification of polymers on the basis of molecular weight and special arrangement viz. linear, branched and network polymers. Types of macromolecules (synthesized and natural), polymerization by condensation and addition reactions only. Molecular forces and chemical bonding in simple molecules and macromolecules and their effects on the physical properties. Polymer solutions, criteria for polymer solubility, conformations of dissolved polymer chains. Different models for describing the size and shape of dissolved macromolecules, configuration and conformation of macromolecules.

### <u>UNIT – II</u>

Thermodynamics of polymer solutions, thermodynamics of simple liquid mixtures, ideal solutions, regular solutions, lattice model of solutions (Flory ó Huggins Theory), Flory ó Krigbaum theory for dilute polymer solutions. Phase separation in polymer solutions involving binary polymer ó solvent systems, ternary systems and multi ó component systems. Fractionation of polymers by different techniques, theory of swelling of cross ó linked / network polymers.

#### <u>UNIT – III</u>

Measurements of molecular weights and size of macromolecules by osmotic pressure measurement, light scattering method, diffusion measurement, sedimentation and ultracentrifuge methods and viscosity methods. Molecular weights of macromolecules viz., number average and weight average molecular weights and related numerical problems.

#### <u>UNIT – VI</u>

Rheology and Mechanical Properties of Polymers: Brief introduction to rheology and mechanical properties of polymers, phenomena of viscous flow, kinetic theory of ribber elasticity, amorphous polymers and practical importance of their aggregation states, viscoelasticity (experimental and dynamic method), general mechanical models for an amorphous polymer, molecular structure and viscoelasticity. The glassy state and glass transition temperature. The mechanical properties of crystalline polymers.

#### 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 ó linked density).
- 2. Polyelevtrolytes: The water soluble charged polymers and their applications. Ionomers (ion containg polymers) conducting polymers solid polymer electrolytes, mechanism of conductivity, polymer colloids and their applications in commercial and industrial formulations (adhesives, coating, paper, pharmaceutical and medical applications), polymer microgels, biomedical polymers. Polymers in combating environmental pollution and as chemical reagents.

- 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



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# <u>SEMESTER - IV</u> COURSE – XIX (A) IEMISTRY PRACTICAL - SPECIAL)

Time: 12 hrs Max. Marks: 75

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

- 1. Stannic iodide
- 2. Bis(acetylacetonate) oxovanadium (IV)
- 3. Tris (acetylacetonate) siliconchloride.
- 4. Mercuration of phenol.
- 5. Hexa ammine nickel (II) chloride.
- 6. Pyridine perchromate.

#### **INSTRUMENTAL ANALYSIS:**

#### (A) Conductometric Titrations:

- i) Differential behaviour of acetic acid to determine the relative acid strength of various acids and basic strength of various bases.
- ii) Strong acid-strong base titration in acetic acid.

#### B) **Potentiometric Titrations**.

- 1. *Neutralisation reactions*:
  - i) Sodium hydroxide-hydrolchloric 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*:

4.

- i) Silver nitrate-sodium halides.
- Complexation Reactions
  - i) Potassium cyanide-silver nitrate.

#### C) Colorimetric Analysis:

- 1) Verification of Beerøs law for KMNO<sub>4</sub>,  $K_2Cr_2O_7$  solutions and determination of the conc. of KMNO<sub>4</sub>  $K_2Cr_2O_7$  in the given solution.
- 2) Colorimetric determination of Iron (III) with potassium thiocyanate reagent or o-Phenanthroline method.
- 3) Determination of traces of manganese (in steel samples) colorometrically by oxidation to permanganic acid with potassium periodate.
- 4) Spectrophotometric determination of pK value of an indicator (acid dissociation constt. of methyl red)

#### (D) pH metric –titrations

- 1) Copper and cactechol
- 2) Copper and salicylic acid
- 3) Acid base titrations
- 4) Mixtures of acids with a base



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If wave potentials of zinc and manganous ions in potassium

- 3) Determination of cadmium in solution
- 4) Investigation of the influence of dissolved oxygen.

#### (F) Amperometric Titrations:

- 1. Zinc with EDTA
- 2. Lead vs. chromate
- 3. Nickel as isoquilnoline thiocynate

#### (G) Flame Photometry:

- 1) Determination of sodium
- 2) Determination of potassium
- 3) Determination of calcium

#### H) Miscellaneous:

- 1. Determination of stability constants of complexes.
- 2. Determination of magnetic susceptibility of complexes
- 3. Estimation of periodate, iodate and bromate in the same solution.
- 4. Determination of bromide and chloride in the same solution.
- 5. Analysis of a solution containing chloride and iodide.

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



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# <u>SEMESTER - IV</u> COURSE – XIX (B) EMISTRY PRACTICAL - SPECIAL)

Time: 12 hrs Max. Marks: 75

(A) <u>Extraction of Organic Compounds from Natural Sources</u>: 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 Rf value reported). lycopene from tomatoes and - carotene from carrots.

**(B)** <u>**Paper Chromatography:**</u> Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.

#### (C) <u>Spectroscopy:</u>

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

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



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# <u>SEMESTER - IV</u> COURSE – XIX (C) EMISTRY PRACTICAL - SPECIAL)

Time: 12 hrs Max. Marks: 75

- 1. <u>Viscosity Measurements:</u> Verification of the Jones ó Dole equation, determination of viscosity A and B ó coefficients for simple electrolytes in water and in aqueous mixtures of organic solvents.
- **2.** <u>Conductometric Measurements:</u> Kinetics of saponification of ethylacetate by NaOH. Solubility of sparingly soluble salts.
- **3.** <u>Potentiometric Titration:</u> Titration of HCl with NaOH, determination of dissociation constant of acetic acid and phosphoric acid. Oxidation ó reduction titration (ferrous ammonium sulphate with KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>).
- 4. <u>Flamephotometric Measurements</u>: Establishing the calibration plots for Na<sup>+</sup> and K<sup>+</sup> ions and determination of their concentration in the given solution at ppm level.
- 5. <u>Determination of Molar Mass</u>: Cryoscopic and Rastsøs methods. Determination of molar mass of polymer by viscosity measurement.
- 6. <u>Colometery Measurements:</u> Determination of composition ferric ions ó salicylicacid complex using Jobøs method.
- 7. <u>Polarimetry Measurements:</u> Determination of specific and molecular rotation, percentage of tow optically active substances, kinetics of acid catalysed inversion of cane sugar, comparison of strengths of two acids.

- 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



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# <u>SEMESTER - IV</u> (COURSE – XX ) R 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.