

## Shivaji University, Kolhapur

## Department of Chemistry

## M.Sc. Part-II (sem-III and IV) Chemistry

(Inorganic, Organic, Physical and Analytical)

**Revised Syllabus** 

### **Choice Based Credit System Pattern**

To be implemented from June- 2019

Applicable for University Department and Affiliated Colleges PG Center

## M.Sc. Part-II, (Sem-III and IV) Inorganic Chemistry <u>SEMESTER-III</u>

Paper No-IX, ICH 3.1	: INORGANIC CHEMICAL SPECTROSCOPY
Paper No. –X, ICH 3.2	: COORDINATION CHEMISTRY – I
Paper No. –XI, ICH 3.3	: NUCLEAR CHEMISTRY
ELECTIVE PAPERS	
Paper No. –XII(A), ICH 3.4(A)	) : ORGANOMETALLIC AND BIOINORGANIC
	CHEMISTRY
Paper NoXII(B), ich $3.4(B)$	: SELECTED TOPICS IN INORGANIC
	CHEMISTRY
Practical Course	: ICHP-V and ICHP- VI

### **SEMESTER-IV**

Paper No. –XIII, ICH 4.1	: INSTRUMENTAL TECHNIQUES.
Paper No. – XIV, ICH 4.2	: COORDINATION CHEMISTRY-II
Paper No. –XV, ICH 4.3	: CHEMISTRY OF INORGANIC MATERIALS
ELECTIVE PAPERS	
Paper No. –XVI(A), ICH 4.4(A)	: ENERGY AND ENVIRONMENTAL CHEMISTRY
Paper No. –XVI(B), ICH 4.4(B)	: RADIATION CHEMISTRY
Practical Course	: ICHP - VII and ICHP-VIII

### M.Sc. Part-II (Sem- III) Inorganic Chemistry

### Paper No. –IX, ICH 3.1: Inorganic Chemical Spectroscopy

#### **Unit I: Molecular Symmetry and Group Theory**

Introduction to Symmetry, Symmetry operations, Symmetry elements, Point group and its classification (Cn-type, Dn-type, Special-type), Schoenflies symbol for point groups, Determination of point group for AB<sub>2</sub> (Bent), AB<sub>3</sub> (Trigonal pyramid), AB<sub>3</sub> (Trigonal Planar), AB<sub>4</sub> (Square planar), AB<sub>5</sub> (Trigonalbipyramidal), AB<sub>6</sub> (Octahedral), CO<sub>2</sub>, HCl, CO, Ortho–, meta– & para–disubstituted benzene molecules. Symmetry and dipole moment of molecule, Symmetry and optical activity, Group and its Properties, Group multiplication table, Matrix representation of symmetry elements, Reducible and Irreducible representations, Character of a representation (character of matrix), Properties of Irreducible representation, Great orthogonally theorem (without proof) and its importance, Construction of character table for  $C_{2v}$  C<sub>3v</sub> point groups, Mulliken symbolism rules for irreducible representations & its illustrations, Direct product, Standard reduction formula.

### Unit II: IR and Raman Spectroscopy

**A) Infrared spectroscopy:** The vibrating diatomic molecule, The simple harmonic oscillator, The anharmonic oscillator, The diatomic vibrating rotator, Vibration– rotation spectrum of carbon monoxide, Breakdown of Born–Oppenheimur approximation, The vibration of polyatomic molecules, Overtones and combination frequencies, The influence of rotation of the spectra of polyatomic molecules, Techniques and Instrumentation, Applications.

**B)** Raman spectroscopy: Classical and Quantum theory, Pure rotational Raman Spectra, vibrational Raman spectra, Rule of mutual exclusion, Overtone and combination vibrations, Rotational fine structure, Outline of technique and instrumentation, Applications.

Modes of vibrations, Selection Rules for Infrared and Raman Spectra, Normal modes of vibrations in  $AB_2$  (Linear/Bent),  $AB_3$ ,  $AB_4$ ,  $AB_5$ , Octahedral  $AB_6$  molecules with factors affecting band frequencies.

### Unit III:

#### Mass Spectroscopy:

Basic principle, Instrumentation, Electron-impact Induced and Fast Atom Bombardment (FAB) spectrometry, qualitative and semiquantitative theories including QET, concept of metastable ions transitions, Stevensons's rules. Applications to metal compounds containing carbonyl, alkyl, cyclopentadienyl and acetylacetonate.

### 15 Hrs.

#### 15 Hrs.

#### 15 Hrs

### Unit IV:

### A) NMR Spectroscopy:

Principle Instrumentation of NMR, the chemical shift, mechanism of electron shielding and factors contributing to the magnitude of chemical shift. Local & remote effect, spin-spin splitting, applications of spin coupling to structural determination, double Resonance techniques. The contact and Pseudo contact shifts Factors affecting nuclear relaxation, an overview of NMR of metal nucleus with emphasis on <sup>195</sup>Ag &<sup>119</sup>Sn NMR, applications of solid-state NMR technique.

### B) X-ray Photo electron Spectroscopy (XPS)

Introduction and basic theory, Instrumentation, sample selection and preparation, spectral analysis, Ar ion sputtering technique and applications of XPS.

### **Reference Books:**

- 1. K. Burger, Coordination Chemistry-experimental methods, Butterworth's
- 2. R. Drago: Physical method in Inorganic Chemistry, DUSAP.
- 3. Hill & Day advanced methods in Inorganic Chemistry, J.Weily
- 4. F.A. Cotton, chemical application of group theory, Weily eastern
- 5. Figgis, Introduction to ligand field theory field
- 6. Schaefer & Gilman: Basic principles of ligand field Theory, J. Wiely
- 7. P.R. Backer: Molecular symmetry and Spectroscopy A.P.
- 8. Ferraro Ziomeek, Introduction to Group theory, plenum
- 9. Scotland Molecular symmetry DVN
- 10. Dorian: symmetry in Chemistry EWAP
- 11. Hall: Group theory and symmetry in Chemistry MGLt
- 12. Nakamoto Infrared R Raman Spectra of Inorganic & Coordination compounds J.Weily
- 13. Nakanisha: Spectroscopy and structure J. Weily
- 14. Ferroro: Metal ligand and related vibrations
- 15. CNR Rao Spectroscopy in Inorganic Chemistry Vol I, II, III
- 16. Durie: vibrations spectra and structure Vol. I to IV, Elsevier
- 17. Dudd, chemical Spectroscopy Elsevier
- 18. Popel: H.N.M.R. Spectroscopy J.Weily
- 19. R.J. Abraham, J.Fisher and P Loftus Wiley Introduction to NMR spectroscopy.
- 20. P.K. Bhattacharya: Group Theory & Its Chemical Applications
- 21. K.V. Reddy: Symmetry & spectroscopy of Molecules.
- 22. M. R. Litzow and T R Spelding, Mass Spectroscopy of Inorganic & Organometallic Compounds, Elsevier,73

### 7 Hrs

8 Hrs

### Paper No.-X, ICH 3.2: Coordination Chemistry-I

### Unit I

### Metal-ligand bonding:

Crystal Field Theory: Splitting of d-orbital in tetragonal, square planar and trigonal bipyramid complexes. CFSE-factors affecting the magnitude of 10 Dq-evidence for crystal field stabilization, tetragonal distortion from octahedral symmetry, John teller effect, nephelauxetic effect. CFSE and their uses, factors affecting CFSE, Limitations of crystal field theory. M.O. theory for octahedral, tetrahedral and square planar complexes with and without  $\pi$ -bonding.

### Unit II

### Electronic spectra of Transition Metal complexes:

Determining the Energy terms, Spin-orbit (L-S) coupling scheme, Hund's rule, Derivation of the term symbol for a d<sup>1</sup> to d<sup>9</sup> configuration, Electronic spectra of transition metal complexes – Laporte 'orbital' selection rule, spin selection rule. Orgel diagrams for octahedral metal complexes. Racah parameters, calculations of 10 Dq, B and  $\beta$  parameters for octahedral complexes of cobalt and nickel, Tanabe-Sugano diagrams for octahedral complexes, Charge transfer spectra, Selection rule and charge transfer spectra

### Unit III

### Magnetic properties of Transition metal complexes: :

Types of magnetic behaviour, origin of paramagnetism, Spin-orbit interaction, Lande interval rule, Diamagnetism, Pascal constants, Ferromagnetism and antiferromagnetism of metal complexes; temperature dependent paramagnetism, Van Vleck's equation, Its derivation and applications, magnetic anisotropy, anamoulous magnetic moment, Quenching of orbital moment, Spin orbit coupling and magnetic moment, Determination of magnetic susceptibility. Spins crossover phenomenon

### Unit IV

### **Mixed Ligand complexes**

Stabilities of ternary complexes, Dynamics of formation of ternary complexes reaction of Coordination ligand in ternary complexes, Mimicking reactions in biological systems, enzyme models, Amino acids ester hydrolysis, peptide synthesis & hydrolysis, Decarboxylation of  $\beta$ -keto acids, Applications of mixed ligand complexes in catalysis.

### **Reference Books:**

- 1. Jones: Elementary Coordination Chemistry. J. Weily
- 2. Graddon: Introduction to Coordination Chemistry. J. Weily
- 3. Drago: Physical methods of Inorganic Chemistry. J. Weily.
- 4. Graddon: Introduction to coordination Chemistry, Parasmom
- 5. Lewis and Wilkins: Coordination Chemistry. J. Weily
- 6. Msrtel: Coordination Chemistry Vol I, II VNR
- 7. Earnshaw: Introduction to Magneto Chemistry
- 8. Mabbs & Machin Magnetism & transition metal complexes Chamman hall
- 9. Calvin, Magnetic properties of transition metal complexes.

### 15 Hrs

15 Hrs

### 15 Hrs.

15 Hrs.

- 10. L.N. Maley: Magneto Chemistry
- 11. Datta & Shymlal: Elements of Magneto Chemistry
- 12. Martel & Taqui Khan: homogeneous catalysis with metal complexes Vol.I & II AP.
- 13. James E. Huheey: Inorganic Chemistry Principles of Structure and reactivity, Harber and Row, Publishers Inc. New York 1972.
- 14. K.P. Purcell & J.C. Kote: An Introduction to Inorganic Chemistry Holt Sounders, Japan 1980.
- 15. William L. Jolly: Modern Inorganic Chemistry, Mecgrow Hill USA, 1984
- 16. F.A. Cotton & R.G. Wilkinson: Advanced Inorganic Chemistry

### Paper No. –XI, ICH 3.3 : Nuclear Chemistry

### UNIT-I:

### Systematic of alpha, beta and gamma decays

Alpha decay, energy curve, spectra of alpha particles, Giger-Nuttal law, theory of alpha decay, penetration of potential barrier, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect

### UNIT-II:

### Nuclear Structure and Stability

Binding energy, empirical mass equation, The nuclear models, the liquid drop model, Single particle shell model, Fermi gas model & collective/lunified nuclear model, nuclear spin, parity & magnetic moments of odd mass number nuclei and numerical.

### Unit III

### Nuclear reactions and Nuclear fission

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and a symmetric fission, decay chains and delayed neutrons

### **UNIT-IV:**

### **Reactor Theory and Applications of Radioactivity**

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

Tracer technique in the field of analytical chemistry structure determination elucidation of reaction mechanism, isotopic dilution analysis, neutron activation analysis applications in

biological, medical, industrial fields, Age determination.

### **Reference Books**

- 1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley
- 2. B. G. Harvey, Nuclear Chemistry
- 3. Hassinsky: Translated by D. G. Tuck, Nuclear Chemistry and its application: Addison Wiley
- 4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry
- 5. Maeclefort: Nuclear Chemistry: D. Van Nostrand
- 6. An N. Nesmeyannoy: Radiochemistry: Mir
- 7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V. Nost & EWAP
- 8. N. Jay: Nuclear Power Today Tomorrow: ELBS
- 9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
- 10. Essentials of Nuclear Chemistry, W. J. Arnikar, John Wiley
- 11. Nuclear and Radiation Chemistry: B. K. Sharma, Krishna Publication
- 12. A Introduction to Nuclear Physics: R. Babber. And Puri.
- 13. Essential of Nuclear Chemistry by H. J. Arnikar

### Paper No. –XII(A), ICH 3.4(A) : Organometallic and Bioinorganic Chemistry

### **Unit I: Organotransition Metal Chemistry:**

Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways of alkyls and aryls of transition metals. Organocopper in Organic synthesis. Compounds of Transition Metal –Carbon Multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes–synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on ligands, role in organic synthesis.

### **Unit-II: Transition Metal Pi-complexes**

Carbon multiple bonds. Nature of bonding, structural characteristics & synthesis, properties of transition metal Pi-Complexes with unsaturated organic molecules, alkenes alkynes, allyl, diene, dienyl, arene and trienyl complexes. Application of transition metal, organometallic intermediates in oraganic synthesis relating to nucleophilic and electrophilic attack on ligands, role in organic synthesis.

### Unit III: Metal Compounds in Medicine

Medicinal use of metal complexes as antibacterial, anticncer, use of cis-platin as antitumor drug, antibiotics & related compounds. Metal deficiency and disease, iron deficiency, zinc deficiency and copper deficiency, Metal used for dignosis and chemotherapy with particular reference to anti cancer drugs. Chelate therapy, chemotherapy with compounds of some non essential elements; platinum complexes in cancer therapy. Antiviral activity of metal complexes. Gold containing drugs used in the therapy of Rheumatic-Arthritis, Gold complexes as anticancer drug. Lithium in psycho pharmacological drugs. Antimicrobial agents

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### 15 Hrs

### 15 Hrs

15 Hrs

### **Unit-IV: Oxygen Transport and Storage**

Heme proteins and oxygen uptake, structure and functions of haemoglobin, myoglobin, hemocyanins & hemerythrin. Perutz mechanism for structural changes in porphyrin ring system, Oxygenation and deoxygenation. Oxygen adsorption isotherm and cooperativity, physiological significance of haemoglobin, role of globin chain in gaemoglobin, Cyanide poisoning and treatment.

### **Reference Books**

- 1. Yamamoto, Organo Transition Metal Chemistry, Wiley (1986).
- 2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals (4th edn.), John Wiley (2005).
- 3. A. J. Pearson. Metallo-Organic Chemistry, John Wiley & Sons (1985).
- 4. M. Bochmann. Organometallics-I Complexes with Transition Metal-Carbon σ-Bonds, Oxford Chemistry Primers (1994).
- 5. Principles of Biochemistry, A. L. Lehinger, Worth Publications.
- 6. Biochemistry, L. Stryer, W. H. Freeman
- 7. Biochemistry, J. David Rawn, Neil Patterson.
- 8. Biochemistry, Voet and Voet, John Wiley.
- 9. Outlines of Biochemistry, E. E. Conn and P. K. Stumpt, John Wiley.
- 10. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford Univ. Press, 1990.
- 11. J. E. Huheey, E. A. Keiter and R.L. Keiter Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education, 2004.
- 12. F. A. Carey G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley Interscience, 2003
- 13. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Univ. Science Books, 1994.
- 14. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life (An introduction and Guide), John Wiley & Sons, 1994.
- 15. Zagic: Microbial Biogeochemistry, Academic press

### Paper No. –XII(B), ICH 3.4(B) : Selected Topics in Inorganic Chemistry

### **UNIT-I: Catalysis**

### 15 Hrs

15 Hrs

Basic principals, thermodynamic and kinetic aspects, industrial requirements, classification, theories of catalysis, homogeneous and heterogeneous catalysis. Introduction, types & characteristics of substrate-catalyst interactions, kinetics and energetic aspects of catalysis, selectivity, stereochemistry, orbital symmetry and reactivity. Catalytic reactions of coordination and Organometallic compounds including polymerization activation of small molecules, addition to multiple bonds, hydrogenation, Zeigler-Natta polymerization of olefins, monsanto acetic acid process.

### **UNIT-II: Coordination Polymers**

Natural polymers and reactions yielding coordination polymers. Synthesis of coordination

polymers. Use of polymeric ligands in synthesis of coordination polymers. Metal coordination polymers. Silicon polymers. Organosilicon polymers: synthesis and their uses

### **UNIT-III: Non-conventional sources of energy**

### 15 Hrs

a) Alternate source of energy

Solar sources: Photochemical methods, thermodynamic efficiency of energy conversion, energy from solar radiations, transition metal complexes for energy production, solar hydrogen system, photochemical processes at semiconductors electrodes, photo galvanic and Photovoltaic cells based on Inorganic photochemical systems.

- b) Geothermal energy
- c) Energy from biogas sources, biodiesel,
- d) Tidal wind sources
- e) Energy from fission and fusion reaction.

### Unit-IV Supramolecular Chemistry:

Concepts and principles, Host-Guest Chemistry, Non-covalent bonds, crown ethers, cryptands and their metal complexes, Molecular recognition for different types of molecules, spherical recognition, Tetrahedral recognition, cooperativity and multivalency, Design and synthesis of co-receptor molecules and multiple recognition, supramolecular reactivity and catalysis, supramolecular devices, supramolecular photochemistry

### **Reference Books**

- 1. Heterogeneous catalysis 2nd edn. Bond C. Chapman all (1987).
- 2. The application & Chemistry of catalysis by suitable transition metal complexes Parashall. W. Weily N. 1980.
- 3. Homogeneous transition metal catalysis, A general art, Masters C. Chapman and Hall, London 1981.
- 4. Introduction to the principles of heterogeneous catalysis, Thomas J.M., Thomas W.J. Academic press N.Y. 1967
- 5. Inorganic polymers: Mark J.F., Allock H.R. West, Prentice hall
- 6. Inorganic polymers: Ring N.H., Academic Press N.Y. 1978
- 7. The Inorganic heterocyclic chemistry of sulphur, nitrogen, phosphorous, Heal A.G. Acta, Press N.Y. 1980.
- 8. Solar energy Principles of thermal collections and storage, Sukhatme S.P., Tata Macgrow Hill New Delhi 1984.
- 9. Fuel Cells, Bockeris JOM, Sriniwasan S. and Mac grow Hills 1969
- 10. Solar Energy Rai C.D.
- 11. Energy Resources, Simon A.L. 1975
- 12. Direct Energy Conversion, Addison Wesley, 1970, All M and Kottani S.
- 13. Outlines in Chemical Technology Vol I, S.D. Sukla & Pandey G.N.M.

### 15 Hrs

### M.Sc. Part-II (Semester-III) Inorganic Chemistry Practical Course ICHP-V and ICHP-VI

- 1. Ore Analysis -3
- 2. Alloy Analysis 3
- 3. Preparation of coordination complexes
- 4. Ion exchange study of separation of mixtures and estimations
- 5. Spectrophotometry
- 6. Separation and estimation of ions using ion exchange chromatography
- 7. Nephelometry
- 8. Potentiometry
- 9. Conductometry
- 10. Thermal analysis
- 11. Magnetic properties of transition metal complexes
- 12. Spectro Fluorimetry
- 13. Solvent extraction
- 14. Nuclear chemistry
- 15. Soil Analysis
- 16. Data analysis

(Any other experiments may be added when required)

# 11

### M.Sc. Part-II (Sem- IV) Inorganic Chemistry

### Paper No. –XIII, ICH 4.1: Instrumental Techniques

### **Unit I: X-ray Diffraction Techniques**

X-ray Sources (X-ray tube and synchrotron sources with their principle of working characteristics of emission spectrum), Bragg's law of diffraction, methods of diffraction (powder and single crystal), Powder diffraction: instrumentation, use of standards, characteristics of powder XRD pattern, significance of peak intensities, systematic absences of reflections, indexing of powder XRD pattern, determination of lattice parameters and solving cubic crystal structure using powder XRD data, qualitative (identification of the phases) and quantitative analysis (phase quantification), crystallite size determination, determination of relative % crystallinity. Single crystal diffraction: Advantages of single crystal diffraction over powder diffraction, introduction to Laue, rotation photograph and oscillation methods. Introduction to crystallographic database and file formats (raw data files, cif and pdf), Open source computer based crystal structure building and visualization tools.

### **Unit II: Mossbauer Spectroscopy**

Principle of Mossbauer spectroscopy, Recoiless absorption and emission of gamma-rays, Doppler shift, Instrumentation, Isomer shift and its factors affecting, Quadruple splitting, Temperature Dependence of MB parameters, Zeeman Splitting (Six fingered MB lines), MB spectra of iron and tin compounds, Applications, Numericals

### Unit III: Electron Spin Resonance Spectroscopy

Principle of ESR Spectroscopy, Presentation of spectrum, Hyperfine splitting in some proton systems, Rules for evaluating ESR lines (Naphthalene anion radical, Pyrazine anion radical, Isomers of Xylene anion radicals, VO<sup>2+</sup>, Quinoline radical, Isoquinoline radical, Quinoxaline radical, Anthracene radical, Phenanthracne radical, Pyrene radical, Alkyl halide radicals, Quinone & Isoquinone anion radicals, nitrogen/deuterium containing radicals), Superhyperfine splitting, Instrumentation, 'g' value and factors affecting it, Zero field splitting, Karmers's degeneracy, Applications, Numericals.

## Unit-IV: Introduction to Advanced Instrumental Tools for Analysis of Inorganic materials: 15 Hrs.

Time resolved studies of chemical reactions such as material synthesis (solid state, hydrothermal, sol/gel, thin film growth etc., cathode/anode materials in lithium ion batteries during charge/discharge cycles, in situ X-ray diffraction methods for thermal expansion/contraction studies, structural studies as a function of temperature and pressure (XRD methods), Temperature programmed techniques (temperature programmed desorption/oxidation/reduction: TPD/TPR), methods of determination of surface acidity and basicity of solid catalysts, Computer softwares for plotting and analysis of the XRD data, Structure drawing softwares (VESTA)

### 15 Hrs.

### 15 Hrs.

### 15 Hrs.

### **Reference Books**

- 1. Powder Diffraction Theory and Practice, Edited by R E Dinnebier and S J L Billinge, RSC publishing, 2008.
- 2. Catalysis, Principles and Applications, Editors: B. Viswanathan, S. Sivasanker, A.V. Ramswamy, Narosa Publishing House
- 3. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data, K. Momma and F. Izumi (2011), J. Appl. Crystallogr., 44, 1272-1276.
- 4. Elements of X-ray Diffraction, B.D. Cullity, Second Edition, Addison Wesley, 1978. Neutron Scattering in Chemistry, Baun, G.E. Butleworth, London, 1971.
- 5. Mossbaur Spectroscopy, Greenwood N.N., Gibbs T.C., Chapmann Hall, 1971.
- 6. Chemical Application of Mossbaur Spectroscopy, Goldanski V.I & Harber R.H., Academic Press 1968.
- 7. Spectroscopy in Inorganic Compounds CNR Rao & Ferraro G.R., Academic Press, 1970.
- 8. Basic Principles of Spectroscopy Cheney R.Mac Grows Hill, 1971.
- 9. Thermal Method, Wendlandt, W.W. John, Wiley, 1986.
- 10. Principles of Instrumental analysis, Skoog, III rd edn., Sounders, 1985.

### Paper No. –XIV, ICH 4.2: Coordination Chemistry-II

### Unit-I Reaction Mechanism of Transition Metal complexes-I

### 15 Hrs.

Energy profile of reaction. Inert and labile complexes, interpretation of liability and inertness of transition metal complexes on the basis of VBT and CFT. Factors affecting the liability of a complex, transition state or activated complex, substrate, attacking reagents electrophilic and nucleophilic, Nature of central atom. Reactions of metal complexes, ligand substitution reaction, Kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct & indirect evidences in favour of conjugate mechanism, anation reaction.

### Unit-II Reaction Mechanism of Transition Metal complexes-II 15 Hrs.

Substitution reaction in square planer complexes: the trans effect, Theories of Trans effect, uses of trans-effect, cis effect, Electron transfer reactions. Types of electron transfer reactions, conditions of electron transfer, and mechanism of one-electron transfer reactions, outer sphere and inner sphere mechanisms, two electron transfer reactions, complimentary and non-complimentary electron transfer reactions. Marcus Theory, Cross reactions, Inner sphere Reactions, Recimization and isomerisation in transition metal complexes.

### **Unit-III Photochemistry:**

Absorption, excitation, photochemical laws and quantum yield, Electronically excited states and their life-time measurement, Electronically excited states of Metal complexes, type of photochemical reactions, substitutions reactions, rearrangement reactions, redox reaction, Photochemistry of Coordination compounds, LMCT states and MLCT states, Charge transfer spectra, charge transfer excitations, methods for obtaining charge transfer spectra.

### **Unit-IV Applications of Coordination Compounds.**

#### 15 Hrs.

Metal Complexes in Analytical Chemistry Inorganic Qualitative Analysis, The 'brown ring' test, Complexometric Titrations, Complexes in Colourimetry, Coordination Compounds in Gravimetry, Stabilization of Oxidation States, Complexes in Separation of Metals. Metal Complexes in Medicinal Chemistry:-Complexation in Food Poisoning, Metal Complexes in Therapy. Metal Complexes in Industrial Processes:-Heavy Metals-protein Complexes in the Rasching Process, The Ziegler-Natta Catalyst, Metal complexes in alkene conversions, Complexes and Electroplating, Complexes in Metallurgy. Copper Metal dissolves in Aqueous Potassium Cyanide, Complexes in water softening. Metal complexes in Agriculture.

### **Reference Books:**

- 1. R. Gopalan and V. Ramlingam: Concise Coordination Chemistry.
- 2. J. E. Huheey, Ellen A. Keiter and Okhil K. Medhi: Inorganic Chemistry: Principle of Structure and Reactivity.
- 3. K. F. Purcell, J. C. Kotz: An Introduction to Inorganic Chemistry.
- 4. F. Basolo and R. Pearsons: Mechanism of Inorganic Reactions: A Study of Metal Complexes in Solution.
- 5. Obe, M. L. Inorganic reaction mechanism, Nelson, London, 1972.
- 6. Taube, electron transfer reactions of metal complex ions in solution. Academic Press, 1970.
- 7. E. S. Gould, Inorganic Chemistry.
- 8. V. Balzani and V. Cavassiti, Photochemistry of coordination compounds, AP, London, 1970.
- 9. K. Burger, Coordination Chemistry Experimental methods, Butterworths.
- 10. K. K. Rastogi and Mukharjee, Fundamentals of photochemistry, Wiley eastern.
- 11. J. G. Calverts and J. N. Pits, Photochemicals of Photochemistry, John Wiley.
- 12. Wells, Introduction to Photochemistry.
- 13. K. M. Macky, R. A. Macky, Modern Inorganic Chemistry, 4th edn., Blackie, London-1989.
- 14. B. R. Puri, L. R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, Vallabh Publications, Delhi,2005.

### Paper No. -XV, ICH 4.3: Chemistry of Inorganic Materials

### Unit-I: Solid State Materials

A) Bonding incrystals, Crystal systems and Bravais Lattice, Lattice planes and their designation.Metallic Crystal structures:Face-centered cubic (fcc), body-centered cubic (bcc), hexagonal close-packed (hcp) structure.Radius ratio rule (2, 3,4,6,8 co-ordinate structures), octahedral and tetrahedral voids.Isomorphism and polymorphism, Numericals.

#### 13

### 15 Hrs.

### **B)** Simple type structures:

*AB type:*NaCl, CsCl, Zincsulphide (sphalerite or cubic and hexagonal) , *AB*<sub>2</sub> *type:* Fluorite (CaF<sub>2</sub>), TiO<sub>2</sub>(Rutile), CdCl<sub>2</sub>, CdI<sub>2</sub> structures, *AB*<sub>3</sub> *type:* ReO<sub>3</sub>, BiI<sub>3</sub>, *A*<sub>2</sub>*B*<sub>3</sub> *type:* Corundum Al<sub>2</sub>O<sub>3</sub>,  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> ,Mn<sub>2</sub>O<sub>3</sub>., *ABO*<sub>3</sub>*type:* Perovskite Structures (Barium titanate, lead titanate, CaTiO<sub>3</sub>, FeTiO<sub>3</sub>), *AB*<sub>2</sub>O<sub>4</sub> *type-* Spinel structure, Normal & Inverse,Factors causing distortion in spinel, *A*<sub>2</sub>*B*<sub>2</sub>O<sub>7</sub> *type:* Pyrochlores (La<sub>2</sub>Sn<sub>2</sub>O<sub>7</sub>).

### **Unit-II: Imperfections in Materials**

### 15 Hrs.

Perfect &Imperfect crystals, point defects, Interstitial, Schottky defect, Frenkel defect, line defect & other entities, thermodynamics of Schottky& Frankel defects.

Dissociation, theory of dislocation, plane defects-Lineage boundary, grain boundary, stacking fault, 3D defects, Defects & their concentrations, ionic conductivity in solids, Non stoichiometric compounds.

Electronic properties of Non-stoichiometric oxides, solid electrolytes, pyknometric& electrical conductivity methods of study of defects, photoradiation effects on solid nature and properties, photography, colour centers, order-disorder changes, defects, imperfection equilibrium, atom movements, and defect interactions.

### Unit III :Synthesis and Characterization of Nanomaterials 15 Hrs

General Introduction to Nanomaterials, Nanoscience and nanotechnology, History.

**Chemical Methods**: Metal nanoparticles: Reduction method, Semiconducting or composite nanomaterials: Hydrothermal and Solvothermal method, Sol-gel, Arrested Precipitation, and other methods include) Langmuir-Blodgett, Micelles-Microemulsions.

**Characterization Tools:** Electron Microscopy (TEM & SEM), Probe Microscopy (STM & AFM), Diffraction Technique (XRD), UV-Visible-NIR spectroscopy, BET.

### Unit IV : Properties and Applications of Nanomaterials15 Hrs.

**Properties of Nanomaterials:** Optical, Magnetic, Electrical, Mechanical, Structural properties **Illustrative Nanomaterials:** Carbon nanostructures (CNTs, Graphene and its derivatives, fullerenes, Metal oxides (TiO<sub>2</sub> and ZnO)& itscomposites, Quantum dots, Core-Shell nanoparticles, Different morphological nanomaterials.

**Applications in the various fields:** Electronic devices, Energy generation and storage, Automobiles, Sports and toys, Textile Industries, Cosmetics Products, Domestic appliances, Sensors, Biotechnology and medical field, Space and Defense, Catalysis, Environment.

### **Reference Books**

- 1. New Directions in Solid State Chemistry (Second Eds.), C.N.R.Rao and G. Gopalkrishnan, Cambridge Oxford Press.
- 2. A basic course in crystallography, JAK Tareen, TRN Kutty, Universities press.
- 3. Essentials of crystallography, M.A. Wahab, Narosa Publications.
- 4. Synthesis of Inorgnic Materials: Ulrich Schubert, Nicola Hüsing.
- 5. Solid State Chemistry: Lasley E. Smart, Elaine A. Moore.
- 6. Introduction to Solid State Physics: Charles Kittel.

- 7. Solid State Chemistry: A. H. Hanny
- 8. Wilcox : Preparation and Properties of Solid State Materials: Vol I & II, Dekker
- 9. Hagenmuller, Preparative Methods in Solis State Chemistry
- 10. Lohn Wulff, The Structure and Properties of Materials Vol. IV, Electronic Properties (Wily Eastern)
- 11. , Chemistry of Imprefect Crystals (Holland) E.A. Kroger
- 12. Solid State Chemistry A. R. West,
- 13. Principles of the Solid State Chemistry, Wiley Eastern. H. V. Keer:

### Paper No. –XVI(A), ICH 4.4(A) : Energy and Environmental Chemistry

### **Unit I: Energy Conversion Devices**

**Solar Cells:** Solar energy, Solar devices, Efficiency of Solar energy conversion, Generations in Solar devices, Silicon-based solar devices, chalcogenide thin films-based devices, Sensitized solar devices (dye and QDs), Pervoskite solar devices, Mechanism of Solar energy generations, Characterization of solar devices.

**Fuel Cells:**Working of Fuel Cells, Types of fuel cells, Current capabilities/uses, Fuel cell stacks and systems, Hydrogen as a fuel,

**Production of hydrogen:** Electrolysis, Thermochemical Processes, Steam Reformer Processes, Water Gas Processes, Bosch Process, Biosynthesis and Photochemical Processes, Coal Gasification, Steam Iron Process, Partial Oxidation Processes. Storage, Transport, and Handling of Hydrogen

### UNIT II: Energy Storage Devices Batteries

Li-ion batteries: Principle of operation, Battery components and design, Electrode materials (LiCoO<sub>2</sub>, LiNiO<sub>2</sub>, LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub>, LiMn<sub>2</sub>O<sub>4</sub>, LiFePO<sub>4</sub>, graphitic carbon) their synthesis and characterization, Theoretical capacity, Energy density, power density, cycle life,Electrode and battery fabrication, Battery modules and packs, Li-polymer batteries and applications, Electrolytes for Li-ion batteries, All solid state batteries.Future developmentsand beyond lithium batteries: Li-S battery, Li-Air battery, Advanced lead-acid batteries, Sodium-battery, Magnesium battery, Aluminum battery, Silicon battery,Battery Recycling Technologies.

#### **UNIT III:**

### A) Waste Treatment

Electronic waste recycling programs, E-waste – non-recycling impacts, Materials Used in Manufacturing Electrical and Electronic Products,

Solid Waste Management: Gas to Energy projects, Incandescent vs. compact florescent light bulbs, Value-added Material Recovery, Cost effective treatment of refractory organics,

#### **B)** Air and Water Pollution control

### 7 Hrs.

### 15 Hrs.

8 Hrs.

### 15 Hrs.

Control of NOxSOx and particulate pollution, Sewage and industrial waste water treatment, water softening, municipal water purification

### UNIT-IV:

### A) Monitoring, sampling and Analysis of Air and water pollutants 8 Hrs.

Methods of monitoring and sampling of gaseous, liquid and solid pollutants, analysis of CO, CO<sub>2</sub>, NO<sub>2</sub>, SO<sub>2</sub>, H<sub>2</sub>S, analysis of toxic heavy metals, Cd, Cr, Hg, As, Pb, analysis of anions  $SO_4^{2^-}$ ,  $PO_4^{3^-}$ ,  $NO_3^{-}$ , estimation of COD and BOD

### **B)** Techniques in Environmental Analysis

### 7 Hrs.

ND-IR Spectroscopy, FTIR, AAS, ICP-AES, GC, GC-MS, HPLC, Anodic stripping voltammetry with case studies

### **Reference Books:**

- 1) Lithium ion Batteries: Basics and Applications, R. Korthauer, Springer
- 2) Lithium ion Batteries: Fundamentals and applications, Yuping Wu, CRC Press, Taylor & Francis group
- 3) Lithium ion batteries: Materials, Technology and new applications, K. Ozawa, Wiley
- 4) 30 Years of Lithium-Ion Batteries, Advanced Materials, M. Li et al., Vol 30, issue 33, 2018,1800561
- 5) Fuel Cell Fundamentals, R. O'Hayre, et al., John Wiley & Sons, 2016
- 6) George Techobanoglous et al,"Integrated Solid Waste Management" McGraw Hill, 1993.
- 7) Environmental Chemistry, H. Kaur, PragatiPrakashan, 10<sup>th</sup> edition 2016.
- 8) Environmental Pollution, A. K. De
- 9) Environmental Pollution Analysis, S. M. Khopkar
- **10)** Compendium of R&D Projects, Waste Management Technologies (WMT) Programme, Technology Development and Transfer Division, Department of Science and Technology, New-Delhi 2018-2019.
- 11) Environmental Waste Management, Ed. Ram Chandra, CRC Press 2015, 1<sup>st</sup> Edition
- 12) Electronic Waste Management, RSC Publishers, Editors: R E Hester, R M Harrison, 2009

### Paper No. –XVI(B), ICH 4.4(B): Radiation Chemistry

### UNIT-I: A] Isotopes

Difference between Isotopes and Isobars, isotope separation, thermodynamic and kinetic isotope effects, isotope exchange reaction kinetics, determination of exchange rate constant, production and applications of radio isotopes.

### **B**] Biological effects of Radiation

Introduction, genetic and somatic effect on human being, effect of radiation on plants and aquatic Environment.

### **UNIT-II: Radiochemical Separation**

### 8 Hrs

### 7 Hrs

### 15 Hrs.

The need of radiochemical separation techniques, carrier techniques, isotope and nonisotopic carriers, coprecipitation and adsorption, ion exchange, solvent extraction, electrolytes behavior of carrier free tracer radionuclide.

### **UNIT-III: Principle of tracer chemistry**

### 15 Hrs.

Introduction to tracers, application of tracers in physiochemical studies, diffusion studies, isotopic and exchange reactions, tracer in the study of the mechanism of the inorganic chemical reaction, atom transfer and electron transfer mechanisms. Heterogeneous catalysis and surface area measurements, radio carbon dating, tracer studies with tritium, application in metallurgy and preservation of food, geochemical application and hot atom chemistry.

### UNIT-IV: Radiation detection and measurements.

### 15 Hrs.

Ionization current measurements, multiplicative ion collector, methods not based on ion collection, auxiliary Instrumentation and health physical instruments and counting statistics. Working of Scintillation and Geiger Muller Counter.

### **Reference Books**

- 1. Friedlander, Kennedy and Miller, Nuclear and radio Chemistry, ohm Wiley.
- 2. B.G. Harvey, Nuclear Chemistry.
- 3. Haissinsky, Translated by D.G, Tuck, Nuclear physics and Chemistry.
- 4. Mark lefort, Nuclear Chemistry, D.V. Nostrand.
- 5. An N.Nesmeyanov, Radiochemistry, Mir.
- 6. Jacobs, et al, Basic Principles of nuclear science and reactors, V.Nost, EW AP.
- 7. N. Jay, Nuclear power, today tomorrow, ELBS.
- 8. Kenneth, Nuclear power, today and tomorrow, ELBS.
- 9. Essentials of Nuclear Chemistry, J. Arnikar, John Wiley.
- 10. D.C. Dayal, nuclear physics.

### M.Sc. Part-II (Semester-IV)

### **Inorganic Chemistry Practical Course ICHP-VII and ICHP-VIII** Practical courses includes Submission of project work :

### (A) Practicals

- 1. Ore Analysis -3
- 2. Preparation of coordination compounds (Three) and preparations of mixed metal oxides(two)
- 3. Ion Exchange chromatography; separation of multicomponent mixtures
- 4. Solvent extraction
- 5. Spectrophotometry
- 6.  $P^{H}$  Metry
- 7. Conductometry
- 8. Polarography
- 9. Electrogravimetry
- 10. Nuclear and radiochemistry

### **B)** Interpretation exercises

- 1. X-ray powder diffraction analysis of cubic compound
  - a. Determination of lattice constants and geometry
  - b. Partical Size
  - c. Density
- Interpretation of Mossbaur spectrum with reference to determination of a) isomer shift
   b) quadruple splitting c) Internal magnetic field d) general comment
- 3. Interpretation of IR spectrum with reference to stretching vibration 0-2 C=N, C=O, N-, M-O.
- 4. Interpretation of NMR spectrum with reference to calculation of chemical shifts and general comments.
- 5. Interpretation of absorption spectra for
  - a. Verification of position of ligands in spectrochemical series
  - b. Determination of geometry (Octahedral, Square planar, tetrahedral) of a given compound.
- c. Calculation of spectral splitting parameters.
- 6. Interpretation of polar gram for determination of half wave potentials and unknown concentration.
- 7. Calculation of band gap of semiconductors with the help of plots of log Vs.10  $\frac{3}{4}$ .
  - In all 20 experiments with at least five experiments in each course should be completed.Addition of other experiments in place of existing one may be allowed. A variety of small projects designed by teacher based on the interest of students and capabilities should be worked out. (**Project** work or the review report (50 Marks) will be examined by internal and external examiners.

## Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

### M.Sc. Part-II, (Sem-III and IV) Organic Chemistry

### **SEMESTER III**

Paper No. - IX, OCH 3.1

: Organic Reaction Mechanism

Paper No X, OCH 3.2	: Advanced Spectroscopic methods
Paper No. –XI, OCH 3.3	: Advanced Synthetic methods
Paper No XII(A), OCH 3.4(A)	: Drugs and Heterocycles
Paper No. XII(B), OCH 3.4(B)	: Polymer Chemistry
Practical Course	: OCHP-V and OCHP-VI

### **SEMESTER IV**

Paper No. – XIII, OCH 4.1	: Theoretical Organic Chemistry
Paper No. XIV, OCH 4.2	: Stereochemistry
Paper No. – XV, OCH 4.3	: Chemistry of Natural Products
<b>ELECTIVE PAPERS</b> Paper No XVI(A), OCH 4.4(A)	: Organic Industrial Chemistry
Paper NoXVI(B), OCH 4.4(B)	: Bioorganic Chemistry
Practical Course	: OCHP-VII and OCHP-VIII

M.Sc. Part-II (Sem- III) Organic Chemistry

Paper No.- IX, OCH 3.1: ORGANIC REACTION MECHANISM

UNIT-I: Methods of determining reaction mechanism

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**Kinetic Methods:** Order and Molecularity, Methods of following reaction rates, Types of reactions: 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> order reactions; Reversible, Consecutive and Parallel reactions. Energy of Activation, Entropy of Activation, Effect of Ionic strength, Solvent effect and Kinetic isotopic effect

**Non-Kinetic Methods:** Identification of reaction products, Testing of the possible intermediates, trapping of the intermediates, isotopic labeling, Reaction catalysis, Cross-over experiments, Stereochemical studies and Use of physical properties. **Hammett and Taft equations.** 

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### **UNIT—II: Pericyclic reactions**

Molecular orbital symmetry, Frontier orbital of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system, classification of peri cyclic reaction, Wood-ward Hoffman correlation diagrams, FMO and PMO approach, electrocyclic reactions, conrotatory and disrotatary motions, 4n, 4n+2 and allyl systems, cycloaddition, and supra and antara facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes, 1,3-dipolar cycloaddition and chelotropic reactions, sigmatropic rearrangement, supra and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearrangement and Claisen and Cope and Aza Cope rearrangement, Ene reaction.

UNIT - III:(15)

**A) Study of reactive intermediates:** Synthesis and Applications of nitrogen, sulphur and phosphorous ylides. (7)

B) Study of following reactions: Alkyne metathesis reaction, Weinreb ketone synthesis, Petasis reaction, Henry reaction, Corey Kim oxidation. Reactions of carboxylic acids and esters.
 (8)

### **UNIT-IV: Free radical reactions**

Types of free radical reactions, detection by ESR, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity. Allylic hydrogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt, Sandmeyers reaction. Hunsdiecker reaction.

### **RECOMMENDED BOOKS:**

- 1. A guide book to mechanism in organic chemistry (orient- Longmans)- Peter Sykes
- 2. Organic Reaction Mechanism (Benjumin)- R. Breslow

- 3. Mechanism and structure in Organic Chemistry (Holt Reinhartwinston)- B. S. Gould
- 4. Organic chemistry (McGraw Hill)- Hendrikson, cram and Hammond
- 5. Basic principles of organic chemistry (Benjamin) J. D. Roberts and M. C. Caeserio.
- 6. Reactive intermediates in organic chemistry, (J. Wiley) N. S. Issacs.
- 7. Organic reaction mechanism (McGraw Hill ) R. K. Bansal
- 8. Fundamentals of photochemistry K. K. Rohtagi- Mukherji Wiley- Eastern
- 9. Essentials of molecular photochemistry, A. Gilbert and J. Baggott. Blackwell Scientific Publication.
- 10. Molecular photochemistry, N.J. Urro, W. A. Benjamin
- 11. Introductory photochemistry. Cox and T. Camp McGraw -Hill
- 12. Photochemistry R.P. Kundall and A. Gilbert. Thomson Nelson.
- 13. Strategic applications of named reactions in organic synthesis by Laszlo Kurti and Barbara Czako.
- 14. Organic photochemistry J. Coxon and B. Hallon Cambridge University press.

### Paper No. -X, OCH 3.2: ADVANCED SPECTROSCOPIC METHODS

### UNIT-I:

A) Ultraviolet Spectroscopy: Woodward- Fisher rules for conjugated dienes and carbonyl compounds; Calculation of  $\lambda$  max. Ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls. (05)

**B) IR Spectroscopy:** 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; lactams and conjugated carbonyl compounds] Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones; combination bands and Fermi resonance. FT-IR of gaseous; solids and polymeric materials. (10)

### **UNIT-II: NMR Spectroscopy**

General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift values and correlation for protons bonded to carbons [aliphatic; olefinic; aldehydic and aromatic] and other nuclei [alcohols; phenols; enols; acids; ammines; amides and mercaptons]; 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 Simplification of complex spectra; nuclear magnetic double resonance; shift reagent; solvent effect. Fourier transform technique, nuclear overhauser effect [NOE] Resonance of other nuclei – F; P.

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### **UNIT-III: Mass Spectrometry**

Introduction, ion production- EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. 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.

### UNIT – IV:

**A) Carbon-13 NMR Spectroscopy:** General considerations; chemical shift [aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl compounds]; problems associated with <sup>13</sup>C, FT-NMR, proton decoupled off resonance. (07)

## B) Structural problems based on combined spectroscopic techniques (including reaction sequences) (8)

### **RECOMMENDED BOOKS:**

- 1. V.M. Parikh, Application spectroscopy of organic molecules. (Mehta)
- 2. D.W. Williams and Flemming, Spectroscopic methods of organic compound.
- 3. Silverstein and Basslar, Spectroscopic identification of organic compounds V.M. Parikh ORPTION SPECTROSCIPY OF ORGANIC MOLECULES (J. Wiley)
- 4. P.S. Kalsi Spectroscope of organic compounds (New age publisher)
- 5. J.R. Dyer. Application of absorption spectroscopy of organic compounds.
- 6. Jackman and Sterneil, Application of NMR spectroscopy
- 7. Nuclear magnetic resonance. J.D. Roberts (J. Wiley)
- 8. Theory and application of U.V. Jafee and Orchin.
- 9. Mass spectroscopy K. Benjamin.
- 10. The mass spectra of organic molecules. Beynon J H.
- 11. Interpretation of carbon 13 NMR Wehli F.W, Marchand A. P. (J. Wiley)
- 12. Organic Spectroscopy W. Kemp, ELBS
- 13. Instrumental methods of analysis CBS. Willard Merritt and Dean.
- 14. Mass Spectroscopy. Das and Jame
- Organic structural spectroscopy : J. B. Lambert, S. Gronert, H. F. Shurvell, D. Lightneli, R. G. Cooks (Prentice Hall 2<sup>nd</sup> edition)

### Paper No. – XI, OCH 3.3 : ADVANCED SYNTHETIC METHODS

### **UNIT-I: Disconnection approach**

An introduction to Synthons and synthetic equivalents, disconnection approach,

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functional group interconversions. One group C-X and two group disconnections in1, 2; 1, 3 - 1, 4 & 1, 5-difunctional compounds, Retro - synthesis of alkene, acetylenes and aliphatic nitro alcohols and carbonyl compounds, amines. Importance of the Order of events in organic synthesis, Chemoselectivity, Regioselectivity. Protecting groups, Diels-Alder reaction, Michael addition and Robinson annulation. Retro- synthesis of aromatic heterocycles and 3, 4, 5 and 6 membered carbocyclic and heterocyclic rings. Reversal of polarity (Umpolung).

### UNIT–II: Application of the following reagents and reaction in synthesis. (15)

Lithium diisopropylamide(LDA) Dicyclohexyl carbodiimide(DCC), lead tetra acetate, PPA, Diazomethane, ozone, phase transfer catalyst, Woodward-Prevost hydroxylation, Barton and Shapiro reaction, Hoffmann – Loffler-Fretag, Peterson synthesis, Selenium dioxide, Dess-Martin periodinane, periodic acid and iodoisobenzyldiacetate, Olefin metathesis using Grub's catalysts.

UNIT-III:	(15)

### A) Applications of following metal in organic synthesis

### B) Synthesis and applications of following ligands in organic synthesis.

Phosphines, N-heterocyclic carbenes, Oxazoline ligands (08)

### UNIT-IV: Application of the following in synthesis

Synthesis and applications of Merrifield resin, Electro-organic synthesis, Enzyme catalyzed reaction in synthesis, Solvent free synthesis, Multicomponent reactions, Microwave and Ultrasound techniques and their applications.

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### **RECOMMENDED BOOKS:**

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	Designi	ng of org	ganic synt	thesis. S.	Warren
1.	2 USI SIII				

- 2. Organic synthesis J. Fuhrhop & G. Penzlin. (2nd ed.)
- 3. Some modern methods of organic synthesis.Carruthres:
- 4. Modern synthetic reaction. H. O. House
- 5. Reagent in organic synthesis. Fieser & Fieser
- 6. Principle of organic synthesis. R. O. C. Norman
- 7. Advanced organic Chemistry. Carey & Sundharg
- 8. Organic synthesis. P. E. Realand:
- 9. Comprehensive organic Chemistry. Bartan and Ollis :
- 10. Organic reactions. R. Admas:
- 11. Advances in organometallic Chemistry. Stone & West:
- 12. Transition metal intermediate in organic synthesis. C. W. Bird:

- 13. Organometallic in organic synthesis. Swan & black :
- 14. Synthesis of prostaglandins. A. Mitra :
- 15. Total synthesis of natural products. John Apsimon:
- 16. Phosphorus ligands in homogeneous catalysis: Design and synthesis by Paul C. J. Kamer.
- Phosphorus ligands effect in homogeneous catalysis and rational catalyst design by Jason A. Gillespie and Erik Zuidema. Polymers as aid in organic synthesis. M. K. Mathur, C. K. Narang & R. E. Williams:
- 18. Polymer supported reaction in organic synthesis. P. Hodge & D. C. Sherrington:
- 19. Enzyme catalysed reactions.C. J. Gray:
- 20. Electroorganic Chemistry. T. Shona:
- 21. Phase transfer catalyst in organic synthesis. Weber & Gokel :

### Paper No.- XII (A), OCH 3.4(A) : DRUG AND HETEROCYCLES

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### Part- A: Drugs

### UNIT-I:

### A) Drug design

Procedures followed in drug design, **factors affecting development of new drugs**, concepts of prodrugs and soft drugs, **Isosterism, bioisosterism,** Theories of drug activity, Quantitative structure activity relationship, QSAR theory, Concepts of drug receptors. (10)

### **B)** Study of Antibiotics

Classification of antibiotics, Preparation of semi synthetic penicillin, Penicillin G, Penicillin V, conversion of penicillin into cephalosporin. (05)

### UNIT–II: Study of the Following types of drugs

a) Antimalerials: Trimethoprim, Amodiaquine

- b) Analgesic & Antipyretics: Meperidine, Aminopyrine, Diflunisal
- c) Anti- inflammatory: Oxyphenylbutazone, Indomethacin
- d) Antitubercular & antileprotic: Dapsone, Pyrazinamide, Ethionamide
- e) Anaesthetics: Lidocaine, Thiopental
- f) Antihistamines: Cyproheptadine, Cetirizine
- g) Psychoactive drugs: Ethiosuximide, Glutethimide
- h) Antiinfective drugs: Grisefulvin, norfloxacin
- h) Anti AIDS: General study
- i) Cardiovascular: Synthesis of warfarim, Clofibrate, quinidine, methyldopa, atenolol

**j)** Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloraethamine, cyclophosphamide, Mephalan, uracils, mustards. Recent development in cancer chemotherapy. Hormones and natural products.

### **Part-B: HETEROCYCLES**

UNIT-III:	(15)		
A) Small ring Heterocycles: Three membered and four membered Heterocycles- synthesis and			
reactions of aziridines, oxiranes, thiranes, azetidines	(05)		
B) Benzofused five membered Heterocycles : Synthesis and reactions of benzopyrroles,			
benzofurans and benzothiophenes	(05)		
C) Six membered Heterocycles with one heteroatom: Synthesis and reactions of pyrilium salts			
and pyrones, coumarins, chromones.	(05)		

### UNIT – IV:

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A) Six membered Heterocycles with two and more Heteroatoms: Synthesis and reactions of diazines & triazines (08)
 B) Benzofused heterocycles with two hetero atom: Synthesis and reactions of benzimidazole,

benzthiazole and benzoxazole (07)

### **RECOMMENDED BOOKS:**

- 1. Medicinal Chemistry.Burger:
- 2. Medicinal Chemistry A. Kar. (Wiley East)
- 3. Principals of medicinal chemistry.W. O. Foye:
- 4. Text book of organic medical and pharmaceutical chemistry. Wilson, Gisvold & Dorque:
- 5. Pharmaceutical manufacturing encyclopedia.
- 6. D. Sriram, P. Yogeeswari: Medicinal Chemistry
- 7. An introduction to chemistry of heterocyclic compounds. R. M. Acheson :( Interscience).
- 8. Heterocyclic chemistry. Joule &Smith: (Van Nostrand).
- 9. Heterocyclic chemistry. R. K. Bansal: (Wiley E).
- 10. Principals of modern heterocyclic chemistry.L. A. Paquitte:
- 11. The structure and reactions of heterocyclic compounds.M. H. Palamer:
- 12. Advances in Heterocyclic chemistry. A. R. Katritzky: (A.P.).
- 13. Organic chemistry (Vol. 1& 2) Finar.
- 14. Outline of Biochemistry. Cohn &Stumpt
- 15. Introduction to the chemistry of enzyme action.Williams:
- 16. The Organic Chemistry of Drug design and Drug action. R. B. Silverman Academic press.
- 17. Strategies for Organic Drug synthesis and Design. D. Lednicer, J. Willey.
- 18. Heterocyclic Chemistry. Vol-1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Veriag.
- 19. The Chemistry of Heterocycles. T. Eicher and S. Hauptmann, Thieme
- 20. Heterocyclic Chemistry. J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall
- 21. Heterocyclic Chemistry. T. L. Gilchrist, Longman Scientific Technical
- 22. Contemporary Heterocyclic Chemistry. G. R. Nikome and W. W. Poudler, Willey

24. Comprehensive Heterocyclic Chemistry. A. R. Katritzky and C. W. Rees

### PAPER NO. - XII (B), OCH 3.4(B): POLYMER CHEMISTRY (Optional paper for Sem-III)

### UNIT-I:

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**Terminology and basic concepts of Polymers**: Monomers, Functionality, repeat units, degree of polymerization. General structure and naming of polymers. Average molecular weight and average chain dimension concept. Expressions for average molecular weighs. Molecular weight distribution and Polydispersity. Classification based on various considerations-source, preparation methods, thermal behavior, chain structure etc.

Types –Homopolymers and copolymers; linear, branched and network polymers.

**Techniques of polymerization**: Techniques of preparation of addition and condensation polymers.

**Kinetics of Polymerization**: Kinetics and mechanism of addition and condensation polymerization. Kinetics of copolymerization-reactivity ratio and copolymer equation. Free radical chain polymerization- Cationic polymerization – Anionic polymerization – Poly condensation. Glass transition temperature: Glassy solids and Glass transition – associated properties – Factors influencing glass transition temperature – molecular weight – Plasticisers – melting point – importance of glass transition temperature.

### UNIT-II:

**Crystalline Nature:** Crystalline soils and their behaviour towards X-rays – Polymers and X- ray diffraction – Degree of crystallinity – crystallites –factors affecting crystallinity, Helix structures.

**Copolyemerization:** Free radical copolymerization – Ionic copolymerization – Copolycondensation – Individual monomers: Polyethylene, polypropylene, polystyrene, poly acrylonitrile, polymethyl methacrylate, polyesters, polycarbonates, polyamides, polyurethanes, polyvinyl acetate, polyvinyl chloride, poly isoprene's, silicone polymers.

### UNIT-III:

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**Polymer degradation:** Types of degradation, thermal and mechanical – photo degradation – oxidative and hydrolytic degradation. Polymer reactions – Hydrolysis, acidolysis, aminolysis, hydrogenation, addition and substitution reactions – cyclisation, cross-linking reactions – Graft and Block copolymers.

**Experimental methods:** Polymer synthesis, isolation and purification of polymers – Fractional - Molecular weight determination – Molecular weight distribution curve – determination of glass transition temperature. Elastomeric materials – Fibre forming materials – Plastic material Rheology of polymeric materials – compounding and

### UNIT-IV:

**Stereochemistry of polymers**: Geometric and optical isomerism in polymers. Structure, properties and preparation of stereoregular polymers.

Determination of molecular weight: Osmometry and viscometry.

**Thermal Characterization**: Glass Transition and melting-correlation with structure-Factors affecting Tg and Tm. Techniques of thermal characterization: DSC, DTA, DTG and TGA techniques.

**Structural features, properties and uses of commercial polymers:** Polyethylene, polystyrene, PVC, polyesters, polyamides, polyurethanes and polycarbonates. Conducting polymers, liquid crystal polymers and biomedical polymers.

### **RECOMMENDED BOOKS:**

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- 1. Contemporary Polymer Chemistry-H.R. Allcock and F.W. Lampe (Prentice Hall).
- 2. Polymer Science and Technology-J.R. Frird (Prentice Hall).
- 3. Polymer Science: V.R. Gowariker, N.V.Viswanathan & T.Sreedhar
- 4. Principles of Polymer Science- P.Bahadur and N.V.Sastry (Narosa Publishers)
- 5. 'Organic Polymer Chemistry', K.J.Saunders, Chapman and Hall, 1976.
- 6. 'Polymer Chemistry An Introduction', Raymond B.Seymour, Marcel Dekker Inc., New York and Based, 1981.
- 'Text Book of Polymer Science', Fred W.Billmeyer, Jr.John-Wiley and Sons, 3rd Edn. 1984.
- 8. 'Fundamentals of Polymer Science and Engineering', Kumar Gupta, Tata Mc Graw Hill, 1981.
- 9. "Polymer Characterization of Processing Technolgy', Stepak, Academic Press, London.
- 10. 'Inorganic Polymers', Stone, Academic Press, New York.
- 11. Polymer Chemistry, B.K.Sharma, Krishna Prakashan Mandir, Meerut.

Separation, purification and identification of compounds of ternary mixtures using **semi-microanalysis**, TLC, column chromatography and chemical tests. IR spectra tobe used for functional group identification.

### **B.** Quantitative analysis

### **1. Two step Preparations**

- a) Preparation of m-Nitroaniline
- b) Preparation of Benzanilide from benzophenone
- c) Preparation of Phthalimide
- d) Preparation of N-Bromosuccinimide
- e) Preparation of 4-methyl -7-acetoxy coumarin
- f) Preparation of 1, 2, 3, 4- Tetrahydro carbazole
- g) Preparation of p-ethoxy acetanilide
- 2. Colorimetry and pH metry experiments.
- 3. Expt. on Hammett equation
- 4. Structure elucidation by using given spectral data.

### 5. Any other suitable expt. may be added

### **RECOMMONDED BOOKS:**

- 1. Textbook of Practical Organic Chemistry A. I. Vogel.
- 2. Practical Organic Chemistry Mann & Saunders.
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
- 4. Organic Synthesis Collective Volumes by Blat

### M. Sc. Part –II (Sem – IV) Organic Chemistry

### Paper No.- XIII, OCH 4.1: THEORETICAL ORGANIC CHEMISTRY

### **UNIT–I: Molecular Orbital Theory**

Aromaticity in benzenoids, alternant and non alternant hydrocarbon, Huckels rule, energy level of pi- molecular orbital and concept of aromaticity, calculation of energies of orbitals cyclic and acyclic systems. Determination energies and stabilities of different systems calculation of charge densities PMO theory and reactivity index.

### UNIT – II: Non benzonoid aromatic Compounds

Aromaticity in Non- benzenoids compounds Annulenes and heteroannulenes, fullerenes, azulene, fulvene, tropylium salts, ferrocene, five membered systems. Crown ether complexes, cyclodextrins, cryptands, catenanes and rotaxanes, bonding in fullerenes.

### UNIT – III: Green chemistry

Introduction to the principles of green chemistry – prevention of waste, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, reduce derivatives, renewable feedstock, catalysis, design for degradation, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention. Green synthesis, clean routes using supercritical solvents, ionic liquids and water.

### UNIT – IV A) Kinetic and thermodynamic control of reactions (9)

Nitration and Sulphonation of naphthalene, Wittig, Enolization, Friedel-Crafts and Diels Alder reactions.

### B) Non-classical carbocations: Formation, stability and reactivity. (6)

### **RECOMMENDED BOOKS:**

- 1. 1. Lehar and Merchand: Orbital Symmetry.
- 2. R. B. Woodward and Hoffman: Conservation of orbital symmetry.
- 3. P. T. Anastas, J. C. Werner: Green Chemistry: Theory and Practice
- 4. V. K. Ahluwalia: Green chemistry, A textbook
- 5. V. K. Ahluwalia, R. S. Verma: Green Solvents: For Organic Synthesis
- 6. Ginsburg: Nonbenzenoid aromatic compound.
- 7. A. Streitwieser: Molecular orbital theory for organic chemistry.
- 8. E. Cler: The aromatic sextet.
- 9. Lloyd: Carbocyclic non- benzenoid aromatic compounds.
- 10. W. B. Smith: Molecular orbital methods in organic chemistry.
- 11. Grratt; Aromaticity

### Paper No. – XIV, OCH 4.2: STEREOCHEMISTRY

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### UNIT- I: Conformational analysis and reactivity of acyclic and alicyclic compounds (15 h): (A) Conformational analysis of acyclic compounds (4 h)

The difference between configuration and conformation. Klyne-Prelog terminology for torsion strain, Pitzer strain, van der Waals interactions, hydrogen bonding, and gauche effect. Conformations of 2, 3-dimethylbutane, n-propyl chloride, 1, 2-dihaloethanes, glycols, halohydrines, Conformations of diasteroisomers; tartaric acid, ephedrine, pseudoephedrine and other compounds. Conformations around sp3-sp2 (carbonyls; aldehydes and ketones) and sp2-sp2 (alkenes) bonds. Conformations around C-O and O-O bonds.

### (B) Conformational analysis of cyclohexane derivatives (4 h)

Concept of Baeyer ring strain, ring inversion, locking groups. Conformations of mono, di and polysubstituted cyclohexanes (1, 4-di-t-butylcyclohexane, 1, 4-cyclohexanediol, t-butylcuclohexanol, menthol, inositol, hexachlorocyclohexane and other related compounds). Conformations of rings containing sp2 hybridized carbon atoms; cyclohexanone and cyclohexene (substituted cyclohexanones: cyclohexanone-2-bromocyclohexanone, dibromocyclo hexanone, 2-bromo-4, 4-dimethyl cyclohexanone and other related compounds).

### (C) Effect of conformation on reactivity (mechanism) of acyclic and cyclic systems (7 h):

Curtin-Hammett principle. Effect of conformation on the course and rate of reactions in; debromination of 2,3-dibromobutane, semipinacolic deamination of 1,2-diphenyl-1-(p-chlorophenyl)-2-amino ethanol, dehydrohalogination of stilbene dihalide and bromo-1,2-diphenyl propane, stereochemistry of molecular rearrangements; pyrolytic cis-elimination.

Effect of conformation on the course and rate of the reactions in cyclohexane systems illustrated by: (a) SN2 and SN1 reactions. (b) E1, E2 eliminations illustrated by; (i) 4-t-butylcyclohexyl tosylate (ii) 2-phenylcyclohexanol (iii) menthyl and neomenthyl chlorides and benzene hexachlorides. (c) pyrolytic cis-elimination (d) semipinacolic deamination of 2-aminocyclohexanol, (e) esterification of hydroxyl carboxyl groups (methanol derivatives, (f) hydrolysis of esters and equatorial tosylates, (g) oxidation of cyclohexanols by chronic acid (h) epoxidation (formation and cleavage).

## UNIT- II: Conformational analysis and reactivity of cyclic compounds other than six membered (15 h)

### (A) Conformational analysis of cycloalkanes other than cyclohexane

Shapes of four, five, seven, eight and higher membered rings. Concept of 'I' strain and transannular strain. Conformational effects in medium sized rings (8-10 membered rings). Stability of rings and ease of rings formation. Conformational analysis of heterocycles (pyramidal inversion, anomeric effect, Rabbit-ear effect, Hockey-sticks effect). Conformations of dioxanes, monosaccharides and disaccharides.

### (B) Fused rings

Types of fused ring systems; (a) Fused bicycles: cis and trans-decalins, octalins, decalols, octahydronaphthalenes, decahydroquinoline, hydrindane (b) Fused polybicycles: perhydroanthracene, perhydrophenanthrene, steroids. Locking groups of conformations in decalins and steroids.

### (C) Bridged rings

Types of bridged ring systems, nomenclature, stereo chemical restrictions, Bredt's rule.

### (3 h)

(3 h)

(9 h)

### UNIT III: Stereoselective synthesis

### (15 h)

(4 h)

(7 h)

(A) Diastereo and enantio-controlled approaches; chirality transfer. Stereoselectivity and stereospecificity: Kinetic and thermodynamic controls, asymmetric induction. General strategies for asymmetric synthesis: Chiron approaches, acyclic diastereoselective approaches, double asymmetric synthesis. Stereoselective addition of nucleophiles to carbonyl group: Re-Si face concepts, Cram's rule, Felkin Ahn rule, Houk model, Cram's chelate model. Asymmetric synthesis by use of chiral auxiliaries. Nucleophilic addition: use of chiral substrates, auxiliaries, reagents and catalysts; asymmetric conjugate addition; addition of allyl boron derivative; reactions at alpha carbon: enolate formation (regioselectivity and stereoselectivity); stereoselective enolate alkylation (oxazolidinone, oxazoline); asymmetric aldol reaction.

### (B) Asymmetric Oxidations:

Asymmetric epoxidation of allylic alcohols (Sharpless Epoxidation), dihydroxylation of olefins (Sharpless asymmetric dihydroxylation, Upjohn process, Milas hydroxylation), Asymmetric aminohydroxylation of olefins (Sharpless oxyamination), epoxidation of unfunctionalized olefins (Jacobsen epoxidation, Shi epoxidation, Dioxirane catalyst), Catalytic asymmetric epoxidation of aldehydes.

### (C) Asymmetric Diels-Alder Reactions using chiral Lewis acids:

(Narasaka's catalyst, chiral lanthanide, bissulfonamides (Corey's catalyst), chiral acyloxy borane, bis (oxazoline), amino acid salts).

### (D) Asymmetric Catalytic Hydrogenation and Other Reduction Reactions:

Chiral phosphine ligands for asymmetric catalytic hydrogenation, asymmetric reduction of carbonyl compounds.

### UNIT-IV: Stereochemistry of compounds containing no chiral carbon atoms (15 h).

(A) Stereochemistry of allens, sprains and biphenyls, assignment of configuration

(B) Configuration of diastereomers (Geometrical isomerism) based on physical and chemical methods (4 h)

### (C) O.R.D. and C.D.

Linearly and circularly polarized lights, circular birefringence and circular dichroism, ORD and CD curves; cotton effect. Determination of the conformation and configuration, empirical and semi-empirical rules; The octant rule, helicity rule, Lowe's rule, and axial haloketone rule.

### **RECOMMENDED BOOKS:**

- 1. E.L. Eliel: Stereochemistry of carbon compounds.
- 2. D. Nasipuri : Stereochemistry of organic compounds
- **3.** P.S. Kalsi: Stereochemistry, Conformation and Mechanism.
- 4. Eliel, Allinger, Angyal and Morrison: Conformational analysis.
- 5. Hallas: Organic stereochemistry
- 6. Mislow and Benjamin: Introduction to Stereochemistry.
- 7. H. Kagan: Organic stereochemistry.
- 8. Carl Djerassi; Optical Rotatory Dispersion.
- **9.** P. Crabbe : Optical Rotatory Dispersion and C.D.

### Paper No. - XV, OCH 4.3: CHEMISTRY OF NATURAL PRODUCTS

### UNIT-I:

A) Introduction of natural products and Terpenoids: Introduction of natural products: Classification and isolation methods. Terpenoids: Structure and synthesis of camphor, carvone, abietic acid, zingiberene,  $\alpha$ -santonin,  $\beta$ -cuparenone. Biogenesis of abietic acid.

**UNIT-II:** 

**Alkaloid :**Structure, stereochemistry, synthesis and biosynthesis of the following: Morphine, Reserpine, Ephedrine and alpha pinene, Biogenesis of Conin.

### **UNIT-III:**

Steroids: Occurrence, nomenclature, basic skeleton, Diels hydrocarbon.

**Study of the following**: hormones, Cholesterol, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone and cortisone Bile acid (only synthesis) and biosynthesis of lanosterol.

### **UNIT-IV:**

A) Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects, Synthesis of PGE2 and PGF2. (05)

B) Lipids: Classification, Role of Lipids, Fatty acids and glycerol derived from oils and fats.
 (4)

C) Vitamins: Synthesis and structure of biotin, vitamin B<sub>1</sub> and B<sub>2</sub>, Biological functions of Vitamin B<sub>6</sub>, D and E. (06)

### **RECOMMENDED BOOKS:**

- 1. Apsimon: The total synthesis of natural products.
- 2. Manskey and Holmes: Alkaloids
- 3. A.A. Newmen: Chemistry of Terpenes.
- 4. P. D B.Mayo: The chemistry of natural products.
- 5. Simonson: Terpenes.
- 6. T.W. Goddwin: Aspects of terpenoid chemistry and biochemistry.
- 7. Woguer: Vitamins and Co- enzymes.
- 8. P. W. Bently: Chemistry of Natural products,
- 9. Fieser and Fieser: Steriods
- 10. I. Finar: Organic chemistry Vol. II and I

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- 11. J.B. Hendrickson, The molecules of nature.
- 12. Peter Bernfield: The biogenesis of natural products
- 13. R.T. Slickenstaff A.C. Ghosh and G.C. Wole: Total synthesis of steroids.
- 14. The chemistry of natural products, vol. Nakanishi.

15. Biochemistry of Lipids, Lipoproteins and membranes by Neele Ridgway and Roger McLeod.

- 16. Membranes (New comprehensive biochemistry) by J E Vance and E Vance.
- 17. Schaum's easy outline of biochemistry by Philip W Kuchel.

### Paper No. - XVI (A), OCH 4.4(A): ORGANIC INDUSTRIAL CHEMISTRY

### **UNIT-I:**

### A) Agrochemicals

a. Organochlorine pesticides: Introduction, synthesis and mode of action of endrin, aldrin, dieldrin.

b. Herbicides: Synthesis and mode of action of Triazines, triazoles, pyridazinones and Bipyridylium compounds: diquat, paraquat.

f. Juvenile harmone: introduction & structures JHA importance synthesis, IPM (08)B) Synthesis and applications of perfumery

2-Phenylethanol, vanillin and other food flavours, synthetic musk and ionones. (07)

### **UNIT- II Unit Processes**

Introduction, Nitration of hydrocarbons, Becamp reduction, halogenations, sulphonation of aromatic compounds.

### **UNIT-III: Dyes and Intermediates**

Classification and synthesis of important dye intermediates by using nitration, sulphonation, diazotization reactions. Synthesis of Nitro dyes, xanthenes, reactive dyes, Fluorescent brightening agents, thermal sensitive dyes, dispersed dyes and reactive dyes.

### **UNIT-IV: Polymers**

Mechanism of polymerization. Industrial process for synthesis of polyethylene, acrylonitrile, acrylate and methaacrylate polymer, biomedical polymer, Polymer processing, Plasticizers and anti-oxidants for polymers,

### **RECOMMENDED BOOKS:**

- 1. Allan: Colour Chemistry
- 2. K. Venkataraman: Chemistry of Synthetic Dyes Vol-1 to 7
- 3. G. R. Chatwal: Synthetic dyes

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- 4. Abrahart: Dyes & their intermediates
- 5. N. N. Melikov: The Chemistry of Pesticides and formulations
- 6. K. H. Buchel: Chemistry of Pesticides.
- 7. R. Clemlyn: Pesticides
- 8. K. H. Buchel: Chemistry of Pesticides
- 9. H9. R. Alcock and F. W. Lambe: Contemporary Polymer Chemistry
- 10. J. 10M. G. Cowie, Blackie: Physics & Chemistry of Polymers
- 12. I. M. Campbell: Introduction to Synthetic Polymers
- 13. A. L. Gupta: Polymer Chemistry
- 14. M. S. Bhatnagar: A textbook of Polymers
- 15. F. W. Billmeyer: Textbook of Polymer Science
- 16. P. H. Groggins: Unit Processes in Organic Synthesis
- 17. B. Biollot& P. V. Wells: Perfumary Technology
- 18. M. Ash & I. Ash: A formulary of Cosmetic Preparations

#### Paper No. - XVI (B), OCH 4.4(B): BIOORGANIC CHEMISTRY

#### (ELECTIVE CBCS PAPER)

#### **UNIT-I:**

#### **A) Cell Structure and Functions**

Structure of prokaryotic and eukaryotic cells, Intracellular organelles and their functions, comparison of plant and animal cells. Overview of metabolic process- catabolism and anabolism. ATP - the biological energy currency. Origin of life- unique properties of carbon, chemical evolution and rise of living system. Introduction to biomolecules, building blocks of biomacromolecules. (10)

#### **B)** Enzymes

Structure activity and reactions, catalyzed determination of active site, inhibition mechanism chemical transformations using enzymes.

### **UNIT-II: Carbohydrates**

### (15)

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. Naceylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysccharides- cellulose and chitin. Storage polysaccharides- starch and glycogen.

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### (5)

Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoprotines and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

Carbohydrate metabolism- Kerb's cycle, glycolysis, glycogenesis and glycogenolysis, pentose phosphate pathway.

### **UNIT-III: Lipids**

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Fatty acids, essential fatty acids, structures and function of triglycerides, glycerophspholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins-composition and function, role in arthrosclerosis. Properties of lipid aggregates – micelles, bilayers, liposomes and their possible biological functions. Biological member's .Fluid mosaic model of membrane structure. Lipid metabolism -  $\beta$ -oxidation of fatty acids

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### UNIT-IV: a) Amino acids, Peptides and Proteins

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of protein, forces responsible for holding of secondary structures.  $\alpha$ - helix,  $\beta$ -sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein- folding and domain structure. Quaternary structure. Amino acid metabolism- degradation and biosynthesis of amino acids, sequence determination: chemical/ enzymatic/ mass spectral, racemization / detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

### b) Nucleic Acids

Purine and pyrimidine of nucleic acids, base pairing via H – bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (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 poly nucleosides.

### **RECOMMENDED BOOKS:**

- 1. Principles of Biochemistry, A. L. Lehinger, Worth Publications.
- 2. Biochemistry, L. Stryer, W. H. Freeman
- 3. Biochemistry, J. David Rawn, Neil Patterson.
- 4. Biochemistry, Voet and Voet, John Wiley.
- 5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpt, John Wiley.

### M.Sc. Part-II (Semester-IV) Organic Chemistry Practical Course OCHP-VII and OCHP-VIII

# Two or three stage preparations starting with 5g or less and TLC.

# 1. Estimation of Sulphur and Nitrogen.

# 3. Organic preparations

- 1. Preparation of Anthranilic acid.
- 2. Preparation of p- Amino benzoic acid.
- 3. Preparation of p- Chloro nitrobenzene by Sandmeyer reaction.
- 4. Preparation of p- Iodonitrobenzene by Sandmeyer reaction.
- 5. Preparation of Benzylamine
- 6. Preparation of Benzimidazole
- 7. Preparation of 2-acetyl cyclohexanone
- 8. Multicomponent synthesis.

**4. Project:** Literature survey. Studies of reactions, synthesis, mechanism, isolation of natural products, standardization of reaction conditions, use of new methods etc. Identification of organic compounds by spectroscopic methods. External and internal examiners will examine the project (50 Marks) jointly at the time of practical examination.

# 5. Any other suitable experiments may be added.

# 6. Study tour may arrange for M.Sc. Part- II Students to visit Chemical Industries in nearby areas.

# **REFERENCE BOOKS:**

- 1. A Textbook of Practical Organic Chemistry A. I. Vogel.
- 2. Practical Organic Chemistry Mann & Saunders
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke
- 4. Organic Synthesis Collective Volumes.

# M. Sc. Part II( Sem III and Sem IV) Physical Chemistry

# **SEMESTER- III**

# **CORE PAPERS**

Paper –IX, PCH.3.1	: Advanced Quantum Chemistry
Paper –X, PCH.3.2	: Electrochemistry
Paper –XI, PCH.3.3	: Molecular Structure-I

# **ELECTIVE PAPERS**

Practical Course	: PCHP-V and PCHP-VI
Paper -XII( C ), PCH.3.4(C)	: Radiation and Photochemistry
Paper -XII(B), PCH.3.4 (B)	: Advanced Chemical Kinetics
Paper-XII(A), PCH.3.4(A)	: Solid State Chemistry

#### **SEMESTER-IV**

# **CORE PAPERS**

Paper –XIII, PCH.4.1	: Thermodynamics and Molecular Modelling
Paper- XIV, PCH.4.2	: Chemical Kinetics
Paper- XV, PCH.4.3	: Molecular Structure II

# **ELECTIVE PAPERS**

Paper- XVI(A), PCH.4.4(A) : Surface Chemistry

Paper- XVI(B), PCH.4.4(B) : Chemistry of Materials

Paper- XVI(C), PCH.4.4(C): Biophysical Chemistry

Practical Course :PCHP-VII and PCHP-VIII

# M.Sc. Part-II (Sem- III) Physical Chemistry

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# Paper –IX, PCH.3.1 :Advanced Quantum Chemistry

# Unit I: Basic Quantum Chemistry

Introduction. Exact solution of Schrödinger wave equation for rigid rotator, linear harmonic oscillator and hydrogen and hydrogen like atoms. Atomic orbitals, radial and angular shapes of atomic orbitals, ground and excited state energies, ionization potentials for hydrogen like systems. Transition dipole moment integral and selection rules for rotational, vibrational and electronic transitions.

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#### Unit III: Ab initio methods

Self-consistent field (SCF) theory, Hertree-Fock (HF) method, quantum particles and their spins, properties of slater determinant, HF equations, restricted Hartree-Fock (RHF) and unrestricted Hartree-Fock (UHF) models, Fock matrix, HF calculations, Roothan-Hall equations, Koopman's theorem, Basis sets: Slater type orbitals (STO), Gaussian type orbitals (GTO), difference between STO and GTO, energy calculations using such orbitals for multielectron systems, classification of basis sets, minimal basis sets, energy calculations for H-atom using STO basis sets at different levels, double- and triple-zeta basis sets, valence-split basis sets, polarized basis sets, truncation and superposition errors, methods to overcome these errors. Correlation energy.Post Hertree-Fock methods:Configuration interactions, many body perturbation theory, Möller-Plesset perturbation, coupled cluster method. Introduction to various software packages for performing ab initio calculations.

# **Unit III: Density Functional Theory**

Basics of density functional theory (DFT): functionals, electron density and hole functions, fermi and coulomb holes, electron density as basic variable, Thomas-Fermi model, Slater's Approximation of Hartree-Fock Exchange, the Hohenberg-Kohn theorems, energy functionals, minimizing energy, orbitals and the non-interacting reference systems, the Kohn-Sham equations, computing the total energy, Exchange-Correlation energy functional, Solving the Kohn-Sham equations: basis sets, Pseudo-potentials, Plane waves, the self-consistent cycle, Density Functional Perturbation theory: basic formalism, first order energy derivative and atomic forces, second order.

# **Unit IV: Semiempirical Methods**

Introduction, need of semi-empirical methods, differential zero overlap (ZDO) approximation. Variation principle, Secular determinant and secular equations. Hamiltonian in semi-empirical methods, Hückel molecular orbital theory – Assumptions of HMO theory,  $\pi$ electron approximation, Hückel rule and aromaticity, HMO calculations for organic molecules, free valence index and prediction of chemical reactivity, use of molecular symmetry for simplification of HMO calculations. Neglect of differential overlap (NDO) method, complete neglect of differential overlap (CNDO), intermediate neglect of differential overlap (INDO), modified intermediate neglect of differential overlap (MINDO), modified neglect of differential overlap (MNDO), neglect of diatomic differential overlap (NDDO). AM1, PM3, PM5, PM6 etc. methods, comparisons in various above mentioned methods, limitations of semi-empirical methods. Introduction to various software packages for performing semi-empirical calculations.

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#### **Reference Books:**

1. A.K. Chandra, Introductory Quantum Chemistry, 4th Edition, Tata McGraw-Hill, New Delhi, 1994.

2. D. A. McQuarrie, Quantum Chemistry, Viva Books, New Delhi, 2003.

3. P. Atkins and R. Friedman, Molecular Quantum Mechanics, 4th Edition, Oxford University Press, New York, 2005.

4. Leach, A.R. Molecular Modelling. Principles and Applications, 2nd Edition, Prentice-Hall, Harlow, England, 2001.

5. K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.

6. Becker, O.; MacKerell, A.D.; Roux, B.; Watanabe, M. eds. Computational Biochemistry and Biophysics, Marcel Dekker, New York, 2001.

7. F. Jensen, Introduction to Computational Chemistry, 2nd Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.

8. D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.

9. Fabio Finocchi, Density Functional Theory for Beginners: Basic Principles and Practical Approaches, 2011

10. Wolfram Koch, Max C. Holthausen, A Chemist's Guide toDensity Functional Theory, 2nd Edition, Wiley-VCH Verlag GmbH, Weinheim (Germany), 2001.

11. C. Fiolhais F. Nogueira M. Marques (Eds.), APrimer inDensityFunctional Theory, Springer-Verlag, Berlin, 2003.

12. P. Geerlings, F. De Proft, and W. Langenaeker, Conceptual Density Functional Theory, *Chem. Rev.* 2003, *103*, 1793-1873.

# Paper –X, PCH.3.2: Electrochemistry

#### **UNIT-I: Equilibrium Properties of Electrolytes**

(15)

Non-ideal behaviour of electrolyte solutions, Debye – Huckel Theory of inter-ionic attraction, Ionic atmosphere, Time of relaxation, Relaxation and Electrophoretic effects, Debye – Huckel Onsagar equation, Validity of Debye – Huckel equation, factors influencing the degree of dissociation, , Debye – Falkenhagen effect, Wein effect, Debye Huckel limiting law equation, Qualitative and quantitative test of Debye Huckel limiting equation, Debye-Huckel Bronsted equations ,Ionic mobility, Determination of dissociation constant by emf method, Experimental determination of ionic mobility, osmotic coefficient, Bjerrum theory, association constant, Numerical problems.

#### **UNIT-II: Ion-solvent Interactions**

Structure of water, hydration, heats of hydration of electrolytes, individual ions and their comparison, calculation of heats of hydration( Born, Van Arkel & de Boer, Bernal-Fowler methods), entropy of hydration and hydration numbers. Ion transport in solutions, diffusion, chemical potential and work of transport, Ficks laws, expressions for flux and diffusion coefficient. Ionic liquids: Introduction, difference between electrolytes and ionic liquids, diffusion in fused salts, viscosity and diffusion coefficient in molten salts.

#### **UNIT-III: Electrode reactions**

Electrified interface, electron transfer under interfacial electric field, symmetry factor, electrode at equilibrium, exchange current density, over potential, Butler-Volmer equation, high field and low field approximations, Tafel equations, Multistep electrode reactions; Marcus microscopic model of electron transfer. Electrode kinetics of semiconductor/ solution interface; n and p type semiconductor, current-potential relation of n and p type semiconductors Electrocatalysis: Influence of various parameters on water splitting, HER and OER and Application of cyclic voltammetry for characterization of various electrochemical processes, Electrochemical instrumentations. Bioelectrochemistry: Nerve impulses, Membrane potentials, Nernst-Planck equation, Hodgkin-Huxley equations, electrochemical impedance spectroscopy.

#### **UNIT-IV: Fuel cell and Corrosion**

**Fuel cell**: Significance of fuel cells, Hydrogen – oxygen fuel cells, hydrocarbon - air fuel cell, alkaline fuel cells, Phosphoric acid fuel cell (PAFC), Proton exchange membrane fuel cells (PEMFC), Solid oxide fuel cells, Molten Carbonate Fuel Cell (MCFC), Alkaline Fuel cell (AFC), Solid Polymer Fuel Cell (SPFC) and applications.

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**Corrosion:** Introduction, Comparison between dry and wet corrosion, Factors affecting corrosion: Nature of the metal, Nature of the corroding environment, Types of corrosion, Prevention of corrosion: Material selection & Design, protective coatings, corrosion inhibitors.

#### **REFFERENCE BOOKS:**

1. An Introduction to Electrochemistry by Samuel Glasstone, East west press riveted limited. (2005).

2. Callister's Material Science and Engineering adapted by R. Balasubramaniam, Wiley India (p) Ltd.

3. Electrolytic Solutions, by R. A. Robinson and R. H. Strokes

4. Physical Chemistry by P. W. Atkins. ELBS.

5. Electrochemical Methods: Fundamentals and Applications, Bard, A. J. Faulkner, L. R., 2nd Ed., John Wiley & Sons: New York, (2002).

6. Electrochemical Science and Technology: Fundamentals and Applications, Oldham, K. B., Myland, J. C. and Bond, A. M. John Wiley & Sons, Ltd. (2012).

7. Modern Electrochemistry 2A: Fundamentals of Electrodics , 2nd Ed., Springer (2001).Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E.

8 Electrochemistry, Brett, C. M. A. & Brett, A. M. O., Oxford University Press (1993).

9. Principles of Electrochemistry, John Wiley & Sons: NY (1993).

10. Fundamentals of electrochemistry, Bagotsky, V.S., 2nd Ed. Wiley – Interscience, (2006) Hamann, Carl H., Hamneff , Andrew & Vielstich, Wolf., Electrochemistry, 2nd Ed. (2007)

11. Fuel Cell Systems Explained Second Edition by James Larminie Andrew Dicks, John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, England.

# Paper –XI, PCH.3.3: Molecular Structure-I

UNIT- I: Symmetry properties of molecules and group theory (15)

Symmetry elements, symmetry operations and point groups, properties of group, symmetry operations as a group, multiplication table. Classes of symmetry operations, basis, representative and matrix representations of operations. Reducible and irreducible representations, orthogonality theorem. Properties of irreducible representations. Constructions of character table for point groups. Explanations for the complete character table for a point group. Representations of vibrational modes in nonlinear molecules. Infrared and Raman activities of normal modes of vibrations.

#### UNIT– II: Introduction of spectroscopy and Rotational Spectra (15)

Characterization of electromagnetic radiation. The qualification of energy. Regions of Spectrum, transition probability, the width and intensity of spectral transitions. Classification of molecules according to their moment of inertia. Rotational spectra of rigid and non rigid diatomic molecules. The intensities of spectral lines. The effect of isotopic substitution. Polyatomic and symmetric top molecules. The stark effect.

#### UNIT- III: Infrared spectroscopy and Raman Spectroscopy (15)

Diatomic molecules: 1) Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero point energy, isotope effect. The anharmonic oscillator, the diatomic vibrating rotator, the interactions of rotations and vibrations. Polyatomic molecules: Fundamental vibrations and their symmetry, overtone and combination frequencies. The influence of rotations and molecular spin on the spectra of polyatomic molecules. Analysis by Infrared techniques. Raman Spectroscopy: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Polarization of light and the Raman effect . Structure determination from Raman and Infra-red spectroscopy.

#### **UNIT – IV: Electronic Spectroscopy**

General nature of band spectra. Beer- Lambert Law integrated absorption coefficient and oscillator strength. Term symbols for atoms and molecules. The hydrogen atom and hydrogen like species spectrum. Sequences and progressions, the vibrational course structure and rotational fine structure of electronic band. The Franck-Condon principle, dissociation energy and

dissociation products. Birje-Sponer extrapolation. The fortrat diagram. Predissociation, classification of electronic states. The spectrum of molecular hydrogen. Electronic spectra of polyatomic molecules. Chemical analysis by electronic spectroscopy. (d-d), ) and  $(\neg-n^*)$  transitions. Photochemical mechanism of vision.

#### **REFFERENCE BOOKS:**

1. Fundamental of molecular spectroscopy by C. N. Banwell, E. M. McCash, Vth Edn.,

Tata McGrew Hill(2013).

2. Physical Chemistry by P. W. Atkins, J. D. Paula, IXth Edn., Oxford University Press (2010).

3. Chemical Applications of Group Theory, F. A. Cotton, 3rd Edn., Wiley-India(2009).

4. Molecular Symmetry and Group Theory by R. L. Carter, John-Wiley & Sons Inc.(1998)

5. A Text Book of Physical Chemistry by K. L. Kapoor, IVth Edn., Macmillan (2011).

6. Symmetry & spectroscopy of molecules by K. Veera Reddy, IInd revised Edn., New Age International Publishers (2009)

7. Intruduction to spectroscopy by D. L. Pavia, G. M. Lapmann, G. S. Kriz, IIIrd Edn., Thomson(2006).

8. Molecular Structure and Spectroscopy by G. L. Aruldhas, Prentice-Hall of India Pvt. Ltd. (2006).

#### Paper XII (A), PCH-3.4(A): Solid State Chemistry (Elective)

#### **UNIT-I: The solid state**

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Introduction, laws of crystallography, lattice types, X-ray diffraction, Bragg's equation, Miller indices, Bragg Method, Debye-Sherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-Ray intensities, structure factor and its relation to intensity and electron density, phase problem, procedure for an X-ray structure determination.

#### **UNIT –II: Solid State Reactions**

General principle, types of reactions: Additive, structure sensitive, Decomposition and phase transition reactions, tarnish reactions, kinetics of solid state reactions, factors affecting the reactivity of solid state reactions.

#### **UNIT –III: Electronic Properties and Band Theory**

Metals, insulators and semi conductors, free electron theory and its applications, electronic structure of solids, band theory, band structure of metals, insulator, and semiconductors, doping in semiconductors, p- n junction, superconductors, Molecular materials, Organic materials, some examples of organic semiconductors, charge carrier injection and transport, Optical properties of organic semiconductors, applications and devices involving optical properties, luminescence photoluminescence, effect of impurity levels on photoluminescence, light emitting diodes, luminous efficiency, photo-conduction and photoelectric effects, laser, principle of laser action, solid state laser and their applications.

#### **UNIT-IV: Preparation of materials**

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Purification and crystal growth, kinetics of nucleation, radius of nucleus, critical radius, principle of nucleation, crystal growth during casting, zone refining, growth from solution, growth from melt and preparation of organic semiconductors for device applications.

# **Crystal Defect and Non Stiochiometry**

Classification of defects subatomic, atomic and lattice defect in solids. Thermodynamics of vacancy in metals, Thermodynamics of Schottky defects in ionic solids, Thermodynamics of Frenkel defects in silver halides. Calcualtion of number of defects and average energy required for defect.

#### **REFERENCE BOOKS:**

- 1. A guide to laser in chemistry by Gerald R., Van Hecke, Keny K. Karokitis
- 2. Principals of solid state, H. V. Keer, Wiley Eastern,
- 3. Solid state chemistry, N. B. Hannay
- 4. Solid state chemistry , D. K. Chakrabarty , New Age International
- 5. An Introduction to Crystallography : F. G. Philips
- 6. Crystal Structure Analysis: M. J. Buerger
- 7. The Structure and properties of materials:
- Vol. III Electronic properties by John Walss
- 8. Electronic processes in materials : L. U. Azroff and J. J. Brophy
- 9. Chemistry of imperfect crystal : F. A. Krogen
- 10. Elements of X-ray Diffraction by B. D. Cullity, Addison- Weily.
- 11. Solid state Chemistry by A.R.West (Plenum)
- 12. Electronics made simple by Jacobwitz.
- 13. Principles of Physical Metallurgy, by Abhijeet Mallick,
- 14. Solid State Chemistry, An Introduction, by Lesley E. Smart, & Elaine A. Moore,

# Paper XII (B), PCH-3.4(B): Advanced Chemical Kinetics (Elective)

# Unit-I: Hydrogen ion dependence of reaction rates:

Protonation and hydrolysis equilibria, determination of active reactant species form kinetic data, interpretation of hydrogen ion effect with example.

# **Unit-II: Electron transfer reaction:**

Complimentary and non-complimentary reactions, outer and inner-sphere electron transfer reactions, proton transfer, hydride transfer and hydrogen, oxygen and chlorine atom transfer reactions.

# Unit-III: Catalysis:

Trace metal ion catalysis and their mechanisms. Micellar catalysis, Berezini, Menger-Portonoy, cooperative and pseudo-phase ion exchange models and examples.

# Unit-IV: Mechanism of chromium (VI) oxidations:

One and two equivalent reductants oxidation, assumptions, limiting forms of rate laws, Westheimer mechanism and its validity. Catalysis, Induced and cooxidations. Mechanisms other than Westheimer mechanism.

# **REFERENCE BOOKS AND ARTICLES**

1) Chemical Kinetics by K. J. Laidler.

2) Kinetics and Mechanism by A. A. Frost and R. G. Pearson

3) Micellar effect on the kinetics and mechanism of chromium(VI) oxidation of organic

substrates By Asim K. Das, Coordination Chemistry Reviews, Vol 248, p 81-89 ( 2004 ).

4) Some aspects of electron transfer reactions involving organic molecules by B. Sethuram, Allied Publishers, 2003.

5) Surfactants and polymers in aqueous solution by Bo Jonsson, Bjorn Lindman, Krister Holmberg and Bengt Kronberg, John-Wiley & Sons, 1998.

6) Inorganic reaction mechanisms, Part II Edited by John O. Edwards, Interscience, 1972.

# Paper XII (C), PCH-3.4(C) : Radiation and Photochemistry(Elective)

# Unit - I : Radiation Chemistry :

Introduction, Radiation Types, their characteristics, Radiation in chemical processes.

# Unit - II: Lasers and Lasers in Chemistry :

Introduction, characteristics of laser, uses of lasers in chemical process, laser induced chemical reactions, organic photochemistry, lasers as a photochemical tool, laser induced selective bond chemistry, overview, bond selective chemistry of light atom molecules.

# Unit - III: Basics of Photochemistry :

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Electrochemistry of excited states, life time measurements, flash photolysis, energy dissipation by radiative and non-radiative processes, properties of excited states, structure, dipole moment, acid-base strength, reactivity, photochemical kinetics, calculations of rates of radiative process, bimolecular quenching, Luminescence for sensors and switches, charge transfer excited state, photoinduced electron transfer reactions.

# **Unit - IV : Micellaneous Photochemical reaction :**

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Photo-fries reaction of anilides, photo - fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog, photodegradation of polymers, photochemistry of vision.

# **REFRENCE BOOKS**

1) Molecular Photochemistry, N. J. Turro, W.A. Benjamin

- 2) Fundaments of Photochemistry, K. K. Rohatagi Mukherji, Weiley Eastern
- 3) Elements of Inorganic Photochemistry : G. S. Ferraudi , Wiley
- 4) Concepts of Inorganic Photochemistry, A.W. Adamson & P. J. Fleischauer, Wiley
- 5) A Guide To lasers in chemistry, Gerald R. Van Hecke & Kerry K. Karukstis.
- 6) Photochemistry, R.P. Kundall, A Gilbert, Thomson Nelson

# M.Sc. Part-II (Semester-III) Physical Chemistry Practical Course PCHP-V and PCHP-VI

1) Determination of stability constant of ferric thiocyanate complex.

- To determine stoichiometry and stability constant of ferric-salicylate complex by Job's Method and mole ratio method spectrophotometrically.
- 3) Determination of stoichiometry and instability constant silver ammonia complex.
- Determination of transport number of H<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup> etc. ions using moving boundary method
- 5) Determination of the critical micelle concentration of a given surfactant in aqueous and aqueous salt solutions.
- 6) Determination of equivalent conductance at infinite dilution and dissociation constant for weak acid using Kolharausch Law of independent ionic mobility.
- 7) pH-metric determination of dissociation constant of carbonic acid.
- Cryoscopic determination of molecular weight and state of organic acids in nonaqueous volatile solvents.
- 9) Determination of order of reaction for iodination of acetone catalyzed by acid with reference to acetone, iodine and acid catalyst.
- 10) Determination of apparent and partial molar volumes of 1:1 electrolytes in aqueous solutions using pyknometric method of density measurements.
- Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using minimal basis sets.
- 12) Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using correlation consistent basis sets.
- Semi-empirical and quantum mechanical determination of thermochemical properties of small molecules.

# M.Sc. Part-II (Sem- IV) Physical Chemistry

#### Paper -XIII, PCH.4.1: Thermodynamics and Molecular Modelling

#### **Unit I: Modern Theoretical Principles**

Exact and inexact differential expressions in two variables. Total differentials. Techniques of partial differentiations. Transformation of variables. Maxima and mimima. Integrating factors, Paff differential equations, Caratheodary's theorem. Legendre transformations. Derivation of thermodynamic identities. The second law of thermodynamics, classical formulations, mathematical consequences of second law. Entropy changes, Clausius inequality. Free energy concept. General condition of equilibrium. Thermodynamic potentials.

#### **Unit II: Statistical Thermodynamics**

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Ensembles, ensemble average and time average of the property, ergodic hypothesis, partition functions and thermodynamic properties, classical and quantum statistics, properties of photon gas, thermodynamic properties bosons, use of quantum statistics for evaluation of absolute entropies, condensation of helium, Fermi energy, electron gas in metals.Heat capacity of solids, Einstein and Debye specific heat equations. Characteristic temperatures. Debye  $T^3$  law.

#### Unit III: Molecular Mechanics and Molecular Dynamic Simulation Methods (15)

Introduction, microscopic and macroscopic properties, time scale of chemical/biological process, the Morse potential model, harmonic oscillator model, force fields development, various energy terms and non-covalent interactions included in force fields, Lennrad-Jones type and truncated Lennard-Jones potentials, commonly used force fields, parameterization, advantages and limitations of Force Field Methods, molecular dynamics methods, neighbour searching, Trotter decomposition, cut-offs, temperature and pressure coupling methods, integration algorithms: Verlet algorithm, Leap-frog algorithm, Velocity Verlet, Beeman's algorithm, Constraint algorithms: shake, lincs, etc., topology files, energy minimization: steepest descent method, conjugate gradient method, L-BFGS. Solvent models, Solvation, implicit and explicit solvation, heating dynamics, equilibration dynamics, production dynamics, trajectory analysis, particle mesh Edward dynamics, boundary conditions, Exclusions and 1-4 interactions, replica exchange method, conformational analysis, normal mode analysis, free energy calculation: free energy perturbation method, thermodynamic integration method, thermodynamic cycles for free energy calculations, determination of hydration/solvation free energy, protein folding free energy, protein-ligand binding free energy etc. Software packages for performing Molecular dynamic simulation as well as for visualization and analysis trajectories

#### Unit IV: Non-equilibrium thermodynamics

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Conversion of mass in closed and open systems, conservation of energy in closed and open systems. Law of increasing entropy. Non-adiabatic process and clausius inequality, steady state. Thermodynamic equations of motion. Chemical and electrochemical affinities. Coupling reactions. Rates and affinities. Generalized fluxes, forces and their transformation. Phenomenological equations and coefficients. Concepts of reciprocity relations and Onsager theorem of microscopic reversibility. Entropy production in closed and open systems. Entropy production due to heat flow. Chemical potentials. Diffusion, electromotive force, electroosmosis, thermoelectric effect and other reactions involving cross relations. Saxen's relations.

# **Reference Books:**

1. S. N. Blinder, Advanced physical Chemistry, The Macmilan Company, 1967.

2. L. K. Nash, Elements of statistical thermodynamics, 2nd Edition, Addison Wesley, 1974.

3. T.L. Hill, An Introduction to Statistical Thermodynamics, Addison-Wesley, 1960.

4. S. Glasstone, Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists, D. Van Nostrand Company, Inc., 1944.

5. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A molecular Approach, Viva Books, New Delhi, 1998.

6. Allen, M. P., Tildesley, D. J. Computer Simulations of Liquids, Oxford: Oxford Science Publications. 1987.

7. Frenkel, D.; Smit, B. Understanding Molecular Simulation: From Algorithms to Applications, 2nd Edition, Academic Press, San Diego, 2002.

8. K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.

9. F. Jensen, Introduction to Computational Chemistry, 2nd Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.

10. Schlick, T. Molecular modeling and simulation: an interdisciplinary guide, Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2002.

11. D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.

12. Online Manuals for simulation and visualization packages such as GROMACS, VMD, NAMD, AMBER, TINKER, etc.

13. I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Wiley, New York, 1968.

14. R.P. Rastogi, Introduction to Non-equilibrium Physical Chemistry: Towards Complexity and Non-linear Science, Elsevier, Oxford, 2008.

# Paper- XIV, PCH.4.2: Chemical Kinetics

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# **UNIT-I:** Collision Theory

Collision Theory: Definition, Formulation of the total collision rate, The p factor, Reactive collisions, Contour diagrams for scattering of products of a reaction, Forward scattering: the stripping or grazing mechanism, Backward scattering: the rebound mechanism, Scattering diagrams for long-lived complexes, Steady State Approximation Collision theory of gas reaction, collision frequency. The rate constant, molecular diameters, collision theory vs. experiment

#### **UNIT – II: Transition State Theory**

Transition State Theory: Transition state theory, configuration and potential energy, Properties of the potential energy surface relevant to transition state theory, An outline of arguments involved in the derivation of the rate equation, Use of the statistical mechanical form of transition state theory, Comparisons with collision theory and experimental data. Thermodynamic Formulations of Transition State Theory: Determination of thermodynamic functions for activation, the partition function form and the Thermodynamic form of transition state theory, Typical approximate values of contributions entering the sign and magnitude of  $\Delta S^{\#}$ , Unimolecular Theory: Manipulation of experimental results, Physical significance of the constancy or otherwise of k<sub>1</sub>, k<sub>-1</sub> and k<sub>2</sub>, Physical significance of the critical energy in unimolecular reactions, Physical significance of the rate constants k<sub>1</sub>, k<sub>-1</sub> and k<sub>2</sub>. Lindemann, Hinshelwood, theory, Kassel and Slater Theory.

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#### **UNIT-III: Kinetics of Surface Reactions**

Review of adsorption isotherms, Thermodynamics and statistical mechanics of adsorption, Structure of soilid surfaces and adsorbed layers: Detailed structural studies, Induced Heterogenity, Mechanism of surface reactions: Kinetic effects of surface heterogeneity, Kinetic effects of interaction Unimolecular surface reactions: Inhibition, Activation Energies, Bimolecular surface reactions: Reaction between two adsorbed molecules reaction between a gas molecule and an adsorbed molecule, Adsoprtion of two gases without mutual displacement, Inhibition, Activation energies, Parahydrogen conversion, Combination and formation of atoms at surfaces, Exchange reactions,Addition of hydrogen to ethylene, Transition state theory of surface reactions: rates of chemisorptions, rates of desorption, Unimolecular surface reactions,bimolecular surface reactions,comparison of homogeneous and heterogeneous reaction rates, Problems

#### UNIT- IV : Fast Reactions and Organic Reaction Mechanisms (15)

Linear free energy relationships: Hammett plots Hammett equation, substituent and reaction constants and their physical significance, calculation of k and K values, Yukawa-Tsunoequation.Taft equation, steric parameters Solvent effects, Grunwald-Winstein equation.

Kinetics of Fast reactions: Relaxation techniques, pressure jump and temperature jump methods, NMR relaxation, flash photolysis and molecular beam methods.

# **REFERENCE BOOKS**:

- 1) Chemical Kinetics by K. J. Laidler, Third Edition, Pearson.
- 2) Kinetics and Mechanismby A. A. Frost and R. G. Pearson.
- 3) Fast Reactions by Haque.
- 4) Theory of chemical reaction rates by K. J. Laidler, McGrew Hill, New York, 1969.
- 5) Fast Reactions by J. N. Bradley, Clarendon Press Oxford, 1974
- 6) Physical Chemistry by W. J. Moore.
- 7) Physical Chemistry by P.W. Atkins
- 8) Mechanism of Inorganic Reactions by F. Basolo and R. G. Pearson, John Wiley
- & Sons Inc., 2nd Edition, 1967.

9) A Guidebook to Mechanism in Organic Chemistry, Peter Sykes, Orient Longmann, 6th Edition, 2003.

#### Paper- XV, PCH.4.3: Molecular Structure - II

# UNIT – I: The Electrical and Magnetic Properties of Molecules

Electric dipole moment of molecule, polarization of a dielectric, polarizability of molecules, Clausius-Mossotti equation. Debye equation. limitation of the Debye theory, determination of dipole moment from dielectric measurements in pure liquids and in solutions.

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Diamagnetism and paramagnetism. Volume and mass susceptibilities. Lengevins classical theory of diamagnetism and paramangnetism Atomic and ionic susceptibility. Pascal constants, Curie - Weiss law. Van Vleck general equation of magnetic susceptibility. Determination of magnetic susceptibility.

CO: the unit deals with the understanding of behaviour of various materials in presence of applied electrical and magnetic fields.

# UNIT – II: Nuclear Magnetic Resonance Spectroscopy (15)

The nature of spinning particles , interaction between spin and a magnetic field. Population of energy levels, The larmor precession . relaxation times. the meaning of resonance and the resonance condition. NMR experiment, singnificance of shielding constants and chemical shift . the origin and effect spin - spin coupling , factors affecting chemical shift, chemical analysis by NMR. Exchange phenomena , 13C NMR spectroscopy, double resonance and nuclear-overhauser effect.

CO: the student will be able to predict structure of the given compound.

# UNIT – III: Electron Spin Resonance Spectroscopy and Massbauer Spectroscopy (15)

Electron spin and Magnetic moment, Resonance condition in ESR and significance of 'g' value. ESR spectra of organic free radicals, McConnel relation, Electron Exchange reactions, applications of ESR, B) Massbauer Spectroscopy (7) Basic principle of Mossbauer spectroscopy, hyperfine structure, quadrupole splitting, instrumentation and applications of Mossbauer spectroscopy, Problems related to Mossbaur spectra.

CO; the student will be able to understand behaviour of electrons and nucleus of a given molecule in presence of an external force like magnetic field.

# UNIT – IV: Basics of Fluorescence Spectroscopy

Photoluminescence, Instrumentation, Electronic transition in atoms and molecules, Solvatochromism, Fate of excited molecules, structural factors, properties of fluorescence, Fluorescence parameters: fluorescence intensity, quantum yield and fluorescence life time, Corrected emission and excitation spectrum, Relation between emission spectrum and excitation spectrum, inner filter effect, Solvent effect on fluorescence, solvation dynamics, Effect of intermolecular process, Fluorescence Anisotropy, Relation between concentration with fluorescence and phosphorescence intensity, Fluorescence quenching, Energy transfer, Excited state proton transfer, Synchronous spectrum, Fluorescent nanomaterials and its applications.

# **REFFERNCE BOOKS:**

1.Fundamental of molecular spectroscopy by C. N. Banwell, E. M. McCash, Vth Edn., Tata McGrew Hill(2013).

2. Physical Chemistry by P. W. Atkins, J. D. Paula, IXth Edn., Oxford University Press (2010).

3. Introduction to molecular spectroscopy by G. M. Barrow.

4. Molecular spectroscopy by I. N. Levins , Wiley interscience.

5. Nuclear magnetic Resonance by J. D. Roberts , Mcgrew Hill .

6. Introduction to Magnetic resonance by A. Carrrington and A. D. McLachlan. Harper and Row.

7. Intruduction to spectroscopy by D. L. Pavia, G. M. Lapmann, G. S. Kriz, IIIrd Edn., Thomson(2006).

8. Introduction to Magnetochemistry by Earnst Shaw. Academic Press

9. Electrical and optical properties of molecular behavior by M. Davies, Pergmon press.

10. Polar molecules by P. Debye, Dover publications.

11. A Text Book of Physical Chemistry by K. L. Kapoor, IVth Edn., Macmillan (2011).

12. Principles of Fluorescence Spectroscopy, 3<sup>rd</sup> edition, Joseph R. Lakowicz (Springer)

13. Fundamentals of Photochemistry by K. K. Rohatgi-Mukherjee

14. Molecular Fluorescence: Principles and Applications. Bernard Valeur , 2001, Wiley-VCH Verlag GmbH

#### Paper- XVI (A), PCH.4.4(A) : Surface Chemistry (Elective)

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#### **UNIT-I: Surface Chemistry of interfaces**

Types of interfaces, Liquid-vapour interface, Surface tension and interfacial tension, surface tension across curved surfaces, capillary action, methods of determination of surface tension, , vapor pressure of droplet (Kelvin equation), Surface activity and adsorption phenomenon, Trube's Rule, liquid-liquid interfaces, work of cohesion and adhesion, surface spreading , spreading of one liquid on the surface of other liquid, spreading coefficient and derivation for its relation with surface tension, surface films on liquids, criteria for spreading of one liquid on another. Experimental techniques for the study of monomolecular films, states of monomolecular films reaction on monomolecular films, catalytic activity at surfaces.

UNIT –II: Solid-Liquid and Solid - Solid interfaces (15)

Solid-liquid interfaces, Introduction, wetting phenomenon, contact angle and wetting, heat of wetting, methods of determination of contact angle, contact angle hysteresis, wetting agents, selective wetting, applications in detergency, and pesticide affectivity, Solid-Solid interfaces, introduction, Surface energy of solids, adhesion and adsorption, sintering and sintering

mechanism, Tammann temperature, importance of impurities, surface structure and surface composition. Friction and lubrication, mechanism of lubrication, solid state lubricants.

#### **Unit-III: Solid-gas interfaces**

Adsorption, Mechanism of adsorption, Adsorption of gases by solids, Factors affecting adsorption, Characteristics, Experimental methods of determining gases adsorption, Adsorption of solutes from solution, Heat of adsorption, Measurement of heat of adsorption, Chemisorption: kinetics of chemisorption, heat of chemisorptions, Surface film, Catalysis of gases reaction by solid surface, One reactant gases slightly/ strongly/ moderately adsorbed, Retarded reaction, ion exchange adsorption, Applications

#### **UNIT- IV: Colloids and emulsion**

Colloidal solution, classification of colloids, Theories of origin of charge on sol particles, Determination of charge on a colloidal particle, Stability of sols, Association colloids, Spontaneous ageing of colloids, Factors affecting the spontaneous ageing, theories of spontaneous ageing, coagulation, kinetics of coagulation.

**Emulsion**: Types of emulsion, preparation, properties, Characteristics, Identification test between two types of emulsions, emulsifiers, demulsification. Gels: classification, methods for the preparation of gels, properties of gels, Applications of colloid science.

#### **REFFERNCE BOOKS:**

- 1. Physical chemistry of surfaces: A. W. Adamson.
- 2. Introduction to colloid and surface chemistry by D. J. Shaw.
- 3. Surface chemistry by J. J. Bikermann
- 4. The Surface Chemistry of Solids, by S.J. Gregg, Second Edition, Chapman & Hall Ltd. London.

5. Advanced Physical Chemistry, by Gurdeep Raj ,Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP)

- 6. Physical Chemistry by Pahari S. New Central Book Agency (P) Ltd. Kolkata700009.
- 7. Advanced Physical Chemistry J.N. Gurtu, A. Gurtu. 11th Edition Pragati Prakashan.
- 8. Advanced Physical Chemistry D N Bajpai S Chand Publications

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8. Essentials of Physical Chemistry by Arun Bahl, B S Bahl, G D Tuli . S Chand Publications

9. Principles of Physical Chemistry by S H Maron and C F Prutton

#### Paper- XVI (B), PCH.4.4(B) : Chemistry of Materials (Elective)

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#### Unit I: Glasses, Ceramics, Composite and Nanomaterials:

Glassy state, glass formers and glass modifiers, applications, Ceramic structures, mechanical properties, clay products. Reformatories, characterizations, properties and applications. Microscopic composites; dispersion - strengthened and particle - reinforced, fibre - reinforced composites, macroscopic composites. Nanocrystline phase, preparation procedures, special properties, and applications.

#### Unit II: High Tc Materials:

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

#### **Unit III: Polymeric Materials:**

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

#### Unit IV: Materials of Solid Devices:

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

**b)** Materials of Solid Devices: Rectifiers, transistors, capacitors IV-V compounds, low dimensional quantum structure; optical properties.

#### **REFFERNCE BOOKS**

1. Solid State Physics, N. W. Ashcrott and N. D. Mermin, Saunders College

- 2. Material Science and Engineering, An introduction, W. D. Callister, Willey.
- 3. Principals of Solid State, H. V. keer, Willey Eastorn.

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 Willey.
- 6. Text book of liquid crystals, Kelkar and Halz , Chemie Verlag.

# Paper- XVI (C), PCH.4.4(C): Biophysical Chemistry (Elective)

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# Unit - I Chemistry and Biology:

Amino acids, proteins, enzymes, DNA & RNA in living systems, electrolytes, the chirality of biological molecules, the biochemical process, weak and strong interactions, macromolecules and rubber elasticity, polyelectrolytes, biopolymers.

# Unit - II Physical aspects of biopolymers:

X-ray diffraction, electronic absorption & luminescence Spectroscopy, optical activity, magnetic activity, magnetic-optical activity. Osmosis, hydrophobic hydration and interactions. The properties of amino acids and their aqueous solutions.

#### **Unit - III Photo biological Process :**

Photosynthesis, mechanism of vision, the molecular mechanism of photoreceptor.

# Unit - I : Mechano-chemical processes :

Introduction, thermodynamics, nerve conduction and membrane equilibria, muscle and muscle proteins, their chemistry and physics, kinetic properties of muscle, mechano- chemical systems, biomachanics.

# **REFFERENCE BOOKS**

1) Biophysics by M.V. Volhenshfein.

2) Natural products : Chemistry & Biological Significance, J. Mann, R.S.

Davidson, J. B. Hobb's , D. V. Banthrope and J. B. Harborne , Longmar Essex

3) Elements of Inorganic Photochemistry, G. J. Ferrandi, wiley

4) Principals of bioinorganic chemistry , S. J. Lippard and J. M. Beng , University Science Books,

5) Principals of biochemistry, A. L. Lechinger, worth publisher

6) Biochemistry, J. David Rawn, Neil Patterson

7) Hydrophobic interactions by Ben-Naim, Plenum.

# M.Sc. Part-II (Semester-IV) Physical Chemistry Practical Course PCHP-VII and PCHP-VIII

#### Practical courses includes Submission of project work :

- Statistical representation of given experimental data: Estimation of errors in measured and derived properties, reporting data with appropriate significant figures, graphical representation of data with x- and y-error bars.
- Determination of molecular properties of small gaseous molecules from rovibrational spectra.
- 3) Determination of indicator constant and isosbestic point of an indicator.
- 4) Determination of Thermodynamic Parameters for electrochemical reactions: To determine  $\Delta G^0$ ,  $\Delta H^0$  and  $\Delta S^0$  for the formation of 1 mole of cadmium in 1 wt. % amalgam at 25 °C.
- Determination of isoeletric points and dissociation constants for netutral, acidic and basic amino acids using pH-metric technique.
- Cryoscopic determination of mean activity coefficient of 1:1 electrolytes in aqueous solutions.
- Study of the effect of ionic strength on the reaction between persulphate and iodide by visual method.
- Determination of molar enthalpy of solution, molar enthalpy of dilution and partial molar heat content of components in aqueous solutions.
- Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using minimal basis sets.
- Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using correlation consistent basis sets.

- 11) Electronic structure calculations for small molecules and their aggregates.
- 12) Calculation of vibration spectra using *abinitio* techniques.
- 13) Structure and properties of transition states from DFT calculation.
- Determination of thermodynamic properties from Molecular dynamic simulations of some simple systems.

Along-with above experimental and computational lab work, additional new experiments from computational chemistry as well as from experimental techniques will be given whenever required and found necessary for enhancing the knowledge and skill of the students. A research project is compulsory for each student. Project shall be started at the beginning of Sem – III and will be accessed bimonthly for its progress and continuous evaluation will be made. High standard research work is expected from the project and students are encouraged to publish it in national or international journals of high repute.

Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

#### M.Sc. Part-II, (Sem-III IV) Analytical Chemistry

#### SEMESTER-III

Paper No. – IX, ACH 3.1	: Advanced Analytical Techniques
<b>Paper No.</b> – X, ACH 3.2	: Organo Analytical Chemistry
Paper No. – XI, ACH 3.3	: Electroanalytical Techniques in Chemical Analysis
-	
ELECTIVE PAPERS	
Paper No. –XII (A), ACH 3.4(A)	: Environmental Chemical Analysis and Control
Paper No XII (B), ACH 3.4(B)	: Recent Advances in Analytical Chemistry

**Practical** 

Course

: ACHP-V and ACHP-VI

#### SEMESTER- IV

Paper No. – XIII, ACH 4.1: Modern Separation Method in AnalysisPaper No. – XIV, ACH 4.2: Organic Industrial AnalysisPaper No. – XV, ACH 4.3: Advanced Methods in Chemical AnalysisELECTIVE PAPERS: Industrial Analytical ChemistryPaper No. – XVI (A), ACH 4.4(A): Industrial Analytical ChemistryPaper No. – XVI (B), ACH 4.4(B): Quality Assurance and Accreditation

**Practical Course** 

: ACHP – VII and ACHP-VIII

# M.Sc. Part-II (Sem-III) Analytical Chemistry

#### Paper No. -IX, ACH 3.1: ADVANCED ANALYTCAL TECHNIQUES

#### **UNIT-I: Advances in Mass Spectrometry**

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Introduction to Mass spectrometry, diagram of a mass spectrometer and Instrumentation, principles, history, concept of ion free path, classification of mass spectrometry based on nature of compound to be analyzed and the ion sources viz. Electron impact (EI), chemical ionization (CI), Fast ion or atom bombardment ionization (FID/FAB), field desorption (FD), laser desorption ionization (LDI), plasma desorption ionization (PDI), thermospray ionization (TSI), electrospray (ESI), atmospheric pressure ionization, Inductively couple plasma (ICP) etc. Mass Analyzers, Quadrupolar Analyzers, Quadrupole ion trap or Quistor, Ion trap detector, development of high –Mass, High-resolution ion trap, tandem mass spectrometry in the ion trap, time of flight analyzer, magnetic and electromagnetic analyzer, ion cyclotron resonance and FT-MS, and detectors

#### Scanning Tunneling Microscopy (STM) - Introduction, principle, instrumentation, applications Atomic Force Microscopy (AFM) - Introduction, principle, instrumentation, applications

Practical applications and examples in analytical chemistry and research.

#### **UNIT-IV: Advanced Instrumentation Techniques-B**

Raman Spectroscopy- Introduction, principle, instrumentation, applications

X-Ray Fluorescence Spectroscopy (XFS) - Introduction, principle, instrumentation, applications Electron Spin Resonance Spectroscopy (ESR)- Introduction, principle, instrumentation, applications

X-Ray Photoelectron Spectroscopy (XPS)- Introduction, principle, instrumentation, applications Auger Electron Spectroscopy - Introduction, principle, instrumentation, applications

Secondary Ion Mass Spectrometry (SIMS)- Introduction, principle, instrumentation, applications Practical applications and examples in analytical chemistry and research.

#### **Recommended Books:**

- 1) E. De. Hoffmann, J. Charette, V. Stroobant, Mass Spectroscopy: Principles and Applications, John Wiley & Sons, Masson, Paris 1996.
- 2) J. H. Gross, Mass Spectroscopy: A Text book, Springer-Verlag Berlin 2004.
- 3) C. G. Herbert, R. A. W. Johnstone, Mass Spectrometry Basics, CRC Press, Boca Raton, Florida, 2002.
- 4) K. Benjamin : Mass Spectrometry
- 5)
- 6) A. I. Vogel: A text book of Quantitative inorganic Analysis, Longmans.
- 7) G. H. Morrison and H, Freiser : Solvent Extraction in Analytical Chemistry (John Wiley New
- 8) York, 1958)
- 9) Willard, Merrit and Settle : Instrumental Methods of analysis.
- 10) Principles of instrumental analysis- Holler, Skoog and Crouch
- 11) Instrumental methods of Chemical analysis-H. Kaur
- 12) Bhushan, Bharat 2004. Handbook of Nanotechnology. Springer.
- 13) Niemeyer, C.M. & Mirkin, C.A. 2004. Nanobiotechnology- Concepts, Applications and
- 14) Prespectives. Wiley-VCH Verlag.

#### UNIT-II: Introduction to Nanotechnology and Nano Chemistry

Definition of nanomaterials and nanotechnology, significance of nanotechnology, size and properties, types of nanomaterials like 0D (quantum dots), 1D, 2D and 3D, introduction to physical, chemical and biological synthesis of nanomaterials with suitable examples, top down and bottom-up approach, chemical synthesis of nanomaterials-Different types and processes for synthesis of nanomaterials using wet chemical approaches. Fabricating nanomaterials with different morphology intended for specific applications. Applications of Nanotechnology.

#### **UNIT-III: Advanced Instrumentation Techniques-A**

Scanning Electron Microscope (SEM) - Introduction, principle, instrumentation, applications Transmission Electron Microscope (TEM) - Introduction, principle, instrumentation, applications Electron Dispersion Spectroscopy (EDS) - Introduction, principle, instrumentation, applications Energy Dispersive X-ray Analysis (EDAX) - Introduction, principle, instrumentation, applications

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- 15) Zander, C., Enderlein, J. & Keller, R.A. 2002 Single Molecule Detection in Solution. Wiley-VCH Verlag.
- 16) Avouris, P, Klitzing, K. Von, Sakaki, H. & Wiesendanger, R .2003 NanoScience and Technology
- 17) Series. Scanning Probe Microscopy- Analytical Methods (R. Wiesendanger eds), Springer.
- 18) Instrumental Analysis by Skoog
- 19) Nanochemistry, a chemical approach to nanomaterials, G. A. Ozin, and A. C. Arsenault, RSC Publishing, Cambridge, 2005. ISBN 0-85404-664-X.

# Paper No. -X, ACH 3.2: ORGANO ANALYTICAL CHEMISTRY

#### **UNIT–I: Hyphenated Techniques**

Advanced techniques of analysis: UV-Visible, IR, 1H-NMR (Recapitulation), 13CNMR, Mass spectrometry (Basic fundamentals of mass spectrometry, ionization, advanced organic analysis examples); Problems related to structure determination and applications of spectroscopic techniques as analytical tools.

#### **UNIT-II : A) Drug Analysis**

Introduction to drugs, their classification, sources of impurities in pharmaceutical raw materials such as chemical, atmospheric and microbial contaminants etc. Limit tests: Limit test for impurities for Pb, As, Fe, Se, etc. Estimation of moisture (K-F method), halide (Schnoiger's oxygen flask method), sulfate, boron, etc. Analysis of commonly used drugs such as antihistamines, sulfa drugs, barbiturates, etc. using non-aqueous titrations, sodium nitrite titrations, differential UV methods, colorimetric and fluorimetric methods of analysis.

#### **B)** Analysis of vitamins

Analysis of vitamins (thiamine, ascorbic acid, Vit. A, Vit. B6, Vit. K) and hormones (progesterone, oxytocin, insulin) chemical, instrumental and biological assay, wherever applicable.

#### UNIT – III: A) Clinical Analysis

Biological significance, analysis of assay of enzymes (pepsin, monoamine, oxidase, tyrosinase), Composition and detection of abnormal level of certain constituents leading to diagnosis of diseases. Sample collection and preservation of physiological fluids, analytical methods to the constituents of physiological fluids (blood, urine and serum). Blood- Estimation of glucose, chlolesterol, urea, hemoglobin and bilirubin, Urine- urea, uric acid, creatinine, calcium, phosphate, sodium, potassium and chloride.

#### **B)** Body fluid analysis

Composition and detection of abnormal level of certain constituents leading to diagnosis of diseases. Sample collection and preservation of physiological fluids, analytical methods to the constituents of physiological fluids (blood, urine and serum) Blood-Estimation of glucose, chlolesterol, urea, hemoglobin and bilirubin Urine- urea, uric acid, creatinine, calcium, phosphate, sodium, potassium and chloride.

#### UNIT–IV: A) Pesticides Analysis

Introduction, classification of pesticides, sampling, sample pretreatment and processin g, analysis of DDT, gammexane, endosulphan, zinab, ziram, malathion, thiram, thiometon, simazine and

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chloridane. Applications of colorimetric and chromatographic techniques (GC-MS, HPLC-MS) in analysis of pesticide residue. Introduction to EPA regulatory body. Practical applications and examples in analytical chemistry and research.

#### **B)** Forensic Analysis

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Special features of forensic analysis, sampling, sample storage, sample dissolution, classification of poisons, lethal dose, significance of LD-50 and LC-50. General discussion of poisons with special reference to mode of action of cyanide, organophosphate and snake venom. Estimation of poisonous materials such as lead, mercury and arsenic in biological samples. Practical applications and examples in analytical chemistry and research.

# **Reference Books:**

- 1) F. J. Welcher: Standard methods of Chemical analysis, 6th Ed. Vol. I and II( D. Van Nostard Comp.)
- 2) I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I & II
- 3) F. D. Snell: Encyclopedia of industrial Chemical Analysis Vol. 1 to 20 (John Wiley)
- 4) Riech: Outline of Indutrial Chemistry.
- 5) K. H. Buchel: Chemistry of Pesticides (John Wiley)
- 6) Indian, Pharmacopoeia, British Pharmacopoeia and U. S. Pharmacopoeia.
- 7) V. M. Parikh: Absorption spectroscopy of organic molecules (Addision Wesley)
- 8) Willard, Merrite, Dean and Settle: Instrumental methods of analysis (CBS)
- 9) D. H. Williams and J. Fleming: Specroscopic methods in organic chemistry (Mc Graw Hill)
- 10) Silverstein : Spectroscopic Identification of organic compounds (John Wiley)
- 11) Jackmann and Sternhill : Applications of NMR spectroscopy of organic Chemistry (Pergamon Press)
- 12) J. D. Roberts : Nuclear Magnetic Resonance (Mc Graw Hill)
- 13) K. Benjamin : Mass Spectrometry
- 14) Nichollas: Aids to the Analysis of foods and Drugs.
- 15) A. H. Beckett and J. B. Stanlake; Practical Pharmaceutical Chemistry Vol. I & II (CBS publishers)
- 16) S. Ranganna:Handbook of analysis and quality control for fruits and vegetable products (McGraw Hill)
- 17) Ramalu: Analysis of pesticides

# Paper No. -XI, ACH 3.3: ELECTROANALYTICAL TECHNIQUES IN CHEMICAL ANALYSIS

#### **UNIT-I: Voltammetry Techniques**

Introduction, Principle, excitation signals in voltammetry, basic instrumentation based on operational amplifiers, voltammetric electrodes

Cyclic Voltammetry: Instrumentation, Determination of analytes using cyclicvoltammetry, Applications. Pulse voltammetry: Introduction, Normal Pulse Voltammetry, Reverse pulse voltammetry, Differential pulse voltammetry, Square wave voltammetry. Stripping voltammetry: Cathodic and Anodic stripping voltammetry, Electrodeposition step, Voltammetric completion of the analysis, adsorptive striping methods, voltammetry with microelectrodes. Practical applications in analytical chemistry and research.

# **UNIT-II:**

# a) Ion selective electrodes & Electrochemical sensors:

Introduction, types and construction of electrodes, glass electrode, solid state and precipitate electrodes, liquid – liquid membrane electrodes, enzyme and gas electrodes, Chemically modified electrode, Enzyme based electrode, catalytic electrodes, ultramicroelectrodes and applications.

# b) Electrogravimetry

Introduction, Types of electrogravimetric techniques, Diffusion Migration, Convection, instrumentations, applications.

# UNIT –III: Particle Size Analysis

Introduction, Low angle LASER light scattering: Instrumentation, theoretical models, Mie theory, Fraunhofer diffraction theory, particle size distribution analysis, Applications. Dynamic Light Scattering: Introduction, Instrumentation, photodetector sample cell and sample handling, Applications, Photosedimentation: Setting velocity and particle size, Stokes equation, Instrumentation, sedimentation modes, Particle size distribution analysis, photometric measurements and applications. Comparison with particle size measurements using XRD, SEM and TEM. Practical applications in analytical chemistry and research.

# UNIT –IV: Electrophoresis:

Introduction, Paper electrophoresis Principle, Factors governing migration of ions, Supporting media (gel, paper, cellulose, acetate, starch, polyacrylamide, agarose, sephedax and thin layers) Techniques of electrophoresis: Low and high voltage, iso electric focusing, continuous electrophoresis, capillary electrophoresis, Zone, gel, isotaechophoresis and miceller electro kinetic capillary chromatography, instrumentation, detection and applications and Applications, Numericals.

# **Reference Books:**

- 1) R.D. Braun, Introduction to Instrumental Analysis.
- 2) D.A.Skoog, F. J. Holler, Principles of Instrumental Analysis, 6th edition.
- 3) Willard, Deritt, Dean and Settle, Instrumental methods of Analysis.
- 4) F. J. Welcher, Standard Methods of chemical Analysis Vol.3, PartA & B.
- 5) G.W. Ewing, Instrumental Methods of Analysis 4th and 5th editions.
- 6) Chatawal and Anand, Instrumental Methods of Analysis.
- 7) Bassett, Denney-Jeffer and Mendham, Vogel's Textbook of Quantitative Inorganic Analysis,(5th edition).
- 8) Electro-analytical chemistry, edited by H.W. Nurnberg.
- 9) Stulic, Ion selective electrodes (John Wiley).
- 10) Introduction to instrumental analysis by R. D. Broun, Mc Graw Hill (1987)
- 11) Instrumental methods of chemical analysis by H. Willard, D.Merrit, J.A. Dean and F.A. Settle. Sixth edition CBS (1986)
- 12) Fundamentals of Analytical Chemistry by D. A. Skoog, D. M. West and H. J. Holler sixth edition (1992) and Principles of Instrumental Analysis Skoog, West, Niemann
- 13) Vogel Text Book of quantitative analysis 6th Ed.

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#### **ELECTIVE PAPERS**

#### Paper No. -XII(A), ACH 3.4(A): ENVIRONMENTAL CHEMICAL ANALYSIS AND CONTROL

#### **UNIT-I:** Sampling in analysis

Definition, theory and techniques of sampling, sampling of gas, liquids and solids, Criteria of Good sampling, Minimization of Variables, transmission and storage of samples, high pressure ashing techniques (HPAT), particulate matter, its separation in gas stream, Filtering and gravity separation. Analysis of particulate matter like asbestos, mica, dust and aerosols etc

#### **UNIT-II: Electrochemical and spectral methods Environmental analysis**

Introduction to instrumental techniques, principle instrumentation and applications with respect to environmental analysis of Conductometry, Potentiometry, Ion selective electrodes, Amperometry, Coulometry, Atomic absorption spectrometry, Atomic fluorescence spectrometry, Inductively coupled plasma spectrometry, Turbidimetry, Non Dispersive Infrared Analysis (NDIR).

#### **UNIT-III:** Air and Water Pollutant Analysis

Chemistry of Air pollutants, characterization. source, methods of analysis of air pollutants; CO, CO<sub>2</sub>, NO<sub>X</sub>, NH<sub>3</sub>, H<sub>2</sub>S, SO<sub>2</sub> etc. Monitoring Instruments, Potable and Industrial water, major and minor components, dissolved oxygen (DO) Chemical oxygen demand(COD) Biochemical oxygen demand (BOD) and their measurements. Analysis of Pd, Cd, Hg, Cr, As and their physiological manifestations. Quality of industrial waste water analysis for organic and inorganic constituents. Chemistry of odour and its measurements.

#### **UNIT-IV: Organic Pollutants and Their Analysis**

Sources, disposal, treatment and analysis of phenolic residues, methods of recovery of phenols from liquid effluents, Organomercurials and its analysis, Analysis of organochlorine pesticides, volatile organic pollutants and their analysis

#### **Recommended books:**

- A.K. De : Standard Methods of Waste and Waste water analysis. 1)
- P. M. S. Monk Fundamentals of Electroanalytical chemistry-John Wiley & Sons (2001) 3. 2) Instrumental methods of chemical analysis H. Kaur
- S.M. Khopkar, Environmental Chemistry; Environmental pollution analysis 3)
- M.S. Creos and Morr, Environmental Chemical Analysis, American publication(1988) 4)
- 5) A.K. De, Environmental Chemistry, New Age International publishers. Moghe and Ramteke, Water and waste water analysis : (NEERI)
- A.C. Stern, Air pollution: Engineering control Vol.IV(AP) 6)
- P.N.Cheremisinoff and R.A.Young, Air Pollution controland Design.Hand Book Vol.I&II 7) (Dekker)
- 8) R.B.Pohasek, Toxic and Hazardous waste disposal, Vol.I & II (AAS)
- 9) M.Sitting, Resources Recovery and Recycling, Handbook of industrial Waste.
- B.K.Sharma, Industrial Chemistry. 10)

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UNIT-I: Ultra Purity and Ultra trace Analysis

11) S.P.Mahajan, Pollution Control in Process Industries.

UNIT-I: Ultra Purity and Ultra trace Analysis (15) Ultra purity and ultra trace analysis, laboratory dosing, purification of reagents, Preconcentration Techniques, Methods of trace analysis such as NAA, XRF, AAS and ICP, High purity materials for electronic industry, contamination control during analytical operations.

Paper No. – XII(B), ACH 3.4(B): RECENT ADVANCES IN ANALYTICAL CHEMISTRY

# **UNIT-II: Radio-analytical Chemistry**

Separation methods, Precipitation, solvent extraction and chromatographic methods. Activation analysis, basic principles, fast neutron activation analysis, radiochemical methods in activation analysis, Applications if Geo-chemistry, oxygen in metals. Isotope dilution analysis: Principles and applications. Sub-stoichiometric determination of traces of metals: Principles, techniques and experimental methods in the determination of As, Pb and Hg.

# UNITS-III: Advanced Techniques in Analysis

# Nuclear Magnetic Resonance Spectroscopy (<sup>1</sup>H NMR):

Elementary ideas (Recapitulation); Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

# <sup>13</sup>C Nuclear Magnetic Resonance Spectroscopy

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

#### **UNIT-IV: Electron Spin Resonance Spectroscopy**

Electron behavior, ESR spectrometer, Spectra, Hyperfine interaction, free radical and interpretation of the spectra, Applications in quantitative analysis. Numerical problems.

#### References

- 1) Garen W. Ewing, Analytical Instrumentation, Handbook, Marcel Dekker Inc. (1997).
- 2) Mereitt, Dean, Settel, Instrumental methods of Chemical Analysis.
- 3) M. Zeif and J.W.Mitchell, Contamination Control in trace elemental analysis.
- 4) Ajuja, Ultrapurity.
- 5) Minczewski, Chwastowska and Dycozynski, Separation and pre-concentration methods in Inorganic trace analysis. Ellis Haward.
- 6) Cali, trace Analysis of semiconductor Materials Pergamon.
- 7) Overman and Cleark, Radioisotopes techniques MGH.
- 8) Tolgyessy, Brown and Kyrs, Isotope dilution analysis.
- 9) Leniham and Thomson, Activation Analysis(AP)
- 10) Ruzica and Stary, Substopchiometry in Radiochemical Analysis. Pergamon.
- 11) Ladd and Lee, Radiochemistry.
- 12) Clerk, Handbook of Radiochemical methods
- 13) Price, Nuclear radiation detections.

# 12) R.A.Horne, Chemistry of our Environment.

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# M.Sc. Part-II (Sem-III)

# Analytical Chemistry Practical Course ACHP-V and ACHP-VI List of Experiments:

# Major:

- 1. Estimation of Sn, Zn, Cu and Pb from Bronze alloy (volumetric, gravimetric or colorimetric techniques can be used)
- 2. Estimation of Ca and Fe from milk powder
- 3. Analysis of Galena ore
- 4. Analysis of Benzoic acid and salicylic acid from medicated powder
- 5. Analysis of vitamin A in food products
- 6. Estimation of Aspirin
- 7. Kjeldahl's method of protein estimation in foods and feeds
- 8. Analysis of Lindane in BHC powder.
- 9. Determination of pK value of an indicator.
- 10. Polarographic estimation of traces of Cu, Cd, Ni, Zn and Fe in sample solution.
- 11. To study the complex formation between Fe(III) and salicylic acid and determine the stability constants of the complex by Job's variation method.
- 12. To determine the equivalence conductance and dissociation constant using Kolharach Law at infinite dilution independent of ionic mobility of weak electrolyte.
- 13. Any other suitable experiment may be added when required.

# Minor:

- 1. Analysis of plaster of Paris for calcium content
- 2. Fertilizer analysis for P (colorimetrically), K (Flame photometrically).
- 3. Determination of Barium ions by Turbidimetry.
- 4. Analysis of iodized table salt.
- 5. Analysis of soda ash.
- 6. Estimation of copper fungicide
- 7. Analysis of sulpha drug
- 8. Analysis of vitamin-C in juices and squashes.
- 9. Analysis of ethambutol
- 10. Identification of organic compounds by their IR spectra
- 11. Determination of strength of acetic acid in commercial vinegar by conductometric method.
- 12. Determination of chloride content from saline water by potentiometry.
- 13. Estimation of bicarbonate and carbonate by potentiometric method.
- 14. Estimation of Fe by ceric sulphate and potassium dichromate titration potentiometrically.
- 15. XRD and Thermal analysis Kaolinite, cobalt oxalate and zinc oxalate.
- 16. Estimation of vitamin B2 in the medicinal tablets fluorimetrically.
- 17. Kinetic study of hydrolysis of ethyl acetate in presence of OH ions conductometrically.
- 18. Determination of pK of given dibasic acid pH-metrically.
- 19. Determination of relative strength of acetic acid, chloroacetic acid and trichloro acetic acid by conductometrically.

(At least 10 major and 10 minor experiments should be carried out)

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# M.Sc. Part-II (Sem-IV) Analytical Chemistry

# Paper No. -XIII, ACH 4.1: MODERN SEPARATION METHODS IN ANALYSIS

# **UNIT-I:** Advanced Gas Chromatographic Techniques

Principles, Plate theory, Instrumentation and working of a Gas Chromatograph, sampling, sample pretreatment, sample injection types, columns, Detectors, programmed temperature G.C., Applications. Pyrolysis gas and vapour phase chromatography-instrumentation and techniques, advantages and applications. Gas chromatography-Mass Spectrometry, interface, instrumentation and applications. Introduction to TGA-MS/TGA-GC-MS and significance. Practical applications and examples in analytical chemistry and research.

# **UNIT-II: Advanced Liquid Chromatographic Techniques**

High Performance Liquid Chromatography (HPLC) and Ultra Performance Liquid Chromatography (UPLC)-Principle, instrumentation, mobile phase, Stationary support in HPLC, detectors and applications. Super critical fluid chromatography (SCFC), characteristics, instrumentation and applications. Comparison of HPLC and GLC with SCFC. Liquid Chromatography-Mass Spectrometry interface, instrumentation, advantages and applications. Practical applications and examples in analytical chemistry and research.

# **UNIT-III: Ion Chromatography**

Principles, structure and characteristics of resins, eluent, supressor columns and detectors used in Ion Chromatography, commercial scope, analytical applications, environmental speciation by Ion Chromatography. Practical applications and examples in analytical chemistry and research.

# UNIT –IV: A) Modern extraction and separation techniques

Basic principles, classification of solvents extraction systems, extraction equilibria, factors affecting extraction process, application of  $\beta$ - diketones,  $\delta$ Hydroxyquinoline, dithicarbamaes, xanthenes, Thio, separation of non metals and metals. Separation of transition metal ions using ion exchangers.

Solid phase extraction, solid phase microextraction, sonic extraction, accelerated solvent extraction, soxhlet extraction.

#### **B) Extractive Chromatographic Separations**

Introduction, Theoretical aspects of extraction chromatography, solvent extraction and extraction chromatography with chelating ligands, extraction chromatography by ion pair formation, extraction chromatography by solvation, extraction equilibria, nature of stationary phase in extraction chromatography, inert support, techniques in extraction chromatography, extraction chromatography with tributyl phosphate and other applications. Practical applications and examples in analytical chemistry and research.

#### **Recommended Books:**

- 1) A.I.Vogel, a text Book of Quantitative Inorganic Analysis.
- 2) W H Willard, L L Merritt and J A Dean, Instrumental Methods of Analysis.
- 3) S. M.Khopkar, Basic Concepts in Analytical Chemistry.
- 4) LR. Shyder and C.H.Harvath, An Introduction to separation Science. Wiley Interscience.
- 5) James S Fritz and George H.Schenk Jr. Quantitative Analytical Chemistry, 2nd editions Allyn and Bacon Inc. Bosten.
- 6) J.G.Dick, Analytical Chemistry.

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- 7) R.L.Pescok and L.D.Shield, Modern Methods of Chemical Analysis.
- 8) O.Samuelson : Ion Exchange separation in analytical chemistry (Jhonwiley , 1963)
- 9) Y. Marcus and A. S. Kertes : Ion Exchange and solvent Extraction of metal complexes (Wiley Interscience, 1969)
- 10) J. A. Marinsky and Y. Marcus : Ion exchange and solvent Extraction (Marcel Dekker, INC , New York, 1973)
- 11) G. H. Morrison and H, Freiser : Solvent Extraction in Analytical Chemistry (John Wiley, New York, 1958)
- 12) A. K. Da, S. M. Khopkar and R. A. chalmers :solvents Extraction of metals (Von Nostrant Ravinhold, 1970)

# Paper No. -XIV, ACH 4.2: ORGANIC INDUSTRIAL ANALYSIS

# UNIT – I: Industrial Analysis

# A) Analysis of oils, fats and Soaps

Introduction to natural fats and oils; isolation of oils from natural resources and their purification. Analysis of oils and fats: Softening point, Congeal point, Titre point, Cloud point, Iodine, saponification, acid, hyroxyl, R-M and Polenske value, Elaiden test, etc.

Introduction to soaps, manufacture of soaps (in brief), analysis of soaps: total anhydrous soap and combined alkali, potassium, water, free fatty acids, saponifiable and non-saponifiable matter in soaps, estimation of phenol, copper and germicidal agents in soaps, determination of inorganic fillers and soap builders, and other additives, estimation of soap in detergents (THAM method)

# **B)** Analysis of Detergents

Classification of detergents, analysis of raw materials, separation as alcohol soluble and alcohol insoluble matter, additives in detergent formulation (chlorides, sulfates, phosphates, silicates, borates, oxygen releasing substances, CMC, EDTA, etc.), their role and analysis; analysis of active ingredients in detergents (methylene blue and Hyamine-1622 method).

# UNIT – II: Food and Food Additive Analysis

#### A) Food Analysis

Food flavors, food colors, food preservatives, analysis of milk and milk products, adulterants in milk and their identification, analysis of honey, jam and their major component. Practical applications and examples in analytical chemistry and research.

# B) Food Additive Analysis

Additives in animal food stuff: Antibiotics: penicillin, chlorotetracyclin, oxytetracyclin in diet supplements; Identification and estimation of growth promoting drugs such as. sulfaquinoxaline, methyl benzoquate, sulfanitran, pyrimethamine, nitrovin, nitrofurazone, acinitrazole, etc

# **UNIT-III: Analysis of cosmetics products**

Introduction to cosmetics, definition, types of cosmetics, background, development in cosmetic industry, issues in cosmetic industries (contamination and adulteration), future scope and role of analytical chemistry.

# A) Analysis of cream and lotions

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Composition of creams and lotions, determination of water, propylene glycol, non-volatile matter and ash content; estimation of borates, carbonates, sulphates, phosphates, chlorides, ammonia, nitromethane, oxalic acid, 4- hydroxy benzoic acid, sodium iodate, free formaldehyde, H<sub>2</sub>O<sub>2</sub>, mercatoacetic acid, titanium and zinc oxides. Practical applications and examples in analytical chemistry and research.

# **B)** Analysis of face powder

Composition of face powder, estimation of boric acid, Mg, Ca, Zn, Fe, Al and Ba. Analysis of deodorants and antiperspirants-composition, analysis of fats and fatty acids, boric acid, magnesium, calcium, zinc, iron, titanium, aluminium, phenol, methanamine, hexachlorophenone, sulphonates, urea, etc. Practical applications and examples in analytical chemistry and research.

# **UNIT-IV:** Analysis of Paints, pigments and petroleum products

# A) Analysis of Paints and pigments

Composition of paint, preliminary inspection of sample, test on the total coating, separation and estimation of pigments, binder and thinner of latex paints; modification of binder, flash point of paints. Practical applications and examples in analytical chemistry and research. (07)

# (B)Analysis of petroleum products

Introduction, constituents and petroleum fractionation, quality control; - specific gravity, viscosity, Cloud point, pour point, flash point, vapor pressure, Doctor test, sulphuric acid absorption, aniline point, and colour détermination, cloud point, pour point. Determination of water, neutralization value (acid and base numbers), ash content, sulphur and mercaptan sulphur. Determination of lead in petroleum; Analysis of coal and coke: Types, composition, preparation of sample, proximate and ultimate analysis calorific value by Bomb Colorimetry.

# **Reference Books:**

- 1) S. R. Junk and H. M. Pancoast: Hand book of sugars(AVI)
- 2) B. Bilot and B. V. Well: Perfumary technology (JW)
- 3) I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I and II
- 4) D. Pearson: Laboratory techniques in food analysis.
- 5) S. Ranganna: Handbook of Analysis and Quality control for fruits and vegetable products, 2nd Ed.(Mc Graw Hill.)
- 6) Nicholls : Aids to the analysis of foods and drugs.
- 7) G. J. Mountrey: Poultry product technology (AVI)
- 8) Karamer Twig: Quality control for food industry (AVI)
- 9) G. F. Longonan: the analysis of detergents and detergent products (JW)
- 10) A. Davidsohn & B. M. Mlwidaky : Synthetic detergents (Book center, Mumbai)
- 11) M. Ash and L. Ash: A formulary of cosmetic preparations. (G. Goodwin)
- 12) Kurl Bauer, Dorothea Garhe, Horst Surburg: Common fregrance and flavour materials, (VCH publisher, New York)
- 13) F. J. Welcher: Standard Methods of Chemical analysis Vol I & II (6th Ed.)
- 14) S. N. Mahendru: Analysis of food products (Swan Publishers)

# Paper No. - XV, ACH 4.3: ADVANCED METHODS IN CHEMICAL ANALYSIS

# **UNIT-I : Fluorescence and Phosphorescence Spectrophotometry**

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Fluorimetry, types of luminescence, Instrumentations, theories of fluorescence and phosphorescence, electronic transition, structural factors, solvatochromism, solvation dynamics, faith of excited molecules, solvent effect on fluorescence, effect of intermolecular process, fluorescence anisotropy and time domain fluorescence life time measurements. Relation between concentration with fluorescence and phosphorescence intensity, fluorescence quenching mechanism, resonance energy transfer. Chemiluminescence, Fluorescence sensing, Synchronous spectrum, Fluorescent nanomaterials. Practical applications, examples and problems in analytical chemistry and research.

#### **UNIT-II: Kinetic Methods of analysis**

Theoretical basis of kinetic methods of analysis, methods of determining amount of the substance, Tangent Method, Fixed Time and Concentration method. Addition Method, Oxidation Reactions of H2O2 with thiosulphate, iodide and amino, Enzyme catalyzed reactions. Inhibitors and Activators.

# **UNIT – III: Photoelectron spectroscopy**

Basic principles, photoelectric effects, Photoionization process, Koopman's theorem, photoelectron spectra of simple molecules, ESCA, chemical shift, Auger electron spectroscopy – basic idea.

# **UNIT-IV: X-ray spectroscopy**

Introduction, X-Ray generation, Properties of X-radiation, X-Ray, Instrumentation, X-Ray Absorption, Fluorescence and Diffraction methods of analysis and their applications

#### **Recommended Books:**

- 1) Gary D Christian, Analytical chemistry 6<sup>th</sup> edition. John Willey and sons INC (2003) H.
- 2) Kaur, Instrumental Methods of Chemical Analysis. Pragati Prakashan, Meerut.
- 3) W H Willard, L L Merritt and J A Dean, Instrumental Methods of Analysis.
- 4) S. M.Khopkar, Basic Concepts in Analytical Chemistry.
- 5) D. Skoog and D. West, Principle of Instrumental Analysis.Holl Seamlers.
- 6) E. Berlin, Principles and Practice of X-Ray Spectrometric Analysis, Plenum, NewYork.
- 7) J. Winefordner, S. Schulman and T O Haver :Luminescence Spectrometry in
- 8) Analytical Chemistry. Wiely Interscience NewYork.
- 9) H. Mark and G Rachnitz, Kinetics in Analytical chemistry. Interscience NY.
- 10) 8.Gary D Christian, Analytical chemistry 6<sup>th</sup> edition. John Willey and sons INC (2003)
- 11) Engineering chemistry, R Gopalan, G. S. Nagrajan.
- 12) 10 Engineering chemistry B. K. Sharma

# **ELECTIVE PAPERS**

#### Paper No. -XVI(A), ACH 4.4(A): INDUSTRIAL ANALYTICAL CHEMISTRY

#### **UNIT-I: Spectrochemical Methods of Analysis**

Introduction to spectrochemical methods. Electronic spectra and molecular structure, NIR spectrometry for nondestructive testing. Solvents for spectrometry ,FTIR spectrometer ,fluorometry, optical sensors. Analysis of ores –bauxites, dolomites, monazites. Analysis of Portland cement.

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# UNIT-II: Analysis of metals and alloys

Foundry materials, ferroalloys, and special steels, slags, fluxes. Analysis of alloys ,bronze, brass, Alnico and Nichrom

# UNIT-III: Analysis of soil and fertilizers

Method of soil analysis, soil fertility its determination, determination of inorganic constituents of plant materials, Chemical analysis as measure of soil fertility, analysis of fertilizers.

# **UNIT-IV: Analysis of Commercial materials**

Analysis of explosive materials, TNT, RDX, lead azide, EDNA (ethylene dinitramine). Analysis of conducting polymer, resins and rubber. Analysis of luminescent paints, Analysis of lubricants and adhesive.

# **Recommended Books:**

- 1) Hillebrand Lhundel, Bright and Hoffiman, Applied Inorganic Analysis, John Wiley.
- 2) Snell and Biffen, Commercial Methods of Analysis.
- 3) P.G. Jeffery, Chemical Methods of Rock Analysis, Pergamon.
- 4) Buchel, Chemistry of Pesticides. J Wiley.
- 5) Rieche, Outlines of Industrial Organic Chemistry, ButterWorth.
- 6) F.A.Henglein, Chemical Technology, Pergamon.
- 7) Kent, Riegl's Industrial Chemistry, Rainhold.
- 8) Chopra and Kanwar, Analytical Agriculture Chemistry, Kalyani Publishers.
- 9) Aubert and Pintes, Trace Elements in Soils.
- 10) Bear, Chemistry of Soil.
- 11) Hauson, Plant Growth Regulators, Noyes.
- 12) P.G.Jeffery and D.J. Hatchinson, Chemical Methods of Rock Analysis.
- 13) F.J.Weleher, Standard Methods of Chemical Analysis, A Series of Volumes Robert and Krigeger Publishing Company.
- 14) I. M.Kolthoff and PJ Ewing, Treatise o Analytical Chemistry, A series of Volumes.
- 15) R.D. Reeves and R.R. Brooks, Trace element Analysisof Geological Materials, John Wiley & Sons NewDehli.
- 16) W.M. Johnson and J.A.Maxwell,Rock and Mineral Analysis, John Wiley and Sons, NewYork.
- 17) W. F. Hildebrand, G H C Landell and HABrighot, Applied Inorganic Analysis, John Wiley 2nd Edition.
- 18) K. J. Das, Pesticide Analysis(MD).

#### Paper No. -XVI(B), ACH 4.4(B): QUALITY ASSURANCE AND ACCREDITATION

#### **UNIT-I: Quality Assurance**

Introduction to Quality Control and quality assurance: Concepts and significance. Quality control and statistical techniques: Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, use of blind samples in quality control, use of proficiency evaluations in quality control. Calibration and maintenance of Instruments / Equipment: Instrument calibration – linear calibration curves, equipment calibration, frequency of calibration, calibration of common laboratory instrument and equipment (Analytical balances, volumetric glassware, ovens, furnaces, UV / Visible spectrophotometer, pH

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meter, conductivity meter, IR spectrophotometers, AAS, GC, HPLC etc.,). Maintenance of instruments and equipment

#### UNIT-II: Documentation for Quality Assurance: Raw Data

Type of notebooks, control of notebook distribution and data entry. General Reagents and volumetric reagents. Sampling – sampling methods, sample labelling, sample login/register. Sample analysis, reporting, recording and personal training.Instrument calibration and maintenance. Analytical report, Personnel, training, records - professional personnel, technician personnel. Filing quality assurance documentation. Good laboratory practices and personnel, Quality Programme, Instrument and Organisation calibration, Customer Satisfaction.

#### **UNIT-III: Documentation for Quality Assurance: Raw Data**

Computers and quality assurance: Sample handling. Data Acquisition. Quality control data and calculations. Computer generated analytical reports. Security considerations. Hardware and software. Establishing a Quality Assurance program: Management commitment. Define the quality assurance program. Writing standard operating procedures. Topics for standard operating procedures. Consolidating the programme.Monitoring the program – monitoring quality assurance data, reporting quality assurance problems. Writing the quality assurance manuals.

#### **UNIT-IV Quality Accreditation**

(15)

Laboratory Accreditation: Need for laboratory accreditation. International aspects of laboratory accreditation and in India. Criteria for laboratory accreditation. Benefits of laboratory accreditation, Evolution and significance of Quality Management, Background to ISO 9000, comparison between ISO-9001, ISO-9002 & ISO-9003., ISO 9000-2000 series of standards on quality managament system,- evolution of series of standards, introduction to ISO organization, Registration/ certification- benefits of QMS certification. Structure of ISO 9000-2000 family of standards. Advantages of ISO 9000-2000. Requirements of ISO 9001-2000 QMS and applications, Steps for effective implementations. Significance of ISO - 9001, 9002, 9003 & 9004. Requirements of ISO9000/ IS14001. Concepts of OHSMS (BS 8800) Quality Managament Principles in QMS, QMS documentation, Quality Manual, Quality policy, conformities and Nonconformities

#### **Recommended Books:**

- 1) Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York, 1986.
- 2) Applying ISO-9000 Quality Management Systems, International Trade Centre Publishing, UNCTAD/WTO. Geneva, Switzerland, Indian Edition Printed by D.L.Shah Trust.
- 3) How to practice GLP, PP Sharma, Vandana Publications, 2000, New Delhi
- 4) Training manuals on ISO 9000 / 2000 PQM, Girdhar J Gyani, Raj Publishing House, 2001
- 5) Quality Assurance in Analytical Chemistry, B.W. Wenclawiak, Springer, India, 2004.

# M.Sc. Part-II (Sem-IV)

# Analytical Chemistry Practical Course ACHP-VII and ACHP -VIII List of Experiments:

# Major

- 1. Cement analysis
- 2. Analysis of Chrome steel alloy for Cr and Ni content
- 3. Analysis of bauxite ore to estimate the amount of silica, aluminium and iron.

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- 4. Estimation of salicylic acid and zinc oxide from medicated powder
- 5. Determination of saponification value and iodine value of oil
- 6. Estimation of amount of copper (II) with EDTA spectrophotometrically.
- 7. Simultaneous spectrophotometric determination of Cr and Mn
- 8. Analysis of milk.
- 9. Analysis of some common pesticides, insecticides, plastics and detergents.
- 10. Estimation of Urea, Uric acid and creathinine in Urine.
- 11. Estimation of blood sugar, calcium and total nitrogen and non-protein nitrogen in blood.
- 12. Studies on the effect of substituent at ortho position of benzoic acid on its equilibrium constant pH metrically.
- 13. Agricultural analysis of soil sample, animal feeds, soil micronutrients, milk powder for Ca, Fe and P content.

### Minor

- 1. Estimation of Fe from soil sample
- 2. Analysis of Na and K from soil sample
- 3. Determination of chemical oxygen demand of water sample (dye solution)
- 4. Estimation of lactose from milk sample
- 5. Determination of flash point of oil/fuel
- 6. To estimate the amount of glycine from amino acid
- 7. To determine the amount of alkali content of antacid tablet titrimetrically
- 8. Determination of dissociation constant of weak acid pH-metrically.
- 9. Estimation of Zn in the given solution fluorimetrically.
- 10. Determination of pK of tribasic acid, by potentiometry.
- 11. Determination of critical micelle concentration of given surfactants conductometrically
- 12. Estimation of acetyl salicylic acid in the given aspirin tablet by titrating against 0.1N alcoholic KOH potentiometrically.
- 13. To determine the acid base dissociation constant and isoelectric point of amino acid pH metrically
- 14. (Any other experiments may be added when required.)

(At least 6 major and 6 minor experiments should be carried out. More time should be given to project work)

### **B) Project:**

Projects on contemporary issues of societal significance which should include literature survey, synthesis, reaction mechanism and kinetics, analysis of air, water and soil samples, solid state materials, energy generation and storage materials, nanochemistry, green chemistry, organic materials, organo-metallic, bioinorganic materials, novel materials etc. The Project/Review work (50 Marks) will be examined jointly by internal and external examiners at the time of practical examination.

(Any other experiments may be added when required.)

### Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

Equivalence in Accordance wi	th titles and contents of the papers
M. Sc. In Inorganic Chemistry Semester III and Semester IV	

Old Course(2013)	New Course (2018)	
SEMESTER III		
Paper No- ICH-IX : INORGANIC CHEMICAL SPECTROSCOPY	Paper No- IX, ICH 3.1 : INORGANIC CHEMICAL SPECTROSCOPY	
Paper No ICH -X: COORDINATION CHEMISTRY – I	Paper No. –X, ICH 3.2: COORDINATION CHEMISTRY – I	
Paper No ICH-XI: NUCLEAR CHEMISTRY	Paper No. –XI, ICH 3.3 : NUCLEAR CHEMISTRY	
ELECTIVE PAPERS Paper No ICH - XIIA:	ELECTIVE PAPERS Paper No. –XIIA, ICH 3.4(A):	
ENVIRONMENTAL CHEMISTRY	ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY	
Paper No ICH - XIIB: ORGANOMETALLIC CHEMISTRY	Paper No. –XIIA, ICH 3.4(A): ORGANOMETALLIC AND BIOINORGANIC CHEMISTRY	
Paper No ICH - XIIC: SELECTED TOPICS IN INORGANIC CHEMISTRY	Paper No. –XIIC, ICH 3.4(B) : SELECTED TOPICS IN INORGANIC CHEMISTRY	
	TER IV	
Paper No ICH - XIII : INSTRUMENTAL TECHNIQUES.	Paper No. –XIII, ICH 4.1: INSTRUMENTAL TECHNIQUES.	
Paper No ICH - XIV : COORDINATION CHEMISTRY-II	Paper No. – XIV, ICH 4.2: COORDINATION CHEMISTRY-II	
Paper No ICH - XV: CHEMISTRY OF INORGANIC MATERIALS	Paper No. –XV, ICH 4.3: CHEMISTRY OF INORGANIC MATERIALS	
ELECTIVE PAPERS	ELECTIVE PAPERS	
Paper No ICH - XVI(A) : SEPARATION SCIENCE	Paper No. –XVI(A), ICH 4.4(A): ENERGY AND ENVIRONMENTAL CHEMISTRY	
Paper No ICH - XVI(B): RADIATION CHEMISTRY	Paper No. –XVI(B), ICH 4.4(B): RADIATION CHEMISTRY	
Paper No ICH - XVI(B): APPLIED BIOINORGANIC CHEMISTRY	Paper No. –XVI(A), ICH 4.4(A): ENERGY AND ENVIRONMENTAL CHEMISTRY	

Old Course(2013)	New Course (2018)	
SEMESTER III		
Paper No- OCH-IX: Organic Reaction	Paper No-IX,OCH 3.1: Organic	
Mechanism	Reaction Mechanism	
Paper No OCH- X: Advanced	Paper No -X, OCH 3.2: Advanced	
Spectroscopic Methods	Spectroscopic Methods	
Paper No- OCH- XI: Advanced	Paper No-XI, OCH 3.3 : Advanced	
Synthetic Methods	Synthetic Methods	
Paper No- OCH- XII: Drugs and	Paper No-XII(A), OCH 3.4(A): Drugs	
Heterocycles	and Heterocycles	
SEMESTER IV		
Paper No OCH- XIII: Theoretical	Paper No. –XIII, OCH 4.1:	
Organic Chemistry.	Theoretical Organic Chemistry.	
Paper No OCH- XIV :	Paper No. – XIV, OCH 4.2 :	
Stereochemistry	Stereochemistry	
Paper No OCH- XV :Chemistry of	Paper No. –XV, OCH 4.3 :Chemistry	
Natural Products	of Natural Products	
ELECTIVE PAPERS	ELECTIVE PAPERS	
Paper No OCH- XVI : Applied	Paper No. –XVI(A), OCH 4.4 :	
Organic Chemistry	Organic Industrial Chemistry	
Paper No- OCH- XVI(A): Bioorganic	Paper No. OCH 4.4(B): Bioorganic	
Chemistry	Chemistry	

Equivalence in Accordance with titles and contents of the papers M. Sc. In Organic Chemistry Semester III and Semester IV

### M. Sc. In Physical Chemistry Semester III and Semester IV

Old Course(2013)	New Course (2018)
SEMES	STER III
<b>Paper No - PCH - IX</b> : ADVANCED	<b>Paper No-IX, PCH 3.1</b> : ADVANCED
QUANTUM CHEMISTRY	QUANTUM CHEMISTRY
<b>Paper No - PCH -X</b> :	<b>Paper No-X, PCH 3.2</b> :
ELECTROCHEMISTRY	ELECTROCHEMISTRY
<b>Paper No - PCH - XI</b> : MOLECULAR STRUCTURE-I	<b>Paper No-XI, PCH 3.3</b> : MOLECULAR STRUCTURE-I
<b>Paper No - PCH - XII</b> : SOLID STATE	<b>Paper No-XII(A), PCH 3.4(A)</b> : SOLID
CHEMISTRY	STATE CHEMISTRY
ELECTIVE PAPERS	ELECTIVE PAPERS
<b>Paper No - PCH - XII(A)</b> : ADVANCED	<b>Paper No-XII(B), PCH 3.4(B)</b> :
CHEMICAL KINETICS	ADVANCED CHEMICAL KINETICS
<b>Paper No - PCH - XII (B)</b> : RADIATION	<b>Paper No-XII (C) PCH 3.4(C)</b> :
AND PHOTOCHEMISTRY	RADIATION AND PHOTOCHEMISTRY
SEMES	TER IV
<b>Paper No. PCH-XIII</b> :	<b>Paper NoXIII, PCH 4.1</b> :
HERMODYNAMICS AND MOLECULAR	THERMODYNAMICS AND
MODELING	MOLECULAR MODELING
<b>Paper No. PCH-XIV</b> : CHEMICAL KINETICS	<b>Paper No –XIV, PCH 4.2</b> : CHEMICAL KINETICS
<b>Paper No. PCH-VX</b> : MOLECULAR	<b>Paper No-XV, PCH 4.3</b> : MOLECULAR
STRUCTURE-II	STRUCTURE-II
ELECTIVE PAPERS	ELECTIVE PAPERS
Paper No. PCH-XVI (A): SURFACE	<b>Paper No-XVI (A), PCH 4.4(A)</b> :
CHEMISTRY	SURFACE CHEMISTRY
<b>Paper No. PCH-XVI (B)</b> : CHEMISTRY	<b>Paper No-XVI (B), PCH 4.4(B)</b> :
OF MATERIALS	CHEMISTRY OF MATERIALS
<b>Paper No. PCH-XVI (C)</b> : BIOPHYSICAL CHEMISTRY	<b>Paper No-XVI (C), PCH 4.4(C):</b> BIOPHYSICAL CHEMISTRY

SEMESTER III         Paper No. ACH – IX : General Analytical Techniques       Paper No – IX, ACH 3.1: Advanced Analytical Techniques         Paper No. ACH – X : Organo Analytical Chemistry       Paper No– X, ACH 3.2 : Organo Analytical Chemistry         Paper No. ACH – X1 : Electroanalytical Techniques in Chemical Analysis       Paper No – XI, ACH 3.3: Electroanalytical Techniques in Chemical Analysis         ELECTIVE PAPERS       ELECTIVE PAPERS         Paper No. ACH–XII (A) : Environmental chemical analysis and control       ELECTIVE PAPERS         Paper No. ACH-XII (B) : Recent Advances in Analytical Chemistry       Paper No-XII (B). ACH 3.4(B) : Recent Advances in Analytical Chemistry         Paper No. ACH-XII : Chemical Analysis in Agro, Food and Pharmaceutical Industries       Paper No-XII (B). ACH 3.4(B) : Recent Advances in Analytical Chemistry         SEMESTER IV         Paper No. ACH – XII : Modern Separation method in Analysis       Paper No–XIV ACH 4.1: Modern Separation method in Analysis         Paper No. ACH – XIV : Organic Industrial Analysis       Paper No–XVI ACH 4.2: Organic Industrial Analysis         Paper No. ACH – XVI : Organic Industrial Analysis       Paper No–XVI (A), ACH 4.4(A): Industrial Analysis         Paper No. ACH – XVI (B): Paper No. ACH – XVI (B): Techniques in Forensic sciences and Microbiological Analysis       Paper No–XVI (A), ACH 4.4(A): Industrial Analytical Chemistry         Paper No. ACH – XVI (B):       Paper No–XVI (A), ACH 4.4(A): Industrial Analytical Chemistry	Old Course(2013)	New Course (2018)
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	Computational Chemistry	Industrial Analytical Chemistry

### M. Sc. In Analytical Chemistry Semester III and Semester IV

# SHIVAJI UNIVERSITY, KOLHAPUR.



Accredited By NAAC with 'A' Grade

**Revised Syllabus For** 

**Master of Science** 

Part- II

Applied Chemistry CBCS PATTERN

Syllabus to be implemented from

June, 2019 onwards.

### Shivaji University, Kolhapur

### **Department of Applied Chemistry**

### M.Sc. II. Semester III & IV Revised Syllabus under CBCS Pattern

### (To Be Implemented from June- 2019)

### **Programme Specific Outcome:**

M.Sc. Course in Applied Chemistry is a potential base provided by the Shivaji University, Kolhapur on University campus to educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic Laboratories. The M.Sc. course in Applied Chemistry aims to provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on analytical techniques. Particular attention is given to industrial applications of applied & advanced knowledge of Chemistry so that students are completely equipped to move into careers in academic, research, industrial and commercial organizations. The M. Sc. course in Applied Chemistry is providing broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of interdisciplinary branches of chemistry involving applied organic, inorganic, physical, analytical, industrial, pharmaceutical, polymer, nanoscience & technology.

The laboratory course particularly emphasis on green chemistry approach elaborating the need for waste minimization, substitution of non toxic chemicals and increasing the use of microscope and computational techniques. The laboratory courses are designed to provide an exhaustive and hands on working with various modern instruments. Final Semester is dedicated to project work giving students experience in solving real life problem under the supervision of faculty members involved in pursuing research and development projects usually related to industrial problem.

#### **Employment potential of the course:**

To provide properly qualified manpower for academic institutions R & D and QC laboratories of Indian chemical/pharmaceutical industries research organizations and forensic laboratories. M.Sc. course in Applied Chemistry can be helpful to the students to be self employed as it not only allows for an in-depth subject specific knowledge and opportunities to specializing in number of areas at the leading edge of the subject but also encourage students to develop problem solving and reflective working practices.

Title of the Course: M. Sc. Applied Chemistry.

Year of Establishment of Course: June 2007

Duration of the Course: '2' Year (4 Semester)

**Eligibility of Course:** Admission to the M. Sc. Applied Chemistry course will be open to candidates passing B. Sc degree in Chemistry of Shivaji University or any other statutory university, Institution in India or abroad with minimum 55% marks the candidate should have Chemistry as a principal subject of study at B.Sc. Course.

### The structure of M. Sc. Applied Chemistry Course:-

- 1) Theory course
- 2) Practical course
- 3) Seminars/ Tutorials
- 4) Industrial training/ Project work

#### M. Sc. Part – II Applied Chemistry,

### Semester – III

### **Core Papers**

Paper No. IX, APCH. 3. 1: Applied Inorganic Chemistry–I Paper No. X, APCH. 3.2: Applied Organic Chemistry–I Paper No. XI, APCH. 3.3: Applied Physical Chemistry–I

#### **Elective Papers**

Paper No. XII (A), APCH. 3.4 (A): Advanced Organic Chemistry–I Paper No. XII (B), APCH. 3.4 (B): Applied Analytical Chemistry–I Paper No. XII (C), APCH. 3.4 (C): Bioorganic Chemistry-I

Practical Course

: APCHP-V and APCHP-VI

### Semester – IV

### **Core Papers**

Paper No. XIII, APCH. 4. 1: Applied Inorganic Chemistry- II Paper No. XIV, APCH. 4. 2: Applied Organic Chemistry – II Paper No. XV, APCH. 4. 3: Advance Organic Chemistry – II

### **Elective Papers**

Paper No. XVI (A), APCH. 4. 4 (A): Inorganic Chemical Industries Paper No. XVII (B), APCH. 4. 4 (B): Pollution Monitoring and Control Paper No. XVIII (C), APCH. 4. 4 (C): Applied Analytical Chemistry–II

Practical Course

: APCHP-VII and APCHP-VIII

### SEMESTER III **M. Sc. Part II- APPLIED CHEMISTRY**

### Paper No. IX, APCH. 3. 1: Applied Inorganic Chemistry – I

### **UNIT-I: Electronic Properties of Transition Metal Complexes**

Energy terms, States, Microstates, Splitting of terms in weak octahedral and weak tetrahedral ligand field, Spin selection rule, Laporte selection rule, relaxation of selection rule, band intensities and band widths, Orgel diagrams of d<sup>n</sup>- configurations in octahedral and tetrahedral environments, Tanabe-Sugano diagrams(d<sup>2</sup> and d<sup>3</sup>coniguration), calculation of Dq, B and  $\beta$ values, Adjusted crystal field theory, MO diagrams for octahedral and tetrahedral complexes (with and without  $\pi$ -bonding), charge-transfer spectra, spectral properties of Lanthanides and Actinides.

### **UNIT-II: Magnetic Properties of Transition Metal Complexes**

Origin of magnetism, Types of magnetic behavior, Energy terms, Splitting of terms in weak octahedral and weak tetrahedral ligand field, Magnetic behavior of transition metal complxes: valence bond approach and crystal field approach, quenching of orbital angular momentum, temperature-dependent magnetism, measurement of magnetic susceptibility using Gouy and Faraday methods, magnetic properties of Lanthanides and Actinides.

### **UNIT III: Reaction of Transition Metal Complexes**

Labile and inert complexes; Ligand substitution reactions: Nucleophilic Subtitution (S<sub>N</sub>1and S<sub>N</sub>2, dissociative and associative mechanism); Electron transfer reactions (Redox reactions): Outer sphere and inner sphere mechanism, two electron transfers mechanism; Reactions of coordinated ligands; Isomerization reactions: Isomerization involving geometrical isomers.

#### **UNIT-IV: Nanoscience and Nanotechnology**

Introduction to nanoscience and nanomaterials and emergence of nanotechnology; Moore's law; Classification of nanomaterials; 1D, 2D, 3D with their examples, Experimental methods for preparation of nanomaterials: Chemical and Physical, synthesis of nanoparticles of gold, rhodium, silica, palladium, platinum, and silver; Size dependent properties of nanoparticles: optical properties, M.P., surface to volume ratio, Carbon: fullerenes and nanotubes. Applications of nanotechnology & Nanomaterials: Nanobiotechnology, nanosensors, nanomedicines(drug delivery and diagnosis), nanophotonics, environmental remediation etc., Implications of nanotechnology.

### **References:**

- Theoretical Inorganic Chemistry by Cotton & Willkinsons 1.
- 2. Concise Inorganic Chemistry- J. D. Lee
- Principles of Inorganic Chemistry-Puri, Sharma, Kalia 3.
- 4. Concise Coordination Chemistry-R. Gopalan, V. Ramalingam
- Fundamental Concepts of Inorganic Chemistry, Volume 5 and 6- Asim K Das and Madhua Das 5.
- Theoretical Principles of Inorganic Chemistry- Manku 6.
- 7. Elements of Magnetochemistry-Datta and Shymal
- 8. Inorganic chemistry- Alen Sharp
- 9. Nanotechnology: Principles and Practices- Sulbha Kulkarni
- Nanotechnology: Global Strategies, Industry Trends and Applications by J. Schulte. 10.
- Nanotechnology, Volume 1: Principles and Fundamentals by G. Schmid. 11.
- Solid State Chemistry: An Introduction.by L. E. Smart, E. A. Moore. 12.
- 13. Introduction to solid state Physics C. Kittel.

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### (15)

60 h

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### **Course Outcome:**

To understand basic facts and concepts in Electronic and Magnetic Properties of Transition Metal Complexes, its reactions. To be familiarized with the emerging areas of emergence of nanotechnology and their applications in Applied Inorganic Chemistry.

### Paper No. X, APCH. 3.2: Applied Organic Chemistry – I 60 h

### **Unit I: Molecular Orbital Theory**

Introduction, aromaticity in benzonoids, alternant and non alternant hydrocarbon, Huckels rule, energy level of pi molecular orbital and the concept of aromaticity, calculation of energies of orbitals in cyclic and acyclic systems and the stabilities of different systems. Calculation of charge densities, 'PMO' theory and reactivity index.

### **Unit II: Organic Synthesis**

Wolff Rearrangement, Sommelet-Hauser rearrangement, Stevens's rearrangement, Smiles rearrangement, Robinson ring annulations reaction, Simmon-Smith reaction, McMurry reaction, Heck reaction and Vilsmeier-Haack reaction.

### **Unit III:Organic Photochemistry**

Introduction, photochemical processes. Energy transfer, sensitization and quenching. Singlet and triplet states and their reactivity. Photoreaction of carbonyl compounds, enes, dienes, and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, photo-Fries and Di- Pi methane rearrangement reactions. Photoreactions of vitamin-D. Photochemistry of vision and photosynthesis. Singlet oxygen generation and reactions. Applications of photoreactions and their applications for industrial synthesis.

### **Unit IV: Free radical reactions**

Introduction, types of free radical reactions, detection by ESR, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity. Allylic hydrogenation (NBS), oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt, Sandmeyers reaction.

### **References:**

- 1. J. March, Advanced Organic Chemistry, Wiley
- 2. R. O. C. Norman and A. Coxon, Modern Synthetic Reactions, Chapman and Hall
- 3. M. B. Smith Organic synthesis McGraw-Hill
- 4. Organic Chemistry-Clayden, Greeves, Warren, and Woothevs
- 5. R. K. Bansal, Synthetic application in organic chemistry, Narosa
- 6. A guide book to mechanism in organic chemistry (Orient-Longmans)-Peter Sykes
- 7. Organic reaction mechanism Benjomin-R. Breslow
- 8. Mechanism and structure in organic chemistry by B. S. Gould
- 9. Organic Chemistry by Hendrikson, Cram and Hammond
- 10. Basic principles of organic chemistry-J. D. Roberts and M. C. Caeserio.

#### 15 h nt S

15 h

### 15 h

- 11. Reactive intermediates in organic chemistry, (J. Wiley) N. S. Issacs
- 12. Organic reaction mechanism (McGraw Hill) R. K. Bansal
- 13. Fundamentals of photochemistry K. K. Rohtgi-Mukherji Wiley-Eastern
- 14. J. Kagan Organic photochemistry. Academic press
- 15. J. M. Coxon and B. Holton, Organic photochemistry Cambridge university press
- 16. C. H. Dupuoy, and O. L. Chapman, Molecular reaction and photochemistry Prentice Hall
- 17. Essentials of molecular photochemistry, A. Gilbert and J. Baggott. Blackwell Scientific publication.
- 18. Molecular photochemistry, N. J. Urro, W. A. Benjamin
- 19. Introductory photochemistry. Cox and T. Camp McGraw-Hill
- 20. Photochemistry R. P. Kundall and A. Gilbert. Thomson Nelson.
- 21. Organic photochemistry J. Coxon and B. Hallon Cambridge University press.

### **Course Outcomes:**

To impart the students a thorough knowledge about the mechanisms of several reactions of some selected functional groups in organic compounds and also to give an outline of applied organic chemistry and the applications of organic chemistry in various spheres of chemical sciences. To give an elementary idea of organic reactions, molecular orbital theory, free radical reactions and organic synthesis.

#### Paper No. XI, APCH. 3.3: Applied Physical Chemistry

### Unit I: Equilibrium Properties of Electrolytes

Non-ideal behavior of electrolyte solutions, Debye – Huckel Theory of inter-ionic attraction, Ionic atmosphere, Time of relaxation, Relaxation and Electrophoretic effects, Debye – Huckel Onsagar equation, Validity of Debye – Huckel equation, Debye – Falkenhagen effect, Wein effect, Debye Huckel limiting law equation, Ionic mobility, Determination of dissociation constant by EMF method, Experimental determination of ionic mobility, osmotic coefficient, Bjerrum Theory, Association constant, Numerical problems.

### **Unit II: Catalysis : Principles and Applications**

Basic principles of catalysis: adsorption isotherms, surface area pore size and acid strength measurement. Enthalpy and entropy of adsorption: interpretation of chemisorptions based on the structure and the nature of the solid – solid state theories – role of defects in catalysis. Selection, preparation and evaluation of catalysts – test reaction, promoters, carriers and stabilizers. Mechanisms of selected reactions: hydrogenation and dehydrogenation reaction – dehydration of alcohols, olefin hydrogenation, decomposition of nitrous oxide, oxidation of CO- etonization of carboxylic acids, cracking of hydrocarbons.

**Applications:** petrochemical industry – reforming and refining – value added chemicalsenvironmental protection autoexhaust catalysts Novel catalytic material clusters, zeolites, mesoporous materials. Electrocatalysis and Photo catalysis.

### (15h)

## 60 h

### (15h)

### UNIT III: Fuel cell

Fuel cell: Concept, Importance of fuel cells, Different types of fuel cell : Hydrogen – oxygen fuel cells, hydrocarbon - air fuel cell, alkaline fuel cells, Phosphoric acid fuel cell (PAFC), Proton exchange membrane fuel cells (PEMFC), Solid oxide fuel cells, Molten Carbonate Fuel Cell (MCFC), Solid Polymer Fuel Cell (SPFC), Applications of fuel cell

### **UNIT- IV: Corrosion**

Introduction of Corrosion, Theories of corrosion, Comparison between Dry and Wet Corrosion, Factors affecting corrosion: Nature of the metal, Nature of orroding environment, Prevention of corrosion: Material selection & Design, protective coatings, corrosion inhibitors, Types of Corrosion, Passivity: Oxide or Protective Layer Theory.

### **References:**

- 1. G.W.Castellan, "Physical Chemistry", Addision-Lesley Publishing Co.
- 2. E.A.Moelwyn Hughes, "Physical Chemistry, Pergamon Press.
- 3. L.C.Chapoy, "Recent Advances in Liquid Crystalline Polymers",
- 4. D.R.Crow, "The Principles of Electrochemistry", Chapman and Hall
- 5. J.O.M.Bokris and A.K.N.Reddy, "Modern Electrochemistry", Plenum Rosatta
- 6 Physical chemistry of surfaces: A. W. Adamson.
- 7. Introduction to colloid and surface chemistry by D. J. Shaw.
- 8. Surface chemistry by J. J. Bikermann

9. Advanced Physical Chemistry, by Gurdeep Raj ,Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP)

- 10. Physical Chemistry by Pahari S. New Central Book Agency (P) Ltd. Kolkata700009.
- 11. Advanced Physical Chemistry J.N. Gurtu, A. Gurtu. 11th Edition Pragati Prakashan.
- 12 Advanced Physical Chemistry D N Bajpai S Chand Publications
- 13 Essentials of Physical Chemistry by Arun Bahl, B S Bahl, G D Tuli . S Chand Publications
- 14 Principles of Physical Chemistry by S H Maron and C F Prutton.

### **Course Outcomes:**

This paper will provide an insight into some of the fundamental concepts in Equilibrium Properties of Electrolytes specifically Debye – Huckel Onsagar equation, Debye – Falkenhagen effect, Wein effect, , Bjerrum Theory and principle and applications of catalysis, fuel cell and corrosion . This will give the students a basic understanding of Applied Physical Chemistry concept.

### (15h)

### (15h)

### Paper No. XII (A), APCH. 3.4 (A): Advanced Organic Chemistry – I

### **Unit I: UV and IR Spectroscopy**

UV: Introduction, principle, Woodward- Fisher rules for conjugated dienes and carbonyl compounds; Calculation of  $\lambda$  max. Ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls.

**IR:** Introduction, principle, 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; lactams and conjugated carbonyl compounds] Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones; combination bands and Fermi resonance. FT-IR of gaseous; solids and polymeric materials.

### **Unit II: NMR Spectroscopy:**

General introduction and principle, definition; chemical shift; anisotropic effects and coupling constants in organic compounds. Spin -spin interaction in typical systems. Analysis of 1st order spectra. Impliffication methods for complex spectra, use of high field NMR, shift reagents, chemical exchange and double resonance. Introduction of FT that's pulse NMR NOE, DEPT and 2DNMR. Karplus curve variation of coupling constant with dihedral angle. Simplification of complex spectra; shift reagent; solvent effect. Fourier transform technique, nuclear overhauser effect [NOE].

### **Unit III: Mass Spectroscopy**

Introduction and principle, ion production methods: EI, CI, and FAB, Electrospray and MALDI. Magnetic, TOF, Quandrupole and ion cyclotron mass analyzers. MS technique. Characteristic EIMS fragmentation modes and MS rearrangements.

### Unit IV: Carbon-13 NMR Spectroscopy and Structural problems

General considerations; chemical shift [aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl compounds]; problems associated with <sup>13</sup>C, FT-NMR, proton decoupled off resonance. Structural problems based on UV, IR, NMR, Mass and Carbon-13 NMR Spectroscopy.

#### **References:**

- 1. V.M. Parikh, Application spectroscopy of organic molecules. (Mehata)
- 2. D.H. Williams and Flemming, Spectroscopic methods of organic compound.
- 3. Silverstein and Basslar, Spectroscopic identification of organic compounds V.M. Parikh ORPTION SPECTROSCIPY OF ORGANIC MOLECULES (J. Wiley)
- 4. P.S. Kalsi Spectroscope of organic compounds (New age publisher)
- 5. Jackman and Sterneil, Application of NMR spectroscopy
- 6. Nuclear magnetic resonance. J.D. Roberts (J. Wiley)
- 7. Theory and application of U.V. Jafee and Orchin.
- 8. Mass spectroscopy K. Benjamin.
- 9. The mass spectra of organic molecules. Beynon J H.
- 10. Interpretation of carbon 13 NMR Wehli F.W, Marchand A. P. (J. Wiley)
- 11. Organic Spectroscopy W. Kemp, ELBS

### 15 h

#### 15 h

### 15 h

60 h

- 12. Mass Spectroscopy. Das and Jame
- 13. Organic structural spectroscopy : J. B. Lambert, S. Gronert, H. F. Shurvell, D. Lightneli, R. G. Cooks (Prentice Hall 2<sup>nd</sup> edition)

### **Course Outcomes:**

To get a brief idea about promising branches in chemistry like UV & IR Spectroscopy, NMR Spectroscopy, Mass spectroscopy, Carbon-13 NMR Spectroscopy its applications. Also, to learn the principles, spectroscopic problems and its applications of various spectroscopic techniques. To know the basic aspects and idea of the spectroscopy. To get an overview about research process and to gain the ability to apply in various research fields by this spectroscopic techniques

### Paper No. XII (B), APCH. 3.4 (B): Applied Analytical Chemistry– I 60 h

### Unit I: Fundamentals of Polymers and Their Processing

Basic Concepts, classification, importance of polymers, monomers, initiators, inhibitors, retarders, techniques of polymerization: mass, solution, suspension, emulsion and gas phase; control of molecular weight and their determination, step polymerization, radical/chain polymerization, living and non-living chain polymerization, co-ordination polymerization, co-polymerization, ionic polymerization, ring opening polymerization, introduction, compounding of plastics and rubber, type, nature and role of additives, pre- compounding operations, mixing of polymers and additives, compression molding, transfer, injection and blow molding, extrusion, calendering, thermoforming, roto- molding, casting, sintering and compaction, deep coating, mold design, analysis of defects in molded products.

### **Unit II: Analytical Principles**

Evaluation of analytical data: Accuracy and precision. Standard deviation, variance and coefficient of variation. Student 't' test. Confidence limits. Estimation of detection limits. Errors: Classification, distribution, propagation, causes and minimization of error. Significant figures and computation rules. Correlation analysis: Scatter diagram. Correlation coefficient, r. Calculation of r by the method of least squares.

Volumetric methods: Classification of reactions in volumetry. Theories of indicators: Acid-base, redox, adsorption, metallochromic, fluorescent and chemiluminescent indicators. Complexation titrations: Titrations using EDTA, NTA and Titriplex. Precipitation titrations. Redox titrations. Gravimetric methods: Mechanism of precipitate formation. Aging of precipitates. Precipitation from homogeneous solutions. Coprecipitation and postprecipitation. Contamination of precipitates. Washing, drying and ignition of precipitates. Organic reagents used in gravimetry: Oxine, dimethylglyoxime and cupferron.

Thermal methods of analysis: Principles and instrumentation of TG and DTA. Complementary nature of TG and DTA. Differential scanning calorimeter (DSC). Applications of thermal methods in analytical chemistry and in the study of minerals and polymers.

#### 15h

### Unit III: Science of Corrosion and Corrosion Control

Corrosion, theories of corrosion. Kinetics of corrosion, Evan's diagram, thermodynamics of corrosion-Pourbaix diagram. Forms of corrosion. Corrosion prevention: modification of materials, corrosion inhibitors, protective coatings, cathodic and anodic protection.

Corrosion testing techniques: Evaluation of corrosion effect- XRD, ESCA, FTIR and surface techniques Corrosion in industries with special reference to oil and mining industries.

### **Unit IV: Electroanalytical Methods**

Potentiometric methods: Reference electrodes and indicator electrodes. The hydrogen, calomel, Ag-AgCl electrodes. The glass electrode – its structure, performance and limitations. Measurement of pH. Petentiometric titrations. Redox and precipitation titrations. Electrogravimety: Principle and method. Determination of Cu. Separation of metals. Conductometry: Principle and method. Conductance measurements. Conductometric titrations. Coulometry: Principle and method. Coulometric titrations.

### **References:**

- 1. M.C.Day and j.Selbin, "Theoretical Inorganic Chemistry", Affiliated East-West Press
- 2. F.A.Cotton and G.Wilkinson, "Advanced Inorganic Chemistry, John Wiley & Sons
- 3. J.E.Huheey, "Inorganic Chemistry Principles of Structure and Reactivity", Harper Collins College Publishers.
- 4. A.I.Vogel, "A Text Book of Quantitative Inorganic Anaysis", Longman
- 5. D.A.Skoog, D.M.West and F.J.Holler, "Fundamentals of Analytical chemistry", Saunders College Publishing.
- 6. W.W.Wendlandt, "Thermal Methods of Analysis", John Wiley & Sons
- 7. G.Friedlander and J.W.Kennady, "Introduction to Radiochemistry", John Wiley & Sons
- 8. Injection Moulds & Moulding, J.B Dym, Van Ronstrandt-Reinhold, New York, 1980.
- Polymer Process Engineering, E.A Grulke, PTR Prentice Hall, Eaglewood Chiffs, New Jersey, 1994.
- 10. Principles of Polymer Engineering, N.G Mccrum, C.P Buckley & C.P Bucknell, Oxford Engineering Press, Oxford, 1988.
- 12. Extrusion of Plastics, E.G Fisher, Newness-Butterworth, London, 1976.

14. Principles of Polymer Processing, R.T. Fenner, Macmillan, London, 1979

### **Course Outcomes:**

This course will promote understanding the facts and concepts in Applied Analytical Chemistry. This will give the students a basic understanding of Fundamentals of Polymers and their processing, Corrosion control, Electroanalytical methods and Analytical principle and applications.

15h

### Paper No. XII (C), APCH. 3.4 (C): Bioorganic Chemistry-I

### UNIT I: Cell structure and metabolism

and eukaryotic cells; Intracellular organelles and their functions; Comparison of plant and animal cells; Metabolic processes – catabolism and anabolism; ATP – currency of biological energy; Energy-rich and energy-poor phosphates.

### Carbohydrates

Structure and function of sugar derivatives (deoxy, amino, branched chain sugars); Polysaccharides of biological importance,dextran, sialic acid; Cell-cell recognition andblood group substances.

### **UNIT II: Metabolic Reactions**

Fatty acid metabolism: Biological importance of fatty acidsand lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, calorific value of foods, bological membranes, properties and function of lipid bilayers and liposomes. Protein-related transformations: Amino acid degradation (C3, C4, C5family), urea cycle, uric acid and ammonia formation; Enzymatic hydrolysis of proteins to peptides; Amino acid sequencing; amino acid metabolism (biosynthesis and degradation).

### UNIT III Nucleic Acids

Chemical and enzymatic hydrolysis of nucleic acids; Structure and function of mRNA, tRNA, rRNA; Polymorphic nature of DNA, B- and Z-DNA, multi-stranded DNA; DNA sequence determination by chemical and enzymatic methods, Genetic code – origin, salient features, wobble hypothesis; Gene expression – transcription and translation; Gene mutation and carcinogenesis

### **UNIT IV Enzymes and Co-enzymes**

(a) Co-enzyme chemistry:Cofactors derived from vitamins, coenzymes, prosthetic groups, apoenzymes; Structure & biological function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid and vitamin B12; Mechanisms of reactions catalyzed by above co-factors.

(b) Enzyme models: Host-guest chemistry, chiral recognition and catalysis, molecular recognition, diometric chemistry, crown ether, cryptates; Cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes.

### **References:**

- 1. Stryer, L. Biochemistry(4th edn.), W. H. Freeman & Co. (1995).
- 2. Zubay, S.. Biochemistry, Addison-Wesley (1983).
- 3. Sindell, R. P. DNA Structure and Function, Academic Press (1994).
- 4. Saenger, W. Principles of Nucleic Acid Structure, Springer-Verlag (1984).
- 5. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons (1997).
- 6. Dugas, H. & Penny, C. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Springer Verlag (1998).
- 7. Palmer, T. Understanding Enzymes, Prentice Hall (1995).
- 8. Price, N. C. & Stevens, L. Fundamentals of Enzymology, Oxford University Press (1989)
- 9. Trevan, M. D. Immobilized Enzymes: An Introduction and Applications Biotechnology, John Wiley (1980).

### 15h

## 15h

15h

### 60 h

15h Prokaryotic

- 10.Fersht, A. & Freeman, W. H. Enzyme Structure and Mechanism, W.H. Freeman, New York (1985).
- 11.Metzler, D. E. Biochemistry: The Chemical Reactions of Living Cells, Academic Press (2001).

### **Course Outcomes:**

To have a basic idea about Cell structure and metabolism such as Prokaryotic and eukaryotic cells, Carbohydrates, Structure and function of sugar, Metabolic Reactions, Enzyme and coenzyme, nucleic acids structure and function of mRNA, tRNA, rRNA Polymorphic nature of DNA etc.

### M.Sc. Part II Semester-III Applied Inorganic Chemistry Practicals

### **A: Non-instrumentation Practicals**

- 1. Ore Analysis 2
- 2. Alloy Analysis 2
- 3. Preparation of coordination complexes (four)
- 4. Ion exchange study of separation of mixtures & estimations
- 5. Solvent extraction
- 6. Soil analysis
- 7. Data analysis
- 8. Synthesis and Characterization of transition metal nanoparticles

### **B: Instrumentation Practicals**

- 1. Spectrophotometry
- 2. Nephelometry
- 3. Potentiometry
- 4. Conductometry
- 5. Thermal analysis
- 6. Magnetic properties of transition metal complexes
- 7. Spectro Fluorimetry
- 8. pH Metry
- 9. Polarography
- 10. Electrogravimetry
- 11. Nuclear and radiochemistry

(Any other experiments may be added when required)

### **References:**

- 1. A.I.Vogel, "A Textbook of Quantitative Inorganic Anaysis", Longman
- 2. Gurudeep Raj, Advanced Practical Inorganic Chemistry, Krishna Prakashan.
- 3. W.G.Palmer, "Experimental Inorganic Chemistry", Cambridge University Press

- 4. Shikha Gulathi, J. L. Sharma and Shagun Manocha, Practical Inorganic Chemistry, CBS publisher and Distributors.
- 5. J. B. Yadav, Advanced Practical Physical Chemistry, Krishna Publishers.
- 6. I.M.Kolthoff, V.J.Elving and Sandell, "Treatise on Analytical Chemistry", Interscience.
- 7. I.M.Kothoff and Strenger, "Volumetric Analysis", Interscience
- 8. Fruman and Welcher, "Standard Methods of Inorganic Analysis", Van Nostrand
- 9. G.Schwarzenback, "Complexomtric Titrations", Interscience
- 10. D.A.Skoog and D.M.West, "Analytical Chemistry An Introduction", Reinholdt.
- 11. R.S.Drago, "Physical Methods in Inorganic Chemistry", Affiliated East-West Press
- 12. Instrumental Methods for Chemical Analysis-H. Kaur
- 13. Spectroscopy- B. K. Sharma
- 14. Instrumental Methods of Analysis-Willard, Merritt, Dean, Settle
- 15. Nanotechnology: Principles and Practices- Sulbha Kulkarni
- 16. Principles of Inorganic Chemistry-Puri, Sharma, Kalia
- 17. Concise Coordination Chemistry-R. Gopalan, V. Ramalingam
- 18. Elements of Magnetochemistry-Datta and Shymal
- 19. G.Zhong Cao. Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press (2004).
- 20. T. Pradeep, Nano The Essentials: Understanding Nanoscience and Nanotechnology.

### M.Sc. Part II Semester-III Applied Physical Chemistry Practicals

- 1) Statistical representation of given experimental data: Estimation of errors in measured and derived properties, reporting data with appropriate significant figures, graphical representation of data with x- and y-error bars.
- 2) Determination of indicator constant and isobestic point of an indicator.
- 3) Determination of stoichiometry and instability constant silver ammonia complex.
- 4) Determination of Thermodynamic Parameters for electrochemical reactions. (To determine  $\Delta G^0$ ,  $\Delta H^0$  and  $\Delta S^0$  for the formation of 1 mole of cadmium in 1 wt. % amalgam at 25 °C).
- 5) Determination of equivalent conductance at infinite dilution and dissociation constant for weak acid using Kolharausch Law of independent ionic mobility.
- 6) pH-metric determination of dissociation constant of carbonic acid.
- 7) To determine the dissociation constant of orthophoshoric acid by pH metrically.
- 8) Determination of order of reaction for iodination of acetone catalyzed by acid with reference to acetone, iodine and acid catalyst.
- 9) Determination of apparent and partial molar volumes of 1:1 electrolytes in aqueous solutions using pyknometric method of density measurements.
- 10) Indexing X-ray diffractometer pattern of CsBr.
- 11) To determine equilibrium constant of reaction  $KI + I_2 \rightarrow KI_3$  spectrophotometrically
- 12) Determination of latent heat of fusion of a given solid.

### **References:**

- 1. Text Book of Quantitative inorganic analysis : A.I. Vogel.
- 2. Practical Physical Chemistry : B. Viswanathan and P.S. Raghavan, 2nd edition, (2012).
- 3. Systematic Experimental Physical Chemistry :S.W. Rajbhoj and T.K. Chondhekar.

4. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.R. Denko. R.M.W. Richett (Pergamon Press).

- 5. Experiments in Physical Chemistry by Carl Garland, Joseph Nibler, David Shoemaker 8th Edition, Kindle Edition.
- 6. Laboratory manual of physical chemistry by H.D. Crockford, J.W. Nowell John Wiley & Sons, INC.

### M.Sc. Part II Semester-III Applied Organic Chemistry Practicals

### A. Qualitative analysis:

Separation, purification and identification of compounds of ternary mixtures using Semi-microanalysis,

TLC, column chromatography and chemical tests, IR spectra to be used for functional group identification.

### B. Quantitative Analysis:

### 1. Two step preparation

- a) Preparation of m-nitroaniline
- b) Preparation of Benzaanilide from benzophenone
- c) Preparation of pthalimide
- d) Preparation of N-bromosuccinimide
- e) Preparation of 4-methyl-7-acetoxy coumarin
- f) Preparation of 1,2,3,4-Tetrahydro carbazole
- g) Preparation of p-ethoxy acetanilide

### 2. Colorimetry & P<sup>H</sup> metry experiments

### 3. Experiment on Hammet equation

4. Structure elucidation by using given spectral data.

### 5. Any other suitable experiment may be added.

### **RECOMMONDED BOOKS:**

- 1. A Textbook of Practical Organic Chemistry A. I. Vogel
- 2. Practical Organic Chemistry
- 3. Handbook of Quantitative and Qualitative Analysis- H. T. Clarke
- 4. Organic Synthesis Collective Volumes by Blat.

### **SEMESTER IV**

### **M. Sc. Part-II APPLIED CHEMISTRY**

### Paper No. XIII, APCH. 4. 1: Applied Inorganic Chemistry- II

Unit I: a) Infrared and Raman Spectroscopy

Molecular vibrations, force constants, Diatomic model, simple harmonic oscillator, anharmonic oscillator, Raman Spectroscopy, classical and quantum mechanical theory of Raman effect, Use ofsymmetry considerations to determine the no. of lines in IR and Raman Spectra: Mutual exclusion rule, Selectionrule in Inorganic structure determinations: Hydrogen bonding and infraredspectra, metal ligand and related vibrations, applications of Raman and Infrared spectroscopy.

### b) Microwave spectroscopy

Basic concept, rotation spectra of simple inorganic compounds, Classification ofmolecules, rigid rotor model, effect of isotopic substitution on transitionfrequencies & intensities non rigid rotor, stark effect nuclear and electron spininteraction and effect of external field. Applications of Micro wave Spectroscopy.

### **Unit II: Electron Spin Resonance Spectroscopy**

Principle, fine, hyperfine, superhyperfine and zero field splitting, ESR of d1 and d9 transition metal ions; g values and factors affecting on g values, instrumentation and applications. Mossbaur Spectroscopy: Introduction, Principles, Mossbaur nuclei, Mossbaur effect, Instrumentation, isomer shift, Quadrapole splitting and hyperfine interactions, applications.

### Unit III: Spectroscopic & Microscopic Characterization techniques of Inorganic Materials (15)

**Spectrometric techniques:** UV-Vis-NIR spectroscopy, Energy dispersive X-ray spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS)

Microscopic techniques: Transmission Electron Microscopy [TEM]; High resolution Transmission Microscopy [HRTEM]; Scanning Electron Microscopy [SEM]; Scanning Tunneling Microscopy [STM]; Atomic Force Microscopy [AFM]

### Unit IV: Instrumentation for Characterization of Inorganic Materials

- a) X-ray Diffraction (XRD)
- b) Superconducting Quantum Interface (SQUID) Maganetometry
- c) Brunauer-Emmett-Teller Gas Absorption Surface Area Measurement and
- Pore Structure Analysis (BET Method)
- d) Dynamic light scattering (DLS)

### **Reference:**

- 1. Instrumental Methods for Chemical Analysis-H. Kaur
- 2. Spectroscopy (Atomic and molecular)- Gurudeep R. Chatwal and Sham K. Anand
- 3. R. S. Drago, Physical Methods in Chemistry, Saunders College Publishers (1977).
- 4. Spectroscopy- B. K. Sharma
- 5. Instrumental Methods of Analysis-Willard, Merritt, Dean, Settle
- 6. Nanotechnology: Principles and Practices- Sulbha Kulkarni
- 7. K J Klabunde, Nanoscale materials in Chemistry, Wiley Interscience 2001

### 60 h (15)

### (15)

### 8. A R West, Basic Inorganic Chemistry, II Ed, Jhon Wiley & Sons (1999)

9. C. N. Benwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, TataMcgraw Hill, New Delhi (2006).

### **Course Outcomes:**

To understand the concept of Infrared and Raman Spectroscopy, microwave spectroscopy, some microscopic characterization techniques such as Transmission Electron Microscopy [TEM]; High resolution Transmission Microscopy [HRTEM]; Scanning Electron Microscopy [SEM], Scanning Tunneling Microscopy [STM] and to gain skill of various characterization techniques in material science for research purposes.

## Paper No. XIV, APCH. 4. 2: Applied Organic Chemistry – II

### **Unit I : Chemistry of Biopolymers**

Amino acids: Introduction and classification, protection and deprotection of N-terminus and Cterminus of amino acids, Peptides and their synthesis. Solid phase peptide synthesis (SPPS) Proteins: Structure and classification, Chemistry of nucleic acid bases A.G.C.T and U and their synthesis, structure of DNA. Structure of starch, cellulose Glycogen and Chitin.

### **Unit II: Pericyclic Reactions**

Molecular orbital symmetry, Frontier orbitals of ethylene 1, 3 butadiene, 1, 3, 5, hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions – conrotatory and disrotatory motion, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacialaddition, 4n and 4n+2 systems, 2+2 addition of ketens, 3, 3, dipolar cycloadditions. Sigmatropic rearrangements – Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3, 3, and 5, 5 sigmatropic rearrangements. Ene reaction.

### Unit III: Chemistry of Drugs & Pharmaceuticals

- A) Drugs:Classification of drugs based on activity. Synthetic procedure for the present commonly used dregs of each type, Manufacturing of few important drugs.
- B) Vitamins: Type of vitamins, synthetic of Vit A and Vit E, Vitamine II of niacinamide.

### **Unit IV: Heterocycles**

Six membered Heterocycles with one heteroatom:Synthesis and reactions of pyrillium salts and pyrones and their comparison pyridinium and thiopyrylium salts and pyridines. Synthesis and reactions of coumarins, chromones.

Six membered heterocycles with two and more heterocycles: Synthesis and reactions of diazines and triazines.

Seven membered heterocycles: Synthesis and reactions of azepines, oxepines and thiepines.

### 15 h

### 15 h

### 15 h

## 60 h

### **References:**

- 1. Text book of polymer science, F. W. Billmeyers Jr Wiley
- 2. Polymer science, V. R. Gowarikar, N. V. Vishwanathan and J Shreedhar, Wiley
- 3. Functional monomers and polymers, K. Takemote, Y. Inkiand R. M. Ottanbrite.
- 4. Contemporary polymer chemistry, H. R. Alcoek and F. W. Lambe, Practice Hall.
- 5. H. Arora, Organic Photochemistry and Pericyclic Reactions
- 6. Lendieer and Mitscher: The organic chemistry of drug synthesis (I. W.)
- 7. Burger Medicinal Chemistry.
- 8. A. Kar: Medicinal Chemistry.
- 9. W. O. Foye: Principles of Medicinal Chemistry.
- 10. R. M. Acheson : An introduction to chemistry of heterocyclic compounds (Interscience)
- 11. Joule and Smith: Heterocyclic Chemstry (Van Nostrand).
- 12. R. K. Bansal: Heterocyclic Chemistry (Wiley E).
- 13. L. A. Paquitte: Principles of Modern Heterocyclic Chemistry.
- 14. M. H. Palamer: The structure and reactions of heterocyclic compounds.
- 15. A. R. Katritzky: Advances in heterocyclic chemistry
- 16. Finar: Organic Chemistry (Vol. 1 & 2)
- 17. Cohn and Stumpt: Outline of Biochemistry.
- 18. Williams: Introduction to the chemistry of enzyme action.
- 19. The organic chemistry of drug design and drug action, R. B. Silverman Academic press.
- 20. Strategies for organic drug synthesis and design, D. Lednicer, J. Willey.

### **Course Outcomes:**

The students will understand some fundamental aspects of applied organic chemistry. They will learn mechanism of some organic reactions, classification of pericyclic reactions, Heterocycles and uses of some commercial and natural substances. To sensitise the students to Drug and pharmaceutical applications, heterocyclic applications, Pericyclic reactions and applications of biopolymers. Also, to give awareness of various types of drugs and its advantages.

### Paper No. XV, APCH. 4. 3: Advance Organic Chemistry – II

### Unit I: Aromaticity and some reaction

**Non benzenoid aromatic compounds**: Aromaticity in Non- benzenoids compounds Annulenes and heteroannulenes, fullerenes, tropone, tropolone, azulene, fulvene, tropylium salts, ferrocene, three and five membered systems. Crown ether complexes, cyclodextrins, cryptands, catenanes and rotaxanes, bonding in fullerenes.

**Reaction mechanism**: Alkyne metathesis reaction, Weinreb ketone synthesis, Petasis reaction, Henry reaction, Corey Kim oxidation. Reactions of carboxylic acids and esters.

### Unit II: Kinetic and thermodynamic control of reactions

Nitration and Sulphonation of naphthalene, Wittig reaction, Enolization, Friedel-Crafts and Diels Alder reactions.

Oxidation: Oxidation with Cr and Mn Compounds: oxidation of alcohol, aldehyde, C=C, C-H

#### 15 h

## 60 h

bonds in organic molecules, Pyridinium chloro chromate (PCC), Oxidation with peracids and other peroxides: C=C, Sharpless epoxidation.

Other types: Prevost and Woodward hydroxylation, cis and trans-hydroxylation, glycol cleavage reagent. HIO<sub>4</sub>, Pb(OAc)<sub>4</sub>, mercuric acetate, SeO<sub>2</sub>, DDQ.

### **Unit III: Chemistry of Natural Products**

- A) Terpenoids: Structure and synthesis of alpha-Pinene, Camphor, Cadenine and Caryophyllene. Hofmann, Emde and von Braun degradation.
- **B)** Alkaloids: Structure elucidation of Papaverine, Quinine and Morphine. Synthesis of quinine and Papaverine. Structure and synthesis of beta-carotene, classification and structure of lipids and their biofunctions.
- **C) Prostaglandings:** Nomenclature, structure (not elucidation) and biosynthesis of Prostaglandins PGE<sub>2</sub>, and PGF<sub>IV.</sub>

### **Unit IV: Selected Organic Reactions and Reagents**

Lithium dimethyl cuprate, Trimethyl silyl iodide, Baker Yeast, Phase-transfer catalysts. 1, 3dipolar cycloaddition and chelotropic reactions, sigmatropic rearrangement, supra and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearrangement and Claisen and Cope and Aza Cope rearrangement, Ene reaction.

### **References**:

- 1. L. M. Hardwood, Polar rearrangements, Oxford University
- 2. J. March, Advanced Organic Chemistry, Wiley
- 3. S. N. Issacs, Physical Organic Chemistry, Longman
- 4. P. Y. Bruice, Organic Chemistry, Prentice Hall
- 5. H. Arora, Organic photochemistry and Pericyclic reactions
- 6. C. H. Dupuoy, and O. L. Chapman, Molecular reactions and Photochemistry, Prentice Hall
- 7. J. M. Cozon and B. Holton, Organic Photochemistry, Cambridge University Press
- 8. S. H. Pine, Organic Chemistry by McGraw-Hill
- 9. I. L. Finar, Organic Chemistry Vol W, Longman

### **Course Outcomes:**

To develop interest among students in advanced organic chemistry. To impart essential theoretical knowledge about aromaticity, Kinetic and thermodynamics, natural products and selected organic reactions and reagents.

#### 15 h

### Paper No. XVI (A), APCH. 4. 4 (A): Inorganic Chemical Industries

### **UNIT I: Special materials for electronic Industry**

High purity Silicon, Germanium, Gallium Arsenide (GaAs) Indium phosphide(InP) etc. preparation using Zone refining, Crystal growth and there use inelectronic industry. High temperature materials, High alumina, alumina, SiC, Chromite, Zirconia, Magnesite etc. Ionic & Superionic conductors,  $\beta$ -alumina oxide ion conductors, halideconductors superionic, Fastion conductors- RbAg<sub>4</sub>I<sub>5</sub>, Arrhenious equation.

### **UNIT II: Fertilizer Industries**

**General Principles of plant Nutrition:**Essential plant nutrients, functions of the essential elements, classification of commercial nitrogenous fertilizers. manufacturing of ammonium sulphate, Urea, Ammonia nitrate Commercial phosphatic fertilizers. Manufacturing process and properties of phosphatic fertilizers, single super phosphate, triple superphosphate.

### **Commercial potassic fertilizers:**

Chemicals of potassium compounds, classification, manufacturing process and properties of potassium fertilizer, muriate of potassium, potassium sulphate, mixed fertilizer.

### **Micronutrients:**

Role and deficiency symptom of micronutrients.

### **Biofertilizers:**

classification, demands and production, Present status of fertilizer Industries in India.

### **UNIT III: Glass & Ceramics**

Physical and chemical properties of glasses, Raw materials, manufacturing of special glasses. Ceramics and their properties, raw materials, manufacturing of ceramics, Applications of colours to pottery, use of ceramics.

**Industrial Gases**:Manufacturing and industrial uses of H<sub>2</sub> O<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub>, Cl<sub>2</sub> & acetylene gases. Liquification of gases, production of low temperature.

**Chemicals of Utility**:Inorganic fine chemicals, magnesia, alumina, AlCl<sub>3</sub>, CaCO<sub>3</sub>, Na<sub>2</sub>SiO<sub>3</sub>, MnO<sub>2</sub>, FeSO<sub>4</sub>, PbO<sub>2</sub> and NaOH.

### **UNIT IV: Manufacturing of Inorganic Heavy Chemicals**

Introduction to chemical industry: Flow sheet preparation. Principles of process selection and operation selection. Basic raw materials and routes to major inorganic products. Flow sheets and engineering aspects of the manufacture of sulphuric acid, sodium hydroxide, chlorine, ammonia, phosphoric acid, nitric acid and Portland cement.

### **References:**

- 1. H. V. Keer, Principles of Solid state.
- 2. A. R. West, Solid State Chemistry and its applications, John Wiley & Sons, 2003.
- 3. B. K. Sharma, Engineering chemistry, Krishna Prakashan Media.
- 4. Lowenheim F A (1978) Electroplating MC Graw-Hill Book Company.
- 5. Gable, D: Principal of metal Treatment and protection. Pergaman, Press Oxford(1978)
- 6. G.A. Keneth: Electroplating for Engineering's A Hand Book IIIrd Edn Van Nastrad Reinbold Co London
- 7. F A Lowinbein: Modern Electroplating, Electroplating Publication New Jersey

### 19

### 15 h

### 15h

### 15h

### 15h

- 8. Burke, Progess in ceramic science Vol. IV
- 9. R.R.Iash: afromulary of paints and other coating Vol. I
- 10. Industrial chemistry, B. K. Sharma.
- 11. Engineering chemistry, B. K. Sharma.
- 12. S. D. Shukla & G N Pandey: A text book of chemical technology Vol. 1
- 13. F A. Henglein: Chemical Technology (Pergamon)
- 14. D. Patranabis, Sensors and Transdusers, 2nd Edn, Prentice, Hall of India (2003).
- 15. Rajankumar Basak, Fertilizers, A text Book
- 16. R. Balsubramaniam, Materials Science and Engineering

### **Course Outcomes:**

To learn the important aspects in inorganic chemical Industries such as special materials for electronic industry, fertilizer industry, glass, ceramics and manufacturing of inorganic heavy chemicals. To know the various industrial applications of glass, ceramics, fertilizers and heavy inorganic chemicals.

### Paper No. XVII (B), APCH. 4. 4 (B): Pollution Monitoring and Control 60 h

### **Unit I: Pollution and its Control**

Air pollution: Composition of air. Classification of pollutants. Sources of air pollutants. Industrial pollution: Power plants. Fertilizers. Petrochemicals. Automobile pollution. Water pollution: Water quality criteria for domestic and industrial uses. Analysis of waree and wastewater. Principles of water and wastewater treatments. Removal of organics and harmful inorganics from water and wastewater. Biological treatment of wastewater: Theory and practice. Sludge treatment and disposal.

### Unit II: a] Removal of Heavy Toxic Metals

Chromium, Mercury,Lead, Cadmium, Arsenic analytical methods of determination of small amounts of the metal pollutants, copper recovery, treatment of waste to remove heavy metals, recovery techniques.

**b] Removal of Particulate Matter:** Particulate matter and dynamics of particles separations, Particulate matter in gas stream, filtering, gravity separation, liquid scrubbing cyclone separations, electrostatic precipitations safety of workers analysis of particulate matter.

### Unit III: Removal of Nuclear Hazardous Materials

Sources of Phenolic residues, Analytical methods, treatment by using stream gas stripping, ion – exchange, solvent extraction, oxidation methods, Microbiological treatment. Role of Vapor pressure, role of solubility, effect of pH on solubility, extractive methods of recovery and recycle, Chemical methods of conversion to less soluble nontoxic or biodegradable and products carcinogens. Origin of SO<sub>2</sub> and its hazard, Analysis of SO<sub>2</sub>, SO<sub>2</sub> control methods, desulphurization of fuels, Indian cola and Indian Crude oil. Economics of SO<sub>2</sub> control measures NOx, dissolved NOx, nitrites, ammonia, Urea and other nitrogen containing compounds in the effluents fertilizer explosive, industrial effluents, effluents from nitro aromatic industries.

### 15 h

15h

15h

### 20

### Unit IV: a] Biotechnology in Chemical Industry

elements in biological system Mettallo – proteins and mettallo– enzymes. Metal ions as a charge carriers Health effects due to deficiency and excess of metals of non-metals Biotechnology for the production of chiral compounds. Role of biotechnology in Industry.

### **b]** Polymer Recycling:

Environmental and polymer Industries. Recycling of polymers waste.

### **References:**

- 1. S.P. Mahajan: Pollution control in processes iIndustries (J.W)
- 2. P.N.Chennsioff and R. A Young: Air Pollution control and design Hand Book and recovery (J.W)
- 3. J.R. Holmes: Refuse recycling and recovering (J.W)
- 4. M. Sitting: Resources recovery and recycling Hand Book and Industrial Wastes (NDS)
- 5. J.O. Niagh: Sulphur in the Environment Vol. I & II (J.W)
- 6. P.S.Minor: The Industry/EPA controntation (MGH)
- 7. R.B.Pojaselc: Toxic and Hazardous waste disposal Vol. I &II (AAS)
- 8. S.M.Khopkar: environmental pollution analysis
- 9. A.K.Dey: Environmental Chemistry
- 10. W.Handley: Industrial safety Handbook

### **Course Outcomes:**

To provide basic knowledge of pollution monitoring and its control as well as to study about Pollution, removal of heavy toxic metals, removal of nuclear hazardous materials and biotechnology in chemical industry. The objective of this course is to make the students familiar with pollution monitoring and control study.

### Paper No. XVIII (C), APCH. 4. 4 (C): Chemical Engineering in Applied Chemistry 60 h

### Unit I: Principle of Chemical Engineering

Introduction to chemical engineering. Comparison of academic and industrial Chemistry. Material and energy balances. Units and dimensions, Fluid mechanics. Fluid statistics, Benoulli equation, Flow measurements, pipe fittings and valves. Heat transfer: Steady state heat conduction, unsteady state heat conduction, Heat flow by convection, Heat exchange and evaporators. Distillation: vapor-liquid equilibrium, fractionating column, Comparison of plate columns and packed columns, mass transfer operations, Principles of extraction, leaching and absorption. Chemical reactions: Batch and continuous reactors. Concept of residence time, space time and space velocity.

### **Unit II: Polymers**

Introduction, classification, characteristics and properties of polymers, copolymerization, and addition polymerization: Free radical and ionic polymerization, Plastics: Thermoplastics, Thermosetting plastics, Elastomers or Rubber, Zeigler-Natta catalysts, condensation polymerization, conducting polymers and its application, importance of bio-polymers.

### 15h

#### 00 1

15h

15h Essential

### Unit III: Manufacturing of Organic Chemicals

Raw materials and routes to major organic products. Flow sheets and engineering aspects of the manufacture of important products such as nitrobenzene, linear alkyl enzyme sulphonate, chlorobenzene vinyl chloride, DMT, ethyl acetate, cummene, alkyl benzenes, cyclohexanone, Phallic acid, soaps, detergents and hydogenation of oils. Pharmaceuticals: Manufacturing processes of aspirin, vitamin-A and paracetamol. Pesticides: Manufacture of BHC, DDT, Carbaryl Malathion and Manufacture of dyes.

### Unit IV: Manufacturing of Inorganic Heavy Chemicals

15 h

15 h

Introduction to chemical industry: Flow sheet preparation. Principles of process selection and operation selection. Basic raw materials and routes to major inorganic products. Flow sheets and engineering aspects of the manufacture of sulphuric acid, sodiumhydroxide, chlorine, ammonia, phosphoric acid, nitric acid, ammonium nitrate, urea, glass, ceramics, refractories and Portland cement.

### **References:**

- 1. E.K.Rideal, "Concepts in catalysis", Academic Press
- 2. A.Clark, "The Theory of Adsorption and Catalysis", Academic Press
- 3. R.Pearce and W.R.Patterson (Eds.), "Catalysis and Chemical Processes.", Backie and sons
- 4. J.M.Betty, "Applied Industrial Catalysis", Academic Press
- 5. Coulson and Richardson, "Chemical Engineering", Vol. 1,2, & 3
- 6. McCabe, "Unit Opeartion of Chemical Engineering"
- 7. A. Pahari and B. Chauhan, Engineering Chemistry
- 8. Peter Wiseman, "Industrial Organic Chemistry"
- 9. N.R.Nerris Shreve, "Chemical Process Industries"
- 10. Dridens, "Outline of Chemical Technology"
- 11. B.K.Sharma, "Industrial Chemistry, Goel Publishing House

### **Course Outcomes:**

To provide knowledge regarding the units and dimensions, fluid statistics, Benoulli equation and pipe fittings. Students should an overall idea about polymerization, and addition polymerization: Free radical and ionic polymerization, Plastics: Thermoplastics, Thermosetting plastics, Elastomers, manufacturing of organic chemicals and inorganic heavy chemicals.

### M. Sc. Part II Semester-IV Applied Physical Chemistry Practicals

- 1) Determination of stability constant of ferric thiocyanate complex.
- 2) To determine stoichiometry and stability constant of ferric-salicylate complex by Job's Method and mole ratio method spectrophotometrically.
- 3) Determination of the critical micelle concentration of a given surfactant in aqueous and aqueous salt solutions.
- 4) Determination of isoeletric points and dissociation constants for neutral, acidic and basic amino acids using pH-metric technique.
- 5) Study of the effect of ionic strength on the reaction between persulphate and iodide by visual method.
- 6) Indexing X-ray diffractometer pattern of NaCl.
- 7) To determine pK value of methyl red indicator at room temperature spectrophotometrically
- 8) To determine half wave potential of a given ion using half height method, differential method and wave equation method
- 9) Characterization of the complexes by electronic and IR spectral data.
- 10) Determination of unknown concentration of  $Cd^{+2}/Zn^{+2}$  ions in the given solution by standard addition method.
- 11) Estimation of quinine as quinine sulfate from medicinal tablets by fluorimetrically.

### **References:**

- 7. Findlay's Practical Chemistry Revised by J.A. Kitchner (V edition).
- 8. Text Book of Quantitative inorganic analysis : A.I. Vogel.
- 9. Practical Physical Chemistry : B. Viswanathan and P.S. Raghavan, 2nd edition, (2012).
- 10. Systematic Experimental Physical Chemistry :S.W. Rajbhoj and T.K. Chondhekar.

11. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.R. Denko. R.M.W. Richett (Pergamon Press).

- 12. Experimental Physical Chemistry by D. P. Shoemaker, Mc. Growhill, 7th Edition, 2003.
- 13. Experiments in Physical Chemistry by Carl Garland, Joseph Nibler, David Shoemaker 8th Edition, Kindle Edition.

14. Laboratory manual of physical chemistry by H.D. Crockford, J.W. Nowell John Wiley & Sons, INC.

### M. Sc. Part II Semester-IV Applied Inorganic Chemistry Practicals

### **A: Non-instrumentation Practicals**

- 1. Ore Analysis 2
- 2. Alloy Analysis 2
- 3. Preparation of coordination complexes (four) and preparations of mixed metal oxides (two)
- 4. Ion exchange study of separation of mixtures & estimations
- 5. Solvent extraction
- 6. Soil analysis
- 7. Data analysis
- 8. Synthesis and Characterization of transition metal nanoparticles

### **B: Instrumentation Practicals**

- 1. Spectrophotometry
- 2. Nephelometry
- 3. Potentiometry
- 4. Conductometry
- 5. Thermal analysis
- 6. Magnetic properties of transition metal complexes
- 7. Spectro Fluorimetry
- 8. pH Metry
- 9. Polarography
- 10. Electrogravimetry
- 11. Nuclear and radiochemistry

### **C:** Interpretation exercises

- 1. X-ray powder diffraction analysis of cubic compound
  - a. Determination of lattice constants and geometry
  - b. Partical Size
  - c. Density
- 2. Interpretation of Mossbaur spectrum with reference to determination of
  - a. Isomer shift
  - b. Quadruple splitting
  - c. Internal magnetic field
  - d. general comment
- 3. Interpretation of IR spectrum with reference to stretching vibration C=N, C=O, N-, M-O
- 4. Interpretation of absorption spectra for
  - a. Verification of position of ligands in spectrochemical series.
  - b. Determination of gemetry (Octahedral, square planer, tetrahedral) of a given compound.
  - c. Calculation of spectral splitting parameters.
- 5. Calculation of band gap of semiconductors with the help of plots of log & vs. 10 3/4.

In all 20 experiments with at least five experiments in each course should be completed. Addition of other experiments in place of existing one may be allowed. A variety of small projects designed by teacher based on the interest of students and capabilities should be worked out. (**Project** work or the review report (50 Marks) will be examined by internal and external examiners.

### Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

### M. Sc. Part II Semester-IV Applied Organic Chemistry Practicals

### 1. Two or Three stage preparations starting with 5g or less & TLC.

### 2. Estimation of Sulphur & Nitrogen

### 3. Organic Preparations

- 1. Preparation of anthranilic acid
- 2. Preparatin of p- Amino benzoic acid
- 3. Preparation of p- chloro nitrobenzene by Sandmeyer reaction
- 4. Preparation of p- Idonitrobenzene by Sandmeyer reaction
- 5. Preparation of Benzylamine
- 6. Preparation of Benzimidazole
- 7. Preparation of 2-acetyl cyclohexanone
- 8. Multicomponent synthesis.

### 4. Project:

Project shall be started at the beginning of Sem - III and will be accessed bimonthly for its progress and continuous evaluation will be made. High standard research work is expected from the project and students are encouraged to publish it in national or international journals of high repute. External and internal examiners will examine the project jointly at the time of practical examination.

### 5. Any other experiments as may be added.

### 6. Study tour may arrange for M.Sc. Part-II students to visit Chemical Industries in India.

### **REFERENCE BOOKS:**

- 1. A Textbook of Practical Organic Chemistry A. I. Vogel
- 2. Practical Organic Chemistry
- 3. Handbook of Quantitative and Qualitative Analysis- H. T. Clarke
- 4. Organic Synthesis Collective Volumes by Blat.

### Note: 1. Any other experiments may be added when required.

2. Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

### Laboratory Safety Equipments:

### **Part: I Personal Precautions:**

- 1. All persons must wear safety Goggles at all times.
- 2. Must wear Lab Aprons/Lab Jacket and proper shoes.
- 3. Except in emergency, over hurried activities is forbidden.
- 4. Fume cupboard must be used whenever necessary.
- 5. Eating, Drinking and Smoking in the laboratories strictly forbidden.

### Part: II: Use of Safety and Emergency Equipments:

- 1. First aid Kits
- 2. Sand bucket
- 3. Fire extinguishers (dry chemical and carbon dioxide extinguishers)
- 4. Chemical Storage cabinet with proper ventilation
- 5. Material Safety Date sheets.
- 6. Management of Local exhaust systems and fume hoods.
- 7. Sign in register if using instruments.

### Equivalence in Accordance with titles and contents of the papers

Old Course(2013)	New Course (2018)
SEME	STER III
CORE PAPERS	CORE PAPERS
Paper No. APC-C –IX, APCH 3.1: APPLIED	Paper No.–IX, APCH 3.1: APPLIED
INORGANIC CHEMISTRY – I	INORGANIC CHEMISTRY – I
Paper No. APC-C-X, APCH 3.2: APPLIED	Paper No. –X, APCH 3.2: APPLIED
ORGANIC CHEMISTRY – I	ORGANIC CHEMISTRY – I
Paper No. – APC- C-XI, APCH 3.3:	Paper No. –XI, APCH 3.3: APPLIED
APPLIED PHYSICAL CHEMISTRY – I	PHYSICAL CHEMISTRY – I
ELECTIVE PAPERS	ELECTIVE PAPERS
Paper No. – APC-C-XII (A)APCH 3.4 (A):	Paper No. –XII (A)APCH 3.4 (A): APPLIED
APPLIED ORGANIC CHEMISTRY – I	ORGANIC CHEMISTRY – I
Paper No. – APC-C-XII (B), APCH 3.4 (B):	Paper No. XII (B), APCH 3.4 (B): APPLIED
APPLIED ANALYTICAL CHEMISTRY	ANALYTICAL CHEMISTRY
Paper No. – APC-C-XII (C), APCH 3.4 (C):	Paper No. XII (C), APCH 3.4 (C):
BIOORGANIC CHEMISTRY	BIOORGANIC CHEMISTRY
SEME	STER IV
CORE PAPERS	CORE PAPERS
Paper No. – APC-C-XIII, APCH 4.1:	Paper No. –XIII, APCH 4.1 : APPLIED
APPLIED INORGANIC CHEMISTRY – II.	INORGANIC CHEMISTRY – II.
Paper No. – APC-C-XIV, APCH 4.2:	Paper No. –XIV, APCH 4.2: APPLIED
APPLIED ORGANIC CHEMISTRY – II.	ORGANIC CHEMISTRY – II.
Paper No. – APC-C-XV, APCH 4.3:	Paper No. –XV, APCH 4.3: APPLIED
APPLIED ORGANIC CHEMISTRY – II.	ORGANIC CHEMISTRY – II
ELECTIVE PAPERS	ELECTIVE PAPERS
Paper No. – APC-C-XVI (A), APCH 4.4(A) :	Paper No. –XVI (A), APCH 4.4(A) :
INORGANIC CHEMICAL INDUSTRIES	INORGANIC CHEMICAL INDUSTRIES
Paper No. – APC-C-XVI (B), APCH 4.4(B):	Paper No. –XVI (B), APCH 4.4(B):
POLLUTION MONITORING AND	POLLUTION MONITORING AND
CONTROL	CONTROL
Paper No. – APC-C-XVI (C), APCH 4.4(C):	Paper No. –XVI (C), APCH 4.4(C):
APPLIED ANALTYICAL CHEMISTRY - II	CHEMICAL ENGINEEERING IN APPLIED
	CHEMISTRY

### M. Sc. In Applied Chemistry Semester III and Semester IV

# SHIVAJI UNIVERSITY, KOLHAPUR.



Accredited By NAAC with 'A' Grade

**Revised Syllabus For** 

**Master of Science** 

Part- II

### **INDUSTRIAL CHEMISTRY**

**CBCS PATTERN** 

Syllabus to be implemented from June, 2019 onwards.

### SHIVAJI UNIVERSITY, KOLHAPUR DEPARTMENT OF INDUSTRIAL CHEMISTRY M.Sc. COURSE IN "INDUSTRIAL CHEMISTRY"

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  - 10.4. M.Sc. Part-I, Semester-IV.
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- 12. Nature of Question Paper
- 13. Standard of Passing
- 14. Nature of question paper and scheme of marking
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  - 15.1 Personal Precautions:
  - 15.2. Use of Safety and Emergency Equipment's:
- 16. Credit System:
- 17. Distribution of Credits for Practical's
- 18. M.Sc.IndustrialChemistryequivalenceofpre-revisedandrevisedpapers.

**1. About the Course:** The Indian chemical industries occupy a unique position in the Indian economy interms of contribution to employment and export potential. In spite of a strong natural resource based India's share in the global market is meager one. The experts in Industrial Chemistry have emphasized the need for capital infusion capacity,

modernization and up gradation in various segments of industrial processes to bring about efficiencies and economies of scale in order to achieve in global markets. Keeping in view the need of Indian industries, Shivaji University has started M.Sc. course in Industrial Chemistry from academic year 1993-1994 in the Chemistry. Department to educate and train the science graduates in industrial chemistry to serve the industrial sector as a technical, R & D personnel and quality control production personnel to manage the industrial production and contribute to the development ofnation.

One of the objectives of the M.Sc. Industrial Chemistry Course is to attain new heights in industrial teaching and research and to provide trained man power to vast developing Indian industries to develop the young graduate as a premier precision tool for future creation.

M.Sc. course in industrial chemistry is a potential base provided by the Shivaji University on the University campus to educate the students from rural area who will get employment on large scale in Indian Chemical industries. Since last twelve years, M.Sc. industrial chemistry students have obtained employment on large scale in Indian chemical industries.

**2. Eligibility Criteria for Admission:** Admission to the M.Sc. Industrial Chemistry course will be open to candidates passing B.Sc. degree of Shivaji University or any other statutory university in India or abroad with minimum 55% marks and Chemistry as a principal subject of study.

**3. Selection Procedure:** Selection will be based on common entrance test of Chemistry Department and personal interview. Maximum '30' candidates will be admitted to M.Sc. Industrial Chemistry.

**4. Fee Structure for the Course:** For the detailed fee structure, please see our web site – unishivaji.ac.in

5. Strength of the students:
5.1 For M. Sc. Industrial Chemistry Course
36(18 Open + 18 Reserve) + 4(Other University) = Total 40.
5.2. For elective courses for students of other than Departments: Minimum 10 students per course and maximum 20 students

**6. Duration of the Course:** The duration of the M.Sc. Industrial Chemistry course is – two years consisting of '4' semesters, each semester spanning for 6' months of minimum 120 working days.

### 7. Teaching facilities:

1. Co-ordinator01, Assistant Professor : 2 Teaching Assistant.: 02

2. Inter and intra faculty, contributory staff, professors, readers, lecturers, M.

Tech., B. Tech. Industrial personnel etc. qualification of the teacher for M.Sc.

Industrial Chemistry will be M.Sc., M.Sc., Ph.D., M. Tech., B. Tech.etc.

Scheme of Examination / Assessment with scheme of standard of passing. The

structure of M.Sc. Industrial Chemistry consists of -

- 1) Theory course
- 2) Practical course
- 3) Seminars
- 4) Industrial training#.

Each semester will have theory examination of four papers of 100 marks each (80 marks university examination + 20 marks internal.)

Each Semester will have two practical courses of 100 marks each

Semester-IV will have two practical courses out of which one practical course will have

50 marks project work.

#### #Industrial Tour is compulsory for Semester III and IV Students.

### 8. Choice Based Credit System of M.Sc. Industrial Chemistry

The newly designed choice-based M. Sc. Industrial Chemistry Course consists of total 96 credits. In order to accommodate the excellence achieved by the student in various activities like sports, National Service Scheme, National Cadet Corps and other activities, extra credits of maximum four will be given to the students. The student has to produce sufficient proof in the form of certificate by the competent authority to earn credits for other activities. The Scheme of number of credits given for other activities will be according to the Shivaji University procedure. The total credits that can be earned by a student will be 100 including the credit for other activities. The course consists of Core (Theory, Practical, Seminar and Project) and Elective courses for the third and fourth semester. The elective courses are also offered to the students of other science departments. The M. Sc. Industrial Chemistry consists of total four semesters and the courses offered in the first and second semester are compulsory for students seeking admission. The student admitted to M. Sc. Industrial Chemistry must chose three core courses of theory (of 12 credits), two core courses of practical (of 8 credits) and or Project (of 2 credits) of Industrial Chemistry offered in the third and fourth semesters. He/ she is allowed to choose either the elective theory course of Industrial Chemistry or of other Department of 4 credits under the Choice Based Credit System in each semester. The minimum credits to be obtained by the student to obtain Postgraduate degree in Industrial Chemistry in all the four semesters will be 35% of total marks in each course (Core, Elective, Practical and Project) separately equivalent of 34 credits except for the credit of other activities.

### L= Lecture, T = Tutorial, P = Practical, C = Credits

All core courses for each semester are compulsory for M. Sc. Industrial Chemistry Students. The students are allowed to choose supportive courses from other departments as an alternative for Elective courses of third and fourth semesters.

### 8.1. Total Credits for M. Sc. Industrial Chemistry

A) Sem I (24) (16 T + 8 P) + Sem II (24) (16 T + 8 P) + Sem III (24) (16 T + 8 P) + Sem IV (24) (16 T + 8 P) = 96 (64 T + 32 P) + 4 credits for other activities like sports, N. S. S., N.C.C., etc. = **100 credits.** 

### 8.2. Minimum credits to be chosen from Industrial

Chemistry B) Sem I (24) (16 T + 8 P) Sem II (24) (16 T + 8 P) Sem III (20) (12 T + 8 P) Sem IV (20) (12 T + 8 P) Total = 88(56 T + 32 P)

### 8.3. Maximum credits to be chosen from courses offered by other departments

- **C)** Sem III (4T) + Sem IV (4T) =8T
- **D**) Credits for Other Activities =4

So that B + C + D = A

8.4. Grades and average grade point calculation

Grade	Marks	Grade points	
0	70 and above	7	
Α	60 to 69.99	6	
В	55 to 59.99	5	
С	50 to 54.99	4	
D	45 to 49.99	3	
E	40 to 44.99	2	
F(Fail/ Unsatisfactory)	39.99 and below	0	

- i) Semester grade point average (SGPA): Semester wise index grade of a student SGPA =  $(g_1 x c_1) + (g_2 x c_2) + --(g_6 x c_6)/$  Total credits of a semester.
- ii) Cumulative grade point average (CGPA): Cumulative index grade point average. CGPA =  $(g_1 \times c_1) + (g_2 \times c_2) + (g_6 \times c_6)/$  Total credits of a student up to and including semester for which cumulative average is required.

iii) Final grade point average (FGPA): Final Index of astudent FGPA =  $(\sum g_i x c_i) / (nc_T)$  $\{g_i = \text{grade point secured by the student, } c_i = \text{credit of the course, } c_T = number of credits and n = total number of courses.}$  Illustration with a hypothetical case.

Papers	Ι	II	III	IV				
practical's					Ι	II		
Credits	4	4	4	4	4	4	24	
Grade points secured	7	6	8	6	7	7	41	
$\sum g_i x c_i$	28	24	32	32	28	28	164	
$\sum g_i \ge c_i / c_T$	(164	(164 / 24) = 6.83						
Overall grade	6.83							

### For M.Sc. I, Semester I

The cumulative grade point average is the sum of SGPA of a student of each semester. Suppose it is 164 (6.83) for a semester I, 170(7.08) for semester II, 168(7.0) for semester III and 176(7.33) for semester IV then the CGPA for semester I and II will be = [164 + 170] / 48 = 6.958 = 6.96

The FGPA for all semesters will be = [164 + 170 + 168 + 176] / 96 = 7.0265 = 7.03

### 9.1. M.Sc. Part II, Semester III, Industrial Chemistry

Total credits = 16 Theory + 6 Practical + 2 Seminar = 24, Minimum Credits to be chosen = 12 Theory + 08 Practical = 20Credits to be chosen from the elective courses of other departments =4

No	Paper	Title of the paper		Hours	L	Т	Р	С
	Code							
1	IND 3.1	Core	Organic Chemical Industries-I	60	4	-	-	4
2	IND 3.2	Core	Inorganic Chemical Industries-I	60	4	-	-	4
3	IND 3.3	Core	Methods of Analysis in Industries	60	4	-	-	4
4	IND E01	Elective	General Chemical Technology	60	4	-	-	4
5	IND E02	Elective	Advanced Analytical Techniques in	60	4	-	-	4
			Industry					
6	IND E03	Elective	Chemical Analysis in Agro, Food and	60	4	-	-	4
			Pharmaceutical Industry					
5	IND P05	Core	Practical V	60			8	4
6	IND P06	Core	Practical VI	60			8	4

### 9.2. M.Sc. Part II, Semester IV, Industrial Chemistry

Total credits = 16 Theory + 8 Practical = 24,

Minimum Credits to be chosen = 12 Theory + 08 Practical = 20 Credits to be chosen from the elective courses of other departments = 4

	Wi. Sc. I alt II, Schlester IV							
No	Paper		Title of the paper	Hours	L	Т	P	C
	Code							
1	IND 4.1	Core	Drug and Pharmaceuticals	60	4	-	-	4
2	IND 4.2	Core	Inorganic Chemical Industries-II	60	4	-	-	4
3	IND 4.3	Core	Selected Topics in Industrial	60	4	-	-	4
			Chemistry					
4	IND E04	Elective	Environmental Chemistry	60	4	-	-	4
5	IND E05	Elective	Pharmaceutical Chemistry	60	4	-	-	4
6	IND E06	Elective	Chemistry of Industrially Important	60	4	-	-	4
			Materials					
5	IND P07	Core	Practical VII	45			8	3
6	IND P08	Core	Practical VIII	45			8	3

### M. Sc. Part II, Semester IV

\*\*Includes 50 Marks for Project

### M.Sc. Part-II, Semester-III

### Paper IND 3.1 Organic Chemical Industries – I

### **Unit – I: Dyes and Pigments:**

Dyes, Pigments and Intermediates: Classification of Dyes, Preparation of important dye intermediates, Methods of preparation of commercial dyes of different classes with suitable examples. Typical manufacturing processes of few dyes, Fluorescent brightening agents, and Special dyes: Photosensitive dyes, dyes as food additives, natural dyes.

### **Unit – II: Food Processing and food Additives**

Classification, chemical composition and nutritional value of common food stuffs, properties of foods, food preservation and processing, food deterioration, methods of preservation and processing by heat, cold, chill storage, deep freezing, drying, concentration, fermentation, and radiation. Permitted food additives and their role; antioxidants, coluring agents, sweetners

### **Unit – III: Cane Sugar Based Chemistry**

Introduction, manufacturing processes of Acetic acid, oxalic acid, citric acid, acetic anhydride, furfural from bagasse, anhydrous alcohol, sugar based chemical industries in India. Preparation of organic jaggery, analysis of jaggery

### **Unit – IV: Soap and Detergents**

Oils, soaps and Detergents: Refining of edible oils, Manufacturing of soaps, Detergents, Liquid Soaps, aptholmic solution. Manufacturing of glycerol from fatty acids, greases from fatty acids, turkey - red oil.

Paints: Introduction, properties, manufacture of paint and applications Varnishes and Inks: Constitutions, examples of preparation and applications.

### **REFERENCE BOOKS**

- 1. K. Venkatraman: The Chemistry of Synthetic Dyes Vol. 1-7 (A.P)
- 2. Abranart: Dyes and Their intermediates (Pergaman)
- 3. Beech: Fiber reactive Dyes (Logos Press)
- 4. Frig and David Dyes intermediate
- 5. Allan: Color Chemistry
- 6. Kent: Riehels Industries Chemistry.
- 7. M Ash & I Ash: A formulary of paints & other coatings.
- 8. M Ash & I Ash: A formulary of cosmetic preparation (Godwin)
- 9. P.H. Groggings: Unit Processes in organic synthesis (MGH)
- 10. Kiik& other: Encyclopedia of Chemical technology.

# 15 Hrs

15 Hrs

15 Hrs

- 11. L. W. Aurand, A. E. Woods, Food Chemistry, AVI Publishing Inc.
- 12. L. H. Mayer, Food Chemistry, Affiliated East-West Press Ltd., New Delhi.
- 13. N. Shakuntala Manay, M. Shadakhsara Swamy, Foods-Facts and Principles.
- 14. John M. deMan, Principles of Food Chemistry.
- 15. The Complete Book on Sugarcane Processing and By-Products of Molasses (with Analysis of Sugar, Syrup and Molasses) -H. Panda

### Paper IND 3.2 Inorganic Chemical Industries – I 15 Hrs

Dairy Chemistry: Milk and milk products, composition and structure of milk, milk proteins, enzymes, vitamins, minerals, density and viscosity of milk, effect of heat on milk, milk processing, basic milk categories, butter, ghee and clarified butter.

Leather Chemistry: Introduction, constituents of animal skin, manufacture and preparation of hides, cleaning, soaking, limiting and degreasing, finishing and sharing, tanning; leather, vegetable, chrome, tanning effluents; pollution and control

Unit – II			
TT			

### Hrs

### **Cosmetics and Perfumes**

A general study including preparation and uses of the following: Hair dye, hair spray, Shampoo, Suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Water: Special consideration for cosmetics use. Surfactants: Classification and application in cosmetics - Foaming agents, emulsifiers, and solubilizers. Classification and application in cosmetics Antioxidants, antimicrobial and chelating agents used as preservatives,. Factors affecting effectiveness of antimicrobial preservatives

# Unit-III Hrs

Preparations and applications of Nano materials-Synthesis of nano materials via -gas phase and liquid phase methods, high energy ball milling metal-semiconductor-ceramics and composites- size dependent properties - uniqueness in these properties compared to bulk and microscopic solidsnanomaterials and nanostructures in nature, TiO<sub>2</sub>, ZnO, ZrO<sub>2</sub>, Composites and their applications.

### Unit – IV

### Hrs

Nanotechnology in Agriculture - Precision farming, Smart delivery system - Nanofertilizers: Nanourea and mixed fertilizers, Nanofertigation - Nanopesticides, Nanoseed Science, organic manures, micronutrients, biopestiside, biofertilizers and agrochemicals.

### **REFERENCE BOOKS**

1. F A Henglein: Chemical Technology (pergamon)

2. R.W. Thomas and P. Farago: Industrial Chemistry (HEB)

3. E. Stocchi: Industrial Chemistry, Vol -I, Ellis Horwood Ltd. UK

4. P.C. Jain, M. Jain: Engineering Chemistry, Dhanpat Rai & Sons, Delhi

5. Introduction to Nanoscience and Nanotechnology, Gabor .L et al

6. Fundamentals of Nanotechnology, Hornyak, G. Louis, Tibbals, H. F., Dutta, Joydeep, CRC Press, 2009

7.Nanomaterials: An introduction to synthesis, properties and application, Dieter Vollath, WILE-

# Unit –I:

15

15

### 15

VCH, 2008
8. Lynn J. Frewer, WillehmNorde, R. H. Fischer and W. H. Kampers, Nanotechnology in the Agrifood sector, Wiley-VCH Verlag, (2011)
9. B.K. Sharma: Industrial Chemistry, Goel Publishing House, Meerut

### Paper IND 3.3 Methods of Analysis in Industries

### **Unit – I Voltammetry Techniques:**

Introduction, Modified polarographic techniques, stationary electrode polarography, sinusoidal alternate current polarography, rapid scan polarography, pulse polarography, square wave polarography, Cyclic voltammetry, stripping voltammetry, numerical.

### **Unit – IINMR Spectroscopy:**

General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift values and correlation for protons bonded to carbons [aliphatic; olefinic; aldehydic and aromatic] and other nuclei [alcohols; phenols; enols; acids; ammines; amides and mercapto]; 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, Simplification of complex spectra; nuclear magnetic double resonance; shift reagent; solvent effect. Fourier transform technique; nuclear overhauser effect [NOE] Resonance of other nuclei – F & P.

### Unit – III: Chemical Analysis of surfaces:

Introduction to photoelectron spectroscopy, Ion Scattering Spectroscopy, Secondary Ion Mass Spectrometry, Auger Electron Spectroscopy, Electron Spectroscopy for Chemical Analysis. Basic principles, Instrumentation and applications of these techniques

### Unit – IVGas and Fuel analysis:

Modern concept of fuels, classification of fuels, characteristics of good fuels, Orsat apparatus and its use in gas analysis, Instrumentation and working of bomb calorimetry, boy's calorimeter and numerical, coal analysis, calorific value of fuels, determination of calorific value of a solid or liquid fuel, Flash point, determination of flash point by Abel's method.

### **REFERENCE BOOKS**

- 1. F. J. Welder: standard Methods of chemical analysis Voil. III Part A&B
- 2. H.A. Strobel chemical instrumentation (AW)
- 3. Willard, Merrit& Dean, Instrumental Methods of analysis (FWAP)
- 4. F.D. Snell, Encyclopedia of Industrial: Chemical Inorganic analysis Vol. 1 to 20 (J.W)
- 5. Hillebrand, Lhundell and Hoffman: Applied inorganic analysis (Interscience)
- 6. D.K. Chakrabarty: Solid state Chemistry
- 7. H. Kaur, Instrumental method of analysis.
- 8. .V.M. Parikh, Application spectroscopy of organic molecules. (Mehata)
- 9. D.W. Williams and Flemming, Spectroscopic methods of organic compound
- 10.Silverstein and Basallar, Spectroscopic identification of organic compounds

### 15 Hrs.

### .. 15 Hrs

15 Hrs

15 Hrs

1

11. V. M. Parikh Absorption Spectroscopy for Organic Molecules (J. Wiley)

- 12. P.S. Kalsi Spectroscope of organic compounds (New age publisher)
- 13. Jackman and Sterneil, Application of NMR spectroscopy
- 14.J.D. Roberts, Nuclear magnetic resonance (J. Wiley)
- 15. D.L.Pavia, G.M.Lampman and G.S.Kriz, Introduction to Spectroscopy.
- 16. Analytical Chemistry-Gurudeep R. Chatwal Edited by Madhu Arora, Himalaya publication.
- 17. Instrumental method of chemical analysis- H. Kaur, Pragati prakashan

### Paper IND E01: General Chemical Technology

### Unit-I

## 15 Hrs

### **Chemical reactors and Unit Processes:**

Classification of chemical reactors, continuous reactor and batch reactor, chemical composition of reactor.

**Nitration:** Nitrating agents, Kinetics and mechanism of nitration of aromatic compounds, Nitration of paraffinic hydrocarbons, Nitrate esters, N-nitro compounds, Process equipment. Typical industrial manufacturing processes

### Unit-II

**Sulphonation:** Sulphonating agents, Kinetics and mechanism. Desulphonation Workup Procedures, Industrial equipment and technique, Batch and continuous processes,

Amination by reduction and ammonolysis: Methods of reduction to give amino compounds, Aminating Agents, Manufacture of amino compounds by reduction as well as by Ammonolysis

### Unit-III

**Halogenation:** Kinetics and mechanism. Survey of methods, Catalytic chlorination, photohalogenation, Manufacturing processes for chlorohenzene, Chlorinated methanes, monochloroacetic acid, chloral

**Oxidation:** Oxidising agents with typical applications of each, Liquid phase oxidation with oxidising compounds, Typical manufacturing processes.

### Unit-IV

### 15Hrs

**Esterification:** Kinetics and mechanism. Esterification of carboxylic acid derivatives, Esters by addition to unsaturated systems, Industrial esterifications, Ethyl acetate, butyl acetate, Vinyl acetate, methyl methacrylate.

**Petrochemicals:** petroleum refining, outline of chemicals derived from ethylene, xylene and naphalene

### 15 Hrs

### **REFERENCE BOOKS**

- 1. P. H. Groggins: Unit Processes in Organic Synthesis (MGH)
- 2. F. A. Henglein: Chemical Technology (Pergamon)
- 3. M. G. Rao and M. Sittings: Outlines of Chemical Technology (EWP)
- 4. Clausen, Mattson: Principles of Industrial Chemistry
- 5. H A. Lowenheim and M. K. Moran: Industrial Chemicals
- 6. Kirk and Othmer: Encyclopedia of Chemical technology.
- 7. Kent, Riegel's Industrial Chemistry (N-R).
- 8. S. D. Shukla and G. N. Pandey: A Textbook of Chemical Technology, Vol-II
- 9. J. K Stille: Industrial Organic Chemistry (P.I I.).
- 10. Chemical Reactor Design, Optimization, and Scaleup-E. Bruce Newman 2nd Edition

### Paper- IND E02- Advanced Analytical Techniques in Industries

Basic theory, Instrumentation, Laboratory technique and Applications of following methods Unit – I 15 Hrs X – ray Methods: Diffraction, Fluorescence, absorption, & emission spectroscopy. 15 Hrs Unit – II Thermoanalytical Methods: Thermogravimetric Analysis, Differential Thermal Analysis, Differential scanning calorimetry. Unit – III 15 Hrs ElectroAnalytical Methods: Coulometry, Polarography, Amperometry, electrogravimetry. Unit – IV 15 Hrs Radiochemical Methods of analysis: Radiation Dosimetry, Radiolysis of water, Free Radicals in Water Radiolysis, Radiolysis of some aqueous solutions, A time scale of Radiolytic Events Radiation-induced Color Centers in Crystals: Storing and release of Energy. **REFERENCE BOOKS** 1. H J Arnikar: Essential of Nuclear Chemistry 2. R.D. Braum, Introduction to Instrumental Analysis.

- 3. Willard, Deritt, Dean and Settle, Instrumental methods of Analysis
- 4. G.W. Ewing, Instrumental Methods of Analysis 4th and 5th editions.
- 5. Chatawal and Anand, Instrumental Methods of Analysis.

### Paper- IND E03- Chemical Analysis in Agro, Food and Pharmaceutical Industries.

### Unit – I

15 Hrs

Analysis of soil: Moister, pH, total nitrogen, phosphorous, silica, lime, Magnesia, Manganese, sulfur & alkali salts.

Fuel analysis: Solid, liquid and Gas, ultimate and proximate analysis heating values, grading of cool, liquid fuels, flasks points, aniline point, octane number and carbon residue, gaseous fuels – producer gas and water gas – calorific value.

### Unit-II

Clinical Chemistry and drug analysis: Composition of blood collection, and preparation of samples, clinical analysis - serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulin, barbiturates, acidic and alkaline phosphates, Immunoassay, principals of radioimmunoassay and applications, The blood- gas analysis trace elements in the body.

Drug analysis: Narcotics and dangerous drugs, classification of drugs, screening by gas m thin layer chromatography and spectrophotometric analysis. 15 Hrs

### Unit – III

Food analysis: Moister, ash, crude protein, fat, crud fiber, carbohydrate, calcium, potassium, sodium, and phosphates, food adulteration - common adulteration in food, contamination of food stuffs, microscopic examination of foods for adulterants, Pesticide analysis in food products, Bxdraction and purification of sample, HPLC, gas chromatography for organo – phosphates, thin layer chromatography for identification of chlorinated pesticides in food products

### Unit –IV

15Hrs

Fluorescence in Biological, Medical and Drug Development: Fluorescence instrumentation for analysis, flurophors and their modification, pH - indicators, membrane potential probes, lipid membrane protein, labeling of protein and DNA.

### **REFERENCE BOOKS**

1. Fundamentals of analytical chemistry by D. A. Skoog, D. M. West and F. J. Honer, W. B. Saunders.

2. Chromic phenomenon, The Technological application of color chemistry Peter Bamfield.

### M.Sc. Part-II, Semester – III (Practical V/VI) **Physical Chemistry Practical's**

1. Conductometry

Determination of percentage of acetic acid in commercial vinegar solution 2. Fluorimetry

To determine the amount of riboflavin in given B-complex tablet

3. Latent Heat of fusion

To determine the latent heat of fusion of given solid

4. Polarography

To study the effect of Oxygen supporting electrolyte and maximum suppressor and determine the half wave potential of Cd/Zn in given solution by Half wave potential method. Differential method and half wave equation method.

5. Potentiometry

To determine the dissociation constant of dibasic acid by potentiometric method

6. pH – metry

To determine the dissociation constant of dibasic acid pH – metrically.

7. pH – metry

To determine pH value of various buffer using pH meter and determination of dissociation

constant of acetic acid.

8. Spectrophotometry:

To determine pK value of phenolphthalein indicator by spectrophotometric method.

9. Spectrophotometry:

To study the stoichiometry and stability of ferric sulphate complex by Job's method and Mole ratio method.

### **Organic Chemistry practical's**

1. Preparation of p – amino benzoic acid from p – toluidine

- 2. Preparation of NBS (N bromo Succinimides)
- 3. Preparation of p iodonitrobenzene

4. Estimation of cu from copper fungicide

5. Estimation of Endosulfan

### **Inorganic Chemistry practical's**

Alloy Analysis

1. Chrome -steel alloy

Analyze the given sample of chrome - steel alloy & determine the percentage of

i) Chromium ----- Calorimetrically.

ii) Nickel ----- Gravimetrically.

2. Determine the amount of copper and zinc from given sample of brass alloy

i) Copper, Volumetrically/ Gravimetrically. ii) Zinc, Gravimetrically

3. Cement analysis:

Analyze the given sample of cement for its following constituents. i) SiO<sub>2</sub> - Gravimetrically

ii) Calcium, Volumetrically

iii) Iron, Volumetrically

iv) Magnesium, Complexometrically

36

v) Aluminium, Gravimetrically.

4. Find out the percentage of available chlorine in the given sample of bleaching powder

5. Determine the percentage of calcium present in a given sample of plaster of Paris volumetrically.

6. Find out the amount of Iron present in a given sample of Sulpha - drug; calorimetrically.

7. Determine the percentage of phosphorus present in terms of **P2O5** from a given fertilizer sample volumetrically.

## M.Sc. Part-II Sem-IV

## Paper- IND 4.1- Drugs and Pharmaceuticals

Unit – I

## Drugs, Pharmaceuticals and Pharmaceuticals analysis:

Introduction & classification of thedrugs based upon theirmode of action, Q-SAR, Molecular docking, Manufacturing processes of few important drugs, Aspirin, Ibuprofen, Paracetamol etc.

### Unit– II

Drugs Acting on infectious diseases:

Anthelmintic agents; synthesis of diethyl carbazine, niclosamide

Antitubercular drugs; synthesis of isoniazid, p-amino salicylic acid ethambutol and thioacetazone

Anti-leprosy drugs; synthesis of dapsone and clofazimine.

Sulpha drugs; classification, mode of action, synthesis of sulfadiazine, sulphaisoxazole, sulfadimethoxine.

### Unit – III

**Cancer therapy:**Types of cancers, Causes of cancer and therapy: surgery, radiation therapy, immunotherapy, chemotherapy, combination therapy, adjuvant therapy.

Antineoplastic drugs: Mercaptopurines,6-thioguanine, 5-flurouracil, allopurinol, methotrexate. Alkylating agents, effect of alkylating agents on DNA, DNA intercalating agents. Antimitotic agents and other therapeutic agents.

### Unit– IV

### a) Anti-AIDS:

Introduction& mechanism of HIV multiplication, Pathogenicity of HIV diagnosis, ELISA test, transmission and preventions of HIV, Anti-AIDS drugs

### b) Cardiovascular drugs:

Introduction, synthesis of amyl nitrate, methyldopa, sorbitrate.

### c) Anti-diabetic drugs:

Introduction, synthesis of sequence of A and B chain of insulin, Glibenclamide, metformin.

### **REFERENCE BOOKS**

- 1. Burger: Medicinal Chemistry (I.W.)
- 2. W. O. Foye: Principle of Medicinal Chemistry (I.E)
- 3. Lendieer and Metscher: The Organic Chemistry of Drug Synthesis (I.W.)
- 4. Essentials of Medicinal Chemistry; Editors Korolkovas and J. H. Burkhaltar, John Wiley &Sons
- 5. Wilson and Gisvold: Text Book of Organic Medicinal and PharmaceuticalChemistry.
- 6 O. D. Tyagi: SyntheticDrugs.
- 7. Medicinal Chemistry G. R. Chatwal.
- 8. Principles of medicinal chemistry (4th edition) W.D. Foye, T.L. Lemke, and D. A. Williams.
- 9. Organic chemistry of drug action and design R. B. Siwerman
- 10. Synthetic Drug G. R. Chatwal.
- 11. Handbook of Industrial Chemicals (Vol.-I) K. M. Shah
- 12. Principles of Medicinal Chemistry Vol. I, S. S. Kadam and K.G.Bothara
- 13. A Text Book of Medicinal Chemistry P. Parimo

### 15 hrs

# 15 hrs

15 hrs

15hrs

### Paper- IND 4.2-Inorganic Chemical Industries –II

### Unit – I

**Metallurgy:** Minerals in India, Mineral processing, Ellingham diagrams, manufacture and applications of metal alloys and salts, techniques for using low grade minerals. Iron and steel (Iron, Steel alloy, tool steel and stainless steel), Copper and its alloys, Zinc, Nickel and Aluminum.

### Unit II

**Metal finish technology:** Electro refining of metals, electroplating of nickel, chromium, copper, cadmium, silver and Gold, surface treatment technology, surface coats. Introduction, Electrodeposition, electroplating (Factors affecting, requirements and applications), hot dipping, metal cladding, immersion plating, metal spraying, vapour deposition and chemical and organic coating.

Chloralkali Industries: Soda Ash, Caustic Soda, Chlorine

### Unit III

### 15 Hrs

**Applications of Inorganic compounds in Pharmaceutical chemistry:** Introduction, imprities in pharmaceutical substances and their limit test, antioxidants, gastrointestinal agents, topical agents, dental products, inhalants, expectorants, respiratory stimulants. Compounds of iron, iodine and calcium, antidotes in poisoning, pharmaceutical aids

Unit IV 15 Hrs

**Glass and Refractory materials:** Raw materials, Soda glass, borosilicate glass, Lead Glass, Colored Glass, Refractory: Raw materials, clay pots, Zeolites.

**Industrial Gases:** Manufacture and industrial uses of H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub> & acetylene. Liquefaction of gases, production of low temperatures,

**Chemicals of Utility:** Inorganic fine chemicals, magnesia, alumina, AlCl3, calcium carbonate, sodium silicate, MnO<sub>2</sub>,FeSO<sub>4</sub>,PbO<sub>2</sub>,Na<sub>2</sub>HPO<sub>4</sub> and NaOH.

### **REFERENCE BOOKS**

1. Lowenheim F A (1974) Modern Electroplating III Ed Chapman & Hall, Landon.

2. Gable, D: Principal of metal Treatment and protection. Pergamon, Press Oxford (1978)

3. G.A. Keneth: Electroplating for Engineering's A Hand Book IIIrdEdn Van NastradReinbold Co London

4. F A Lowinbein: Modern Electroplating, Electroplating Publication New Jersey

5. Burke Progess in ceramic science Vol. IV

6. R.R.Iash: afromulary of paints and other coating Vol. I

7. J.D. Gilchrist: Extraction Metallurgy (Pergamon)

8. W.H. Dennis: Foundation of steel and iron Metallurgy (Elsevier)

9. S.D. Shukla & G N Pandey: A text book of chemical technology Vol. 1

10. F A. Henglein: Chemical Technology (Pergamon)

### 15 Hrs

### Paper IND 4.3 Selected Topics in Industrial Chemistry

### **Unit – I Polymer Preparation:**

Polyethylene (HDPE, MDPE, LDPE, LLDPE, UHMWPE, chlorinated PE), Polypropylene (PP), Polyisobutylene (PIB)), Acrylics (PMMA & PAN) Polyvinyl (PVC, PVDC & CPVC), Polystyrene & copolymer (HIPS, SBR, SAN & ABS), Poly (vinyl acetate), Poly ethylene terphalate,(PET) High temperature polymers, Bakelite and other polymers

### Unit-II

Science of corrosion and corrosion control: Introduction, economic aspects of corrosion, theories of corrosion, factors affecting corrosion, kinetics of corrosion, Evans diagram, thermodynamics of corrosion, Fourbaix diagram, corrosion testing techniques, Evaluation of corrosion effect: XRD, ESCA, FTIR surface techniques.

**Corrosion Prevention:** Corrosion inhibitors, protective coating, cathodic and anodic protection. Corrosion problem in India.

### Unit – III

**Mechanical and Rheological Properties of polymers:** Mechanical Properties, tensile strength, stress and strain curves, Maxwell voit model, Boltzmann superposition principle, Impact strength, compressive strength, ultimate polymer properties and structure relationship, Elastomers, Fibers, and Plastics. Rheological Equation of state (RES) fluid – ideal, non-Newtonian, viscous flow, viscoelastic behavior, creep, stress relaxation, dynamic mechanical behavior, Maxwells model, mechanical spectra.

### Unit – IV

Sensor Technology: Introduction, recent trends, classification of sensors, Elector analytical sensors, sensor, electrodes, Metal Membrane electrode sensors, Ionic Conductors, Thin film and thick Film Sensors, Nano - sensors, Application of sensors in Industry.

### **REFERENCE BOOKS**

- 1. Adamson: Surface Chemistry
- 2. D.D. Deshpande: Polymