

## M Sc II YEAR 2020-21

### Compulsory Paper-I

#### **CH-201: GROUP THEORY & INORGANIC SPECTROSCOPY, APPLICATION OF SPECTROSCOPY**

##### **Unit I**

Molecular Symmetry and Group theory (A) : Symmetry elements and operation. Symmetry classification of group, relation between orders of a finite group and its sub groups. Conjugacy relation and classes. Schonflies symbols, representation of groups by matrices ( representation for the  $C_n, C_{nv}, C_{nh}, D_{nh}$  etc. groups to be worked out explicitly types of Matrices, Matrix Multiplications, Transformations of Matrices, ). Characters of representations.

Molecular symmetry and group theory ( B ) : The great orthogonality theorem and its importance, character table and its constructions, use in spectroscopy. Mulliken Symbols for Irreducible representations areas of character tables, reduction formula and its application, unit vector transformation, direct product.

Orbital symmetries and overlap, hybridization in linear trigonal planar, tetrahedral square planar, square pyramidal and trigonal pyramidal molecules. symmetry and hybridization in Buta-1,3-diene and benzene.

##### **Unit II**

Vibrational Spectroscopy: Symmetry and shapes of  $AB_2$   $AB_3$   $AB_4$   $AB_5$  &  $AB_6$  mode of bonding of ambidentate ligands, ethylenediamine and di ketonato complexes, applications of Resonance . Raman Spectroscopy particularly for the study of activesites of metalloproteins.

Electron Spin Resonance Spectroscopy: Hyperfine coupling, spin polarization for atoms and transition metal ion, spin-orbit- coupling and significance of g-tensors, Applications to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as  $PH_4$  ,  $F_2$  and  $[BH_3]$ .

Nuclear Magnetic Resonance of Paramagnetic substances in solution. The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclides with emphasis on  $^{195}Pt$  and  $^{119}Sn$  NMR. Mossbauer

Spectroscopy: Basic principles, spectral display applications of the technique of the studies of (1) bonding and structures of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds including those of intermediate spin, (2)  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds nature of M-L bond, coordination number, structure and (3) detection of oxidation state and in equivalent MB atoms.

### **UNIT III**

#### **Ultraviolet and Visible Spectroscopy**

Various electronic transitions (185-800 nm), Instrumentation, Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

#### **Infrared Spectroscopy**

General introduction, Instrumentation and sample handling, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactames and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT IR. IR, of gaseous, solids and polymeric materials..

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

### **UNIT IV**

#### **Nuclear Magnetic Resonance Spectroscopy**

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines & amides), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification

of complex spectra-nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-F, P.

### **Carbon-13 NMR Spectroscopy**

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

Two dimension NMR spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. Instrumentation of  $H^1$  and  $C^{13}$  NMR and sample handling.

## **UNIT V**

### **Mass Spectrometry**

Introduction, ion production – EI, CI, FD and FAB, factors affecting fragmentative, ion analysis, Instrumentation and sample handling. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

#### **Books Suggested:**

1. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
2. Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J. Martin, Heyden.
3. Spectrometric Identification of Organic Compounds, R.M. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley.
4. Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.
5. Application of Spectroscopy of Organic Compounds, J.R. dyer, Prentice Hall.
6. Spectroscopic Methods in Organic Chemistry, D.H. Williams, I. Fleming, Tata McGraw-Hill.
7. Spectroscopy, P. S. Kalsi New Age Publishers
8. Chemical Applications of Group Theory. F.A. Cotton

9. Physical Methods in Chemistry, R.S.Drago, Saunders College.
10. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V.Parish, Ellis Harwood.
11. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS.
12. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
13. Progress in Inorganic Chemistry vol., 8 ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.

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# CH-202: SOLID STATE CHEMISTRY AND BIO-CHEMISTRY

## UNIT I

### **Solid State Reactions and Non-Stoichiometry**

Crystalline solid, Solid State Reactions - General principles and Experimental procedures, Wagner's theory in reference to MgO and Al<sub>2</sub>O<sub>3</sub>, Enhancement of reactivity of solids, Co-precipitation as a precursor to solid state reaction, Kinetics of solid state reaction

Non-Stoichiometry – Introduction, Classification – Small and Large deviations from stoichiometry, Superlattice ordering of defects

### **Crystal Defects**

Perfect crystal and Crystal Defect, Thermodynamic requirement of defect, Intrinsic and Extrinsic defects, Point defects - Schottky, Frenkel, Interstitial atom, Substitutional impurity atom and Color Centre, Line defect – Dislocation (edge and screw), Plane defects - Lineage boundary, Grain Boundary, Stacking fault, Thermodynamics of Schottky and Frenkel defect

## UNIT II

### **Electronic Structure of Solids**

Introduction to Free electron theory of Metals, Formation of Energy bands, Valence and Conduction bands, Kronig-Penny Model, Band theory of solids, Brillouin zone, Motion of electrons in a band – velocity and effective mass of an electron,  $f_k$  factor, Distinction between metal, semiconductor and insulator on the basis of Band theory

Electrically conducting solids – Conjugated systems, Charge-transfer complexes

## UNIT III

### Semiconductors and Properties of Solids

Intrinsic and Extrinsic semiconductors, p-type and n-type semiconductors, Dependence of conductivity of n-type and p-type semiconductors on temperature, p-n Junction

Optical Properties – Photoconduction and Photoelectric effect

Magnetic Properties: Classification of materials – para-, dia-, ferro-, and antiferromagnet, Effect of temperature on magnetic susceptibility of para-, dia-, ferro-, antiferromagnetic substances, Magnetic Hysteresis

### Superconductor

Superconductivity, Factors affecting superconductivity, Isotope effect, Meissner Effect, Magnetic effects – Type I and Type II superconductors, Persistent current, BCS theory of superconductivity, Cooper pair, Occurrence of superconductivity– conventional, organic and high temperature superconductors, Fullerene as superconductor

## UNIT IV

Metal ions in Biological Systems: Role of metal ions in biological processes.

Dioxygen Uptake: Structure and function of haemoglobin, myoglobin, hemocyanins and hemerythrin, model system and synthetic complexes of iron and Copper. Electron Transfer in Biology: Structure and function of metalloproteins, Cytochromes and iron-sulphur proteins, synthetic models, peroxidases and catalases.

Nitrogenases: Biological nitrogen fixation, molybdenum nitrogenases, model systems

Enzymes: Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, binding energy specificity and regulation. Kinetics of enzyme action that is activation energy, Michaelis- Menten equation, Lineweaver Burk plot & factors effecting enzyme activity. Nomenclature and classification. Fischer's lock and key and Koshland's induced fit hypothesis. Types of inhibition, concept and identification of active site by the use of inhibitors and affinity labeling. Transition state theory, acid-base catalysis and covalent catalysis.

## UNIT V

Co-Enzyme Chemistry: Cofactors as derived from vitamins, coenzyme, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate,

pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, lipoic acid, vitamin B12, Mechanism of reaction catalysed by the above cofactors. Large-scale production and purification of enzymes, techniques.

Bio-energetic and Bio-polymer Interactions: Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.

Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.

Diffraction Methods and Statistical Mechanics in Biopolymers: Evaluation of size, shape, molecular weight by various experimental techniques. Light scattering, X-ray scattering, X-ray diffraction and photo correlation spectroscopy ORD. Chain configuration of macromolecules and calculation of average dimensions. Polypeptide and protein structures, introduction to protein folding.

### **Books Suggested:**

1. Solid State Chemistry and its Applications, A.R. West, Plenum
2. Principles of Solid State, H.V. Keer, Wiley Eastern
3. Solid State Chemistry, D.K. Chakrabarty, New Age International
4. Fundamentals of Solid State Physics, B.S. Saxena, R.C. Gupta and P.N. Saxena
5. Solid State Physics, A. J. Dekkar, Macmillan
6. The Inorganic Chemistry of Biological Processes, M.N.Hughes Wiles (1972).
7. Bioinorganic Chemistry-An Introduction, Enchiroochiai.
8. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M.Berg, University Science Books.
9. Bioinorganic Chemistry, I Bertini, H.B. Gray, S.J.Lipard and J.S. Valentine, University Science Books.
10. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C.Penny, Springer-Verlag.
11. Understanding Enzymes, Trevor Palmer, Prentice Hall.
12. Enzyme Chemistry: Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall.
13. Enzyme Mechanisms Ed. M.I.Page and A.Williams, Royal Society of Chemistry.
14. Fundamentals of Enzymology, N.C. Price and L. Stevens, Oxford University Press.

15. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Tevan, John Wiley.
16. Enzymatic Reaction Mechanisms, C.Walsh, W.H. freeman.
17. Enzyne Structure and Mechanism, A Fersht, W.H. Freeman.
18. Biochemistry: The Chemical Reactions of Living Cells, D.E.Metzler, Academic Press.
19. Principles of Biochemistry, A.L.Lehninger, Worth Publishers.
20. Biochemistry, L. Strver, W.H.Freeman
21. Biochemistry, J.David Rawn, Neil Patterson.
22. Biochemistry, Voet and Voet, John Wiley.
23. Outlines of Biochemistry, E.E.Conn and P.K.Stumpf, Johh Wiley.
24. Bioorganic Chemistry: A Chemical Approach to Enzyme Achon. H. Dugas and C.Penny, Springer-Verlag.
25. Macromolecules: Structure and Function, F.World, Prentice Hall.

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## Group A

### Elective Paper-I

#### **CH-203A: ORGANOTRANSITION METAL CHEMISTRY**

##### **UNIT I**

Organotransition metal compounds : Definition, Classification and nomenclature of organotransition metal compounds. Comparison of bonding between metal carbonyls and Organotransition metal compounds. Organometallic compounds of inner transition elements

##### **UNIT II**

Alkyls and Aryls of Transition Metals: Types, methods of synthesis, thermal stability and decomposition pathways.

##### **UNIT III**

###### **Transition Metal $\pi$ -Complexes**

Transition metal  $\pi$ -complexes with unsaturated organic molecules, alkenes, cyclopentadienyls and arenes, methods of synthesis, properties, nature of bonding and structural features.

##### **UNIT IV**

###### **Homogeneous Catalysis**

Homogeneous catalytic hydrogenation of Alkenes, Zeigler Natta polymerization of olefins, Isomerisation of Alkenes, Hydroformylation, Dimerisation and polymerization of Alkenes and Alkynes.

##### **UNIT V**

Organocopper in Organic Synthesis : Conjugated additions, halogen substitution, alkylation of epoxides, alkylation of allylacetates, ketones from acid chlorides.

#### **Books Suggested:**

1. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
2. The Organomettalic Chemistry of the Transition Metals, R.H. Crabtree, John, Wiley.
3. Metallo-organic Chemistry, A.J. pearson, Wiley.
4. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

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## Group A

### Elective Paper-II

#### **CH-204A: NANOSCIENCE & NANOTECHNOLOGY**

**Unit I Introduction and Preparation:** Introduction to Nano Scale and Nanomaterials, Unique properties of Nanomaterials; Optical, Magnetic, electrical, thermal and chemical properties of Nanomaterials. Bonding, self-assembly, catalysis.

Synthesis of nanomaterial: Chemical Approaches: Chemical reduction; sonochemical synthesis; Sol-Gel Synthesis; Self assembly. Physical Approaches: Aerosol spray; Chemical vapour deposition(CVD) and lithography.

**Unit II Nanostructured materials:** Classification of nano materials based on dimension and configuration, Nanorods, Nanotubes and Nanofibres, wells & wires. Semiconductors quantum dots.

Inorganic nano materials: Metal/Oxide nanoparticles (NPs).

Organic nano materials- Polymer NPs

Carbon nano materials: Graphenes, Fullerenes, Carbon Nano tubes (CNTs)- Single walled carbon nanotubes (SWNTs), Multiwalled Carbon nanotubes (MWNTs)

#### **Unit III Characterization techniques for Nanomaterials-I:**

Electron Microscopy: Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning Probe Microscopy- Atomic force Microscopy (AFM)

#### **Unit IV Characterization techniques for Nanomaterials-II**

Particle size Analyser (Dynamic light scattering), X-ray Diffraction (XRD), Auger Emission Spectroscopy, Electron Spectroscopy for Chemical analysis (ESCA)

#### **Unit V Application of Nanomaterials and Nanotechnology:**

Impact of Nanotechnology in various fields. Pharmaceutical-Advance drug delivery system, Medical & Health diagnosis through biosensors. Environment-water purification and air pollution control. Consumer goods-cosmetics and sports goods, Defence- Light Military platform and soldier protection.

### **Books Recommended:**

1. Essentials in Nanoscience and Nanotechnology, N. Kumar & S. Kumbhat ; John Wiley & Sons.
2. Concise Concepts of Nanoscience & Nanomaterials, N. Kumar & S. Kumbhat ; Scientific Publishers.
3. Charles P. Poole, Jr. and Frank J.Owens ;Introduction to Nanotechnology, , Wiley, 2003
4. G. Cao, Nanostructures and Nanomaterials: Synthesis, Properties and Applications, ICP, London, 2004.
5. C.M. Niemeyer and C.A. Mirkin, Nanobiotechnology, Concepts, Applications and perspectives, WILEY-VCH, Verlag Gmb H&Co, 2004.
6. G.M.Chow and K.E.Gonslaves ;Nanotechnology - Molecularly Designed Materials, (American chemical society)
7. K.P.Jain,Physics of semiconductor Nanostructures: Narosa Publishers, 1997
8. S.P. Gaponenko, Optical Properties of semiconductor nanocrystals, Cambridge University Press, 1980.
9. G. Cao, Nanostructures & Nanomaterials: Synthesis, Properties & Applications, Imperial College Press, 2004.
10. T.Pradeep, “Nano: The essentials, Tata Mc Graw Hill, New Delhi, 2007.
11. Willard, “Instrumental Methods of Analysis”, 2000.

## Group A

### Elective Paper-III

#### **CH-205A: INDUSTRIAL CHEMISTRY**

##### **UNIT I**

###### **Chemistry of colors**

Introduction, Classification of dyes, according to chemical constitution and according to application. General ideas about the synthesis of different dye intermediate and synthetic dyes i.e. direct and reactive dyes, azoic colours, acid and basic dyes, newer cationic dyes for acrylics, Disperse dye, mordant and sulphur dyes. Pigment and fluorescence brighteners. Colour fastness against light, washing, perspiration, rubbing etc. and its evaluation. Methods of colour measurements.

##### **UNIT II**

###### **Industrial/ Commercial polymers and their compounding ingredients:**

General characteristics of Fibers, Plastic, Rubbers and Adhesives-

Structure, properties and preparation of Polyamides, Polystyrene, Polychloride, Polymethylmethacrylate, Polymethacrylate, ABS, Epoxide, IR, SBR, NBR & IIR

Compounding Ingredients: Extenders, Fillers, plasticisers, stabilizers, anti oxidant and anti ozonants, Flame retardants, mould release agents, Sulphur vulcanisation.

##### **UNIT III**

###### **Ores and Minerals**

Inorganic materials of industrial importance, their availability, forms and structure-

Bauxite, clay, mica, zeolites, copper pyrites, zinc blend, dolomite and coal.

##### **UNIT IV**

Characteristic Features of surfactants: Conditions under which interfacial phenomena and surfactants become significant. General structural features and behaviour of surfactants : General use of charge types, general effect of nature of hydrophobic group.

## UNIT V

Micelle Critical micelle concentration (cmc), factors affecting the value of cmc in aqueous medium. factors determining the extent of Solubilization, effect of Solubilization. Formation of emulsions, factors determining emulsion stability, Mechanism of the cleaning process.

### Books Recommended:

1. Hall, A.J.(8<sup>TH</sup> ed.): The Standard Hand Book of Textiles, Butter-Worth, London.
2. Clark, W.: An Introduction to Textiles Printing, A Practical Manual for use in Laboratories College and School of Arts, Bottonworth, London.
3. Shinai, V.A.: technology OF textile processing, Sevak publication, Bombay, Vols. I to IX
4. Chakravarty, R.R. : Glimpses of Textile Technology, Caxton Press, Delhi.
5. Peters, R.H.: Textile Chemistry, Elsevier, Amsterdam, Vol. I to Vol. II
6. Surfactants and Interfacial Phenomenon. Milton J. Rosen, Johan-Wiley, 1978.
7. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
8. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Screehar, Wiley-Eastern.

## Group A

### Elective Paper-IV

#### **CH-206A: POLYMERS**

##### **UNIT I**

###### **Basics:**

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers.

Classification of polymers.

Polymerization: condensation, addition, radical chain-ionic and co-ordination and co-polymerization. Polymerization conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

##### **UNIT II**

###### **Polymer Characterization**

Polydispersion-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 analysis and ultracentrifugation methods.

Analysis and testing of polymers-chemical analysis of polymers, Microscopy.

Thermal techniques: thermo gravimetric analysis, differential thermal analysis, and physical testing-tensile strength, impact. Tear resistance. Hardness and abrasion resistance.

##### **UNIT III**

###### **Structure and Properties**

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology, crystallization and melting. Polymer structure and physical properties-crystalline melting point  $T_m$ -melting points of

homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T<sub>g</sub>-Relationship between T<sub>m</sub> and T<sub>g</sub>, effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

## **UNIT IV**

### **Polymer Processing**

Plastics, elastomers and fibres. Compounding. Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

## **UNIT V**

### **Properties of Commercial Polymers**

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers – Fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

### **Books Suggested:**

1. Textbook of Polymer Science, F.W. Billmeyer Jr. Wiley.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Screedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and RM. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymers, J.M.G. Gowie, Blackie Academic and Professional.
6. J.M.G. Gowie, Blackie Academic and Professional.



## Group B

### Elective Paper-I

#### **CH-203B: PHOTOCHEMISTRY**

##### **UNIT I**

Solar radiation spectrum, Insolation; Photochemical Reactions: Interaction of electromagnetic radiations with matter, types of excitations, fate of excited molecules, quantum yield, transfer of excitation; Properties of excited states: Structure, dipole moment, acid-base strengths, Reactivity; Bimolecular deactivation-quenching. Determination of Reaction Mechanism: Classification, rate constants and life time of reactive energy states- determination of rate constants of reaction, Effect of light intensity on the rate of photochemical reactions, Types of photochemical reaction- photodissociation, gas-phase photolysis.

##### **UNIT II**

Photochemistry of Alkenes and Carbonyl Compounds: Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement 1,4- and 1,5- dienes; Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic,  $\beta,\gamma$  – unsaturated and  $\alpha,\beta$ -unsaturated compounds, Cyclohexadienones; Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

##### **UNIT III**

Photochemistry of Aromatic Compounds : Isomerisations, additions and Substitutions; Miscellaneous Photochemical Reactions; Photo-Fries reaction of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen Reactions; Photochemical formation of smog, Photo degradation of polymers, Photochemistry of vision.

## UNIT IV

Excited states of metal complexes: Comparison with organic compounds, electronically excited states of metal complexes, charges transfer spectra, charge transfer excitations; Ligand field photochemistry: Photosubstitution, Photoreduction, lability and Selectivity, Zero vibrational levels of ground state and excited state, energy content of excited state, zero-zero spectroscopic energy, development of the equations for redox potentials of the excited states; Redox reactions by excited metal complexes: Redox reactions of metal complexes in excited states, excited electron transfer using examples  $[\text{Ru}(\text{bpy})]^{2+}$  complexes and  $[\text{Fe}(\text{bpy})_3]^{3+}$  complex, role of spin-orbit coupling, life times of excited states in these complexes; Metal complex sensitizers: Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction.

## UNIT V

Photochemistry and electricity generation; solar energy conversion and storage; Concepts of solar power, maximum current, open-circuit potential, short-circuit current, i-v characteristics, Energy conversion efficiency, Thermodynamic efficiency limit, Quantum efficiency, Maximum power, Fill factor. Solar power storage; Basic principles, fabrication, characteristics, application and latest status of various solar power techniques like Solar steam generator (solar concentrating solar power), Solar chimney or solar cells, Organic/Polymer solar cells, Nanocrystal solar cells, Multijunction photovoltaic cells, Photoelectrochemical cells, Photogalvanic cells, Point-contact solar cells, Porous Nanoparticulate PEC, Perovskite Solar Cell.

### Books Suggested:

1. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wiley-Easter.
2. Molecular Photochemistry, N.J. Turro, W.A. Benjamin.
3. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill.
4. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
5. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
6. Solar Energy Hand Book, J.F. Kreider and F. Krejth, MacGraw Hill Book Co. 1981.

7. Solar Energy Conversion, R.C. Neville, Elsevier.
8. Alternative Energy Systems, B.K. Hodge, Wiley.
9. Advanced Energy Systems, Second Edition, Nicolai V. Khartchenko; Vadym M. Kharchenko, Taylor & Francis.
10. Non- Conventional Energy Resources, D.S. Chauhan, New Age International
11. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fleischauer, Wiley
12. Inorganic Photochemistry, J.Chem.Educ.vol. 60 No. 10, 1983.
13. Progress in Inorganic Chemistry, Vol. 30ed. S.J. Lippard. Wiley.
14. Photochemistry of Coordination Compounds, V. Balzari and V. Carassiti, Academic Press.
15. Elements in Inorganic Photochemistry, G.J. Ferraudi, Wiley..

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## Group B

### Elective Paper-II

#### **CH-204B: ORGANIC SYNTHESIS I**

##### **UNIT I**

##### **Organometallic Reagents**

Principle, preparations, properties and applications of the following in organic synthesis with mechanistic details.

**Group I and II metal organic compounds-** Li, Mg, Hg, Cd, and Zn compounds.

**Transition metals-** Cu, Pd, Ni, Fe, Co, and Ti compounds.

**Other elements-** Si and B compounds.

##### **UNIT II**

##### **Oxidation**

Introduction, Different oxidative processes.

Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated).

Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids.

Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

##### **UNIT III**

##### **Reduction**

Introduction. Different reductive processes.

Hydrocarbons – alkanes, alkenes, alkynes and aromatic rings.

Carbonyl compounds – aldehydes, ketones, acids and their derivatives

Epoxides.

Nitro, nitroso, azo and oxime groups.

Hydrogenolysis.

## UNIT IV

### Rearrangements

General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements:

Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction.

## UNIT V

### Metallocenes, Nonbenzenoid Aromatics and Polycyclic Aromatic Compounds.

General considerations, synthesis and reactions of some representative compounds.

#### Books Suggested:

1. Modern Synthetic Reactions, H.O. House, W.A. Benjamin.
2. Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.
3. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March, John Wiley.
4. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
5. Advanced Organic Chemistry Part B. F.A. Carey and R.J. Sundberg, Plenum Press.
6. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

### Group B

## Elective Paper-III

### CH-205B: ORGANIC SYNTHESIS II

#### UNIT I

##### **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.

#### UNIT II

##### **Protecting Groups, & Heterocyclic Compounds**

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

##### **Heterocyclic Compounds**

IUPAC of Heterocyclic compounds, saturated heterocyclic compounds containing mono-hetero atom (O, S, N), synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocyclic compounds in organic synthesis.

#### UNIT III

##### **One Group C-C Disconnections**

Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

#### UNIT IV

##### **Two Group C-C Disconnections**

Diels-Alder reaction, 1,3-difunctionalised compounds,  $\alpha,\beta$ -unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Micheal addition and Robinson annelation.

## UNIT V

### Synthesis of Some Complex Molecules

Application of the above in the synthesis of following compounds:

Camphor, Longifoline, Cortisone, Reserpine, vitamin D, Juvabione, Aphidicolin and Fredericamycin A.

#### Books Suggested:

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, Blackie Academic & Professional.
7. Advanced Organic Chemistry Part B, F. A. Carey and R.J. Sundberg, Plenum Press.

## Group B

### Elective Paper-IV

#### **CH-206B: ADVANCED ELECTROCHEMISTRY AND APPLICATIONS**

##### **UNIT I**

###### **Electrochemical Energy Storage**

Properties of Electrochemical energy stores: measure of battery performance, charging and discharging of batteries, storage density, energy density,

Classical Batteries: (i) Lead Acid (ii) Nickel- Cadmium (iii) Zinc- Manganese dioxide

Modern Batteries: (i) Zinc Air (ii) Nickel- Metal Hydride (iii) Lithium battery

Future electricity stores: storage in (i) hydrogen (ii) alkali metals (iii) non aqueous solution

##### **UNIT II**

###### **Electrochemical Energy Generators**

Fuel cells: Hydrogen –Oxygen Cell, Electrochemical solar cell, and Application of Fuel Cell. Comparisons of batteries, fuel cells and super capacitors, electrochemical processes of particular relevance to energy conversion.

##### **UNIT III**

###### **Corrosion and Material Protection**

Electrochemical corrosion: Fundamentals and mechanism , thermodynamics and stability of metals, theories of corrosion, forms of corrosion, corrosion current and corrosion potential- Evans diagrams. Measurement of corrosion rate: Non electro chemical method and electrochemical method. corrosion monitoring and prevention methods. anodic protection ,by alternation in the medium, by alternation in the metal and design consideration, inhibitors, Green inhibitors.

##### **UNIT IV**

###### **Kinetics of Electrode process and their nature**



Kinetically and mass transport controlled electrochemical processes, Mass transport by migration, convection and diffusion. , essential of electrode reaction,. Current density, over potential, Tafel equation, Buttlar- Volmer equation, Potentiostatic and galvanostatic methods including chronoamperometry, chronopotentiometry.

## UNIT-V

### Environmental Electrochemistry

Types of electro-organic reactions, constant current and constant potential, electrolysis, cell design, effect of variable, Techniques of electro organic synthesis, overvoltage, application of sewage waste water treatment, electrochemical incineration of human waste in combined space, electro- organic synthesis of novel drugs.

### Books Recommended:

1. Modern electrochemistry, Vol. I, IIA, Vol. II B, JOM Brockris and A.K.N. Raddy, Plenum publication, New York.
2. Electrochemical methods by Allen J. Bard and Larry R. Faulkner, John Wiley.
3. Techniques of Electro-organic synthesis part I, II and III by N.L. Weinberg, John Wiley.
4. *Corrosion and Corrosion Engineering* chemistry by M.G. Fontana, N.D. Green, McGraw-Hill, New York.
5. Electro chemistry by Carl H. Hamann, Andrew Hamett and Wolf Vielstich. Joh
6. M. G. Fontana "Corrosion Engineering", Mc Graw Hill, New York, 1997
7. "Corrosion Metal Environment Reactions" eds. L L. Shreir, R. A. Jerman, G. T. Burstein, Butterworths, London, 1994
8. D. Gabe "Principles of Metal Surface Treatment and Protection", Merlin Books, London, 1993
9. Corrosion Inhibitors, Principles & Applications, V.S. Sastry, John Wiley & Sons.
10. *Electrochemistry for clean environment by Bockrish*
11. *Electrochemistry by D R crow*
12. *Organic electrochemistry by M.M. Baizer*

## Group C

### Elective Paper-I

#### **CH-203C: BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY**

##### **UNIT I**

Metal storage Transport: Iron storage and Transport;

Oxygen carriers: Hb, Mb , ferritin and transferrin;

Bio-mineralization;

Iron Transport in Microbs: siderophores.

Calcium in Biology: Storage and Transport of Calcium & calcium in Muscle contraction, transport and regulation, intramolecular process, extracellular binding protein,  $\text{Ca}^{2+}$  ATP ase structure,  $\text{Ca}^{2+}$  ATP ase reaction cycle, intracellular  $\text{Ca}^{+2}$  transport.

##### **UNIT II**

Metalloenzymes: Zinc enzymes- carboxy peptidase and carbonic anhydrase. Iron enzymes- Reactivity and structure of catalase, peroxidase and cytochrome P450. Copper enzymes- Reactivity and structure of superoxide dimutase (SOD).

Co enzyme vitamin  $\text{B}_{12}$  – Names of different forms, biochemical function of cobalamin, Vitamin  $\text{B}_{12}$ , special characteristics of  $\text{B}_{12}$  co-enzyme.

##### **UNIT III**

Metals and chelates in medicine, metal deficiency and disease, toxic effect of metals, metal used for diagnosis and chemotherapy with particular reference to anticancer drugs.

##### **UNIT IV**

Supramolecular chemistry: Concepts and language molecular recognition, Principal of molecular receptors designs for different types of molecules, design and synthesis of co- receptor molecules and multiple recognition.

##### **UNIT V**

Supramolecular reactions and catalysis, supramolecular assemblies, Molecular and supramolecular devices, molecular and supra molecular photonic , electronic and ionic devices. supramolecular photochemistry

**Books suggested:**

1. Principles of Bioinorganic chemistry, SJ Lippard and J.M. Berg, University science books.
2. Bioinorganic chemistry, I Bertini, H.B. Garg, S.J. Lippard and J.S. Valentine, University science books.
3. Inorganic Biochemistry, Vol I and II Ed. G.S. Eichhorn, Elsevier progress in inorganic chemistry Vol. 18 and 38 ed. J.J. Lippard, Wiley.
4. Supra molecular chemistry, J.M. Lehn, VCH.
5. Bioinorganic chemistry, A K. Das Books and allied (P) Ltd.
6. Bioinorganic and supra molecular chemistry, Ajay kumar bhagi, G.R. Chatwal Himalaya publishing house.

## Group C

### Elective Paper-II

#### **CH-204C: HETEROCYCLIC CHEMISTRY**

##### **UNIT I**

Nomenclature of heterocycles: Systemic nomenclature of monocyclic, fused & bridge heterocycles.

Three Membered Heterocyclic Compounds With One Hetero Atom:

Aziridines, Oxiranes and Thiiranes

##### **UNIT II**

Four Membered Heterocyclic Compounds with One Hetero Atom:

Azities & Azetidines; Oxitanes, Thietanes

Bicyclic Ring Systems Derived from Pyrrole, Furan and Thiophene:

Benzopyrroles, benzofurans and benzothiophenes

##### **UNIT III**

Five Membered Heterocyclic Compounds with One Hetero Atom:

Tautomerism

Pyrroles, Furans and Thiophenes

Five Membered Heterocyclic Compounds with Two Hetero Atoms:

Pyrazoles, Imidazoles, Oxazoles and Thiazoles

##### **UNIT IV**

Six Membered Heterocyclic Compounds With One Hetero Atom:

Pyridines, Pyrylium salts and  $\alpha$ - and  $\gamma$ -Pyrones

Six Membered Heterocyclic Compounds with Two Hetero Atoms:

Pyrazines, Pyridazines and Pyrimidines,

Cinnolines and Phthalazines

## UNIT V

Seven Membered Heterocyclic Compounds with Two Hetero Atoms:

Azepines, Oxepins and Thiepins

Bicyclic Ring Systems Derived from Pyridine:

Quinoline and Isoquinolone

### **Books Suggested:**

1. Heterocyclic Chemistry Vol. 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer Verlag.
2. The Chemistry of Hetrocycles, T. Eicher and S. Hauptmann, Thieme.
3. Heterocyclic Chemistry, J.A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
4. Heterocyclic Chemistry, T.L., Gilchrist, Longman Scientific Technal.
5. Contemporary Heterocyclic Chemistry, G.R. Newkome and W.W. Paudler, Wiley-Inter Science.
6. An Introduction to the Heterocyclic Compounds, R.M. Acheson, John Wiley.
7. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergamon Press.

### **Group C**

### **Elective Paper-III**

## **CH-205C: CHEMISTRY OF NATURAL PRODUCTS**

### **UNIT I**

#### **Terpenoids and Carotenoids**

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule, biosynthesis.

Structure determination, synthesis of the following representative molecules: Citral, Geraniol,  $\alpha$ -Terpeneol, Zingiberene, Phytol, Abietic acid and  $\beta$ -Carotene.

## UNIT II

### 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, biosynthesis.

Structure, synthesis of the following: Ephedrine, (+)-Cocaine (conine), Nicotine, Quinine and Morphine.

## UNIT III

### Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon, Stereochemistry biosynthesis. Isolation, structure determination of Cholesterol and Bile acids.

## UNIT IV

### Plant Pigments

Occurrence, nomenclature and general methods of structure determination. Isolation structure and synthesis of Apigenin, Luteolin, Quercetin, Myricetin, Vitexin, Diadzein, Butein, Aureusin, Cyanidin, Hirsutidin.

Biosynthesis of flavonoids : Acetate pathway and Shikimic acid pathway.

## UNIT V

### Porphyrins

Structure of Haemoglobin and Chlorophyll.

### Prostaglandins

Occurrence, nomenclature, classification, physiological effects. Synthesis of PGE<sub>2</sub> and PGF<sub>2α</sub>

### Pyrethroids and Rotenones

Structure and reactions.

### Books Suggested:

1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe and J.B. Harborne, Longman, Essex.

2. Organic Chemistry, Vol. 2 I.L. Finar, ELBS.
3. Stereoselective Synthesis: A Practical Approach, M. Nogradi, VCH.
4. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
5. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.
6. Introduction to Flavonoids, B.A. Bohm, Harwood Academic Publishers.
7. New Trends in Natural Product Chemistry, Atta-ur-Rahman and M.I. Choudhary, Harwood Academic Publishers.
8. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

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## Group C

### Elective Paper-IV

#### **CH-206C: ENVIRONMENTAL CHEMISTRY**

##### **UNIT I**

###### **Environment; An Introduction, Atmosphere & Air Pollution**

Concept & scope of Environmental chemistry; Environmental segments; Environmental Pollution; Classification of pollutants; Bio-geological cycles in the environment: Hydrological cycle, C, N, O, S and P cycles in the environment; Bio-distribution of elements;

Structure and Composition of Atmosphere; Particles, Ions & Radicals in the atmosphere; Major sources of Air Pollutants.

Pollution by C, CO, NO<sub>x</sub>, SO<sub>x</sub>, HC, Acid Rain, Smog, Particulates; Green House effect/Global Warming, Ozone Layer; Effects & Control of Air Pollutants; Air quality standards; Sampling, Monitoring.

##### **UNIT II**

###### **Hydrosphere & Water Pollution**

Aquatic environment, Chemical composition of water bodies; Lakes, Streams, Rivers.

Classification of water pollution; Pollution by Pesticides, Polymers, Detergents, Agriculture and Sewage wastes; Purification and Treatment of water;

##### **UNIT III**

###### **Lithosphere: Soil Pollution**

Introduction: Soil formation, composition & classification; Acid-Base and Ion-exchange reactions in Soil; Macro- and Micronutrients, Soil Profile; Soil fertility and Productivity, Soil erosion, Soil Analysis (Moisture, Nitrogen & pH).

Soil Pollution: Sources & Classification, Effects of Pesticides, Fertilizers & Sediments, Control of soil pollution.

##### **UNIT IV**



## **Industrial Pollution & Toxicology**

Classification, Nature and treatment of Industrial Effluents, Industrial Effluents from Distillery, Textile, Cement, Electroplating, Paper & pulp, Dairy & Detergent, Fertilizers, Tanning, .

Toxic Chemicals in the Environment, Biochemical Effects of Ozone, PAN, Carcinogens, Cyanides, Pesticides, Natural & Man-made Disasters.

Solutions to Environmental Problems; Preventive Environmental Management, Better Industrial Processes.

## **UNIT V**

### **Green Chemistry**

Principles and Goals of Green Chemistry, Green chemicals, reagents, catalysts, and solvents. Examples of green synthesis / reactions, Microwave assisted synthesis.

### **Books Recommended/Suggested**

1. Environmental Chemistry: Edited by J. O'M. Bockris, Plenum Press.
2. Environmental Chemistry: S.E. Manahan, Lewis Publications.
3. Environmental Chemistry: H. Kaur, Pragati Prakashan.
4. Environmental Chemistry: AK Day, New Age Int. Publishers.
5. Environmental Chemistry: SM Khopkar, Wiley Estern.
6. Physico-chemical Examination of Water, Sewage & Industrial Effluents: K. Manivasakam.
7. An introduction to Green Chemistry, V Kumar, Vishal Publ..

## Group D

### Elective Paper-I

#### **CH-203D: NUCLEAR AND RADIOCHEMISTRY**

##### **UNIT I**

Stability of the nucleus, Mass Energy relationship for nuclear reactions, Properties of nucleus, Nuclear Models (The shell model, the liquid drop model, the fermi gas model, the collective model and the optical model).

Nuclear reactions, Energetics of nuclear reactions, fission and fusion reactions, spallation, fragmentation, stripping and pick up reactions, photonuclear and thermonuclear reactions.

##### **UNIT II**

Interaction of radiation with matter, passage of neutrons through matter, interaction of radiation with matter; measurement of radiations. Radiolysis of water, counting techniques (GM Ionisation, proportional and scintillation counter), counting statistics.

##### **UNIT III**

Applications of radioactivity, Activation Analysis, isotopic dilution analysis, radiometric titrations, application in chemical investigations and synthesis in physiochemical analysis, in age determination and in prospecting of natural resources. Medical agricultural and industrial applications, source of electricity. Radiation hazards and protection.

##### **UNIT IV**

Nuclear reactors: Basic features, materials and design of nuclear power reactors, Conversion and Breeding, safety features of reactors, Health Physics: Radiation unit (exposure unit), External and doses from various sources of radiations, allowed limit of intake (ALI)

## UNIT V

Applications of radioisotopes in biology & molecular biology: biodistribution, metallic & biochemical pathways for protein synthesis, purine nucleotide synthesis, role of methionine in research, radioligand assay, autoradiography, primer extension, Nick translation , hybridization, nucleic acid sequencing.

### Books Recommended:

1. Essentials of Nuclear Chemistry, H.J. Arnikar.
2. Introduction to Nuclear Science, M.W. Sarton, East West Edition.
3. Theory of Nuclear Structure, M.K. Pal, East West Edition.
4. Principles of Radiochemistry, G.W.A. Newton and V.J. Robinson, Macmilan Education Ltd.
5. Nuclear Chemistry, A. Vertes and I. Kiss.
6. Fundamental of radiation Chemistry, A. Mojumdar, J. David, Morrisey, G. T. Seaborg
7. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J.Holler. Publ. W B Saunders.

## Group D

### Elective Paper-II

#### **CH-204D: MEDICINAL AND PHARMACEUTICAL CHEMISTRY**

##### **UNIT I**

Drug design & Pharmacodynamics

Procedure followed in drug design, Concepts of lead compound and lead modification, concepts of pro drugs & soft drugs, structure-activity relationship(SAR), Theories of drug activity : occupancy theory, rate theory, induced fit theory .

An Introduction of pharmacodynamics, Mechanism of drug action, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides , drug metabolism

##### **UNIT II**

**Antineoplastic agents :**

Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors.

Synthesis of cyclophosphamide , Uracil and mustards .

##### **UNIT III**

**Cardiovascular Drugs :**

Introduction , Cardiovascular diseases, drug inhibitors of peripheral sympathetic function , Synthesis of amyl nitrite, sorbitrate, Methyldopa and atenolol.

## UNIT IV

### Drugs: Psychotic and Antipsychotic –

Introduction, CNS depressants, general anaesthetics, mode of action of; hypnotics, sedatives, anti-anxiety drugs. Anti depressants, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, alprazolam and barbiturates..

## UNIT V

### Antibiotics :

Cell wall biosynthesis , inhibitors ,  $\beta$ -lactam rings , antibiotics inhibiting protein synthesis , synthesis of penicillin –G , penicillin – V, Chloramphenicol and Tetracyclin.

### Books Suggested:

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

## Elective Paper-III

### **CH-205D: PHYSICAL ORGANIC CHEMISTRY**

#### **UNIT I**

##### Principles of Reactivity

Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory. Uses of activation parameters, Hammond's postulate. Potential energy surface model. Reactivity and selectivity principles.

#### **UNIT II**

##### Kinetic Isotope Effect and Structural Effects:

Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

Linear free energy relationships (LFER) The Hammett equation, substituent constants, theories of substituent effects. Interpretation of  $\sigma$ -values. Reaction constant  $\rho$ . Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model,  $\sigma$  I- and  $\sigma$  R-scales.

#### **UNIT III**

##### Solvation and Solvent Effects

Qualitative understanding of solvent-solute effects on reactivity. Thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria. Various empirical indexes of solvation based on physical properties, solvent-sensitive reaction rates, spectroscopic properties and scales for specific solvation.

#### **UNIT IV**

##### Steric and Conformational Properties

Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation, Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

#### **UNIT V**

##### Nucleophilic and Electrophilic Reactivity

Structural and electronic effects on SN1 and SN2 reactivity. Solvent effects. Kinetic isotope effects. Intramolecular assistance. Electron transfer nature of SN2 reaction. SRN1 mechanism. Electrophilic reactivity, general mechanism. Kinetic of SE2-Ar reaction. Structural effects on rates and selectivity.

**Books Suggested:**

1. Molecular Mechanics, U. Burkert and N.L. Allinger, ACS Monograph 177,1982.
2. Organic Chemists' Book of Orbitals. L. Salem and W.L. Jorgenses, Academic Press.
3. Mechanism and Theory in Organic Chemistry, T.H. Lowry and K.C. Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular, Modeling, W.B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N.S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry, Concepts and Perspectives, J.M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

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## Group D

### Elective Paper-IV

#### **CH-206D: CHEMISTRY OF MATERIALS**

##### **UNIT I**

###### **Multiphase Materials**

Classification and properties of materials, Types of phase diagrams, Isomorphous, Eutectic, Peritectic, Monotectic and Eutectoid systems, Calculation of phase amounts from a phase diagram, Phase rule, Ferrous alloys Fe-C phase diagram, Non Ferro alloys, Phase diagrams of brass and tin bronze.

##### **UNIT II**

###### **Ceramic Materials**

Raw materials of glass, Cement and Ceramics, Refractories, Characterization, Properties and Applications, Abrasives, kinds and uses, Powder metallurgy, Manufacturing process, Properties and Applications, Advantages and Limitations.

##### **UNIT III**

###### **Composite Materials**

Traditional composites, concrete, Asphalt and Wood, Synthetic composites, dispersion reinforced, Particle reinforced, Laminated and fiber reinforced composites, applications of composites.

##### **UNIT IV**

**Polymeric and advanced materials** : Brief idea of following :Insulating material, Semiconductors, Superconductors, Fullerenes, Optical fibers, Organic electronic material.

##### **UNIT V**

**Environmental effects of Materials** : Corrosion mechanisms of dry and wet corrosion, Galvanic and concentration cell corrosion, Pitting and stress corrosion, Corrosion control methods, Types, preparation and uses of adhesives, Types and Application of paints and Pigments.

###### **Books Suggested:**



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

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## Marking Scheme for Practicals II YEAR

### Lab Course CH-207

#### Inorganic

- |   |          |
|---|----------|
| 1. Gravimetric Analysis<br>OR<br>Rare earth Mixture | 25 Marks |
| 2. Inorganic Preparation                            | 15 Marks |

#### Analytical

- |                    |          |
|--------------------|----------|
| 1. Instrumental-I  | 20 Marks |
| 2. Instrumental-II | 10 Marks |
| 3. COD/DO etc      | 10 Marks |

#### Organic

- |  |          |
|--|----------|
| 1. Mixture three components                | 20 Marks |
| 2. Extraction<br>OR<br>Organic Preparation | 10 Marks |
| 3. Spectroscopy                            | 10 Marks |

#### Physical

- |                     |          |
|---------------------|----------|
| 1. Major Experiment | 25 Marks |
| 2. Minor Experiment | 15 Marks |

Viva	20 Marks
Record	20 Marks
Total	200 Marks

## LABORATORY COURSE CH-207

### INORGANIC

I. Preparation of some Inorganic coordination compounds/ Complexes.

II. Analysis the given mixture for four rare elements.

III. Estimation of three constituent in the given sample of alloy / Coin (Two gravimetrically and one volumetrically).

### IV. Spectrophotometry

a. Iron- phenanthroline complex: Job's Method of continuous variations.

b. Find out the stability constant of metal complexes by Bjerrum's Method.

### V. Complexometry

a. Estimate Zn in given tablet/ sample complexometrically using xylenol orange as an indicator.

b. Estimate Ni in given sample complexometrically using mureoxide as an indicator.

### ANALYTICAL

#### I. pH metry:

1. To determine the dissociation constants of dibasic and tribasic acids.

2. Titration of mixture of acids (HCl + CH<sub>3</sub>COOH) against strong base.

#### II. Spectrophotometry:

1. Determination of  $P_{ka}$  of an indicator (e.g. methyl red) in (a) aqueous and (b) micellar media.

2. Determination of stoichiometry and stability constant of inorganic (e.g. Iron– salicylic acid) and organic (e.g. Amine – Iodine).

3. To determine the concentration of chromium and Complexes a binary mixture.

### **III. Polarography:**

1. To study oxygen wave by polarography.
2. To characterize and determine  $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$  and  $\text{Zn}^{2+}$  ions by polarography/ cyclic voltammetry

### **IV Fluorometry**

1. Determination of strength of Vitamin B (Riboflavin) and Aluminium.

### **V. Nephelometry**

1. Determination of sulphate content in water sample.
2. Determination of phosphate content in water sample.

### **VI. Flame photometry**

1. Estimation of Mg, K and Ca.
2. Estimation in a mixture (Na and K; K and Ca).

### **VII. Water and Waste Water examination:**

1. DO and BOD determination.
2. COD estimation.
3. Fluoride and nitrate determination.

### **VIII. Cement Analysis**

### **IX. Chromatography: Column**

#### **Books Suggested:**

1. Systematic Qualitative Organic analysis by H. Middleton.
2. Qualitative and Quantitative hand book of Organic analysis by H. Clark
3. Vogel's Text book of practical Organic Chemistry by Vogel

# ORGANIC

## I. Qualitative Analysis

Separation, purification and identification of three components of a mixture of organic compounds (three solids or two liquids and one solid, two solids and one liquid).

## II. Multi-step Synthesis of Organic Compounds

Benzophenone → Benzpinacol → Benzpinacolone

→ Benzophenone → Benzophenone oxime → Benzanilide

Benzoin → Benzil → Benzilic acid

Skraup synthesis: Preparation of quinoline from aniline.

Synthesis using microwaves

To carry out oxidation of alcohols and oxime by PCC.

Synthesis using phase transfer catalyst

Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide.

## III. Extraction of Organic Compounds from Natural Sources

1. Isolation of caffeine from tea leaves.
2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and  $R_f$  value reported).
4. Isolation of piperine from black pepper.
5. Isolation of lycopene from tomatoes.
6. Isolation of  $\beta$ -carotene from carrots.

7. Isolation of eugenol from cloves.

#### **IV. Paper Chromatography / TLC**

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R<sub>f</sub> values.

#### **V. Spectroscopy**

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

##### **Spectrophotometric (UV/VIS) Estimations**

1. Amino acids
2. Proteins
3. Carbohydrates
4. Ascorbic acid
5. Aspirin
6. Caffeine

##### **Books Suggested:**

1. Systematic Qualitative Organic analysis by H. Middleton.
2. Qualitative and Quantitative hand book of Organic analysis by H. Clark
3. Vogel's Text book of practical Organic Chemistry by Vogel
4. Practical Organic Chemistry by N.K. Vishnoi.

# PHYSICAL

## I. Chemical Kinetics

- (i) To investigate the kinetics of the reaction between  $I^-$  and persulphate ion
  - (a) Order of the reaction
  - (b) Energy of activation of the reaction.
  - (c) Effect of ionic strength on rate.
- (ii) To find out the order of the reaction of saponification of ester using unequal concentrations of reactants.

## II. Chemical kinetics

- (i) To investigate the kinetics of the reaction between ceric ammonium sulfate and glycollic acid.
  - (a) Order with respect to ceric ion.
  - (b) Order with respect to glycollic acid.
  - (c) Energy of activation of the reaction.
  - (d) Effect of ionic strength on rate.
- (e) To study the reaction between ceric ammonium nitrate and primary alcohol.

## II. Thermodynamics

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

## III. Phase Equilibrium

- (i) To find out the equilibrium constant for the triiodide formation:

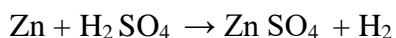
- (ii) To find the formula of complex cuprammonium ion by distribution method.

#### IV. Conductometry

- (i) To find out the equivalent conductance of strong electrolytes at different dilutions and to verify Debye Huckel Onsagar equation.
- (ii) To determine the equivalent conductance of a weak electrolyte at infinite dilution.
- (iii) To determine the dissociation constant of acetic acid/Oxalic acid and verify the Ostwald's dilution law.
- (iv) To determine the degree of hydrolysis and hydrolysis constant of ammonium chloride at room temperature.
- (v) To determine the activity coefficient of zinc ions in the solution of 0.002 M ZnSO<sub>4</sub> using Debye-Huckel's Limiting Law.
- (vi) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by NaOH conductometrically.
- (vii) To determine the solubility and solubility product of sparingly soluble salt (PbSO<sub>4</sub>, BaSO<sub>4</sub>)

#### V. Potentiometry/pH metry

- (i) To determine the dissociation constants of weak acids (oxalic, tartaric, phosphoric) using pH meter.
- (ii) To determine the temperature dependence of emf of a cell.
- (iii) To determine the degree of hydrolysis of aniline hydrochloride for three different solutions at room temperature and hence calculate the hydrolysis constant of the salt and dissociation constant of the base.
- (iv) To study the acid-base titration in a non-aqueous media using a pH meter.
- (v) To find out thermodynamic constants  $\Delta G$ ,  $\Delta S$  and  $\Delta H$  for the reaction by emf measurements.





**Books suggested:**

1. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
2. Findley's Practical Physical Chemistry, B.P. Levitt, Longman.
3. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
4. Advanced Practical Physical Chemistry, J.B. Yadav, Goel Publishing House.
5. Advanced Experimental Chemistry, vol.1 – Physical J.N. Gurtu and R. Kapoor, S. Chand & Co.

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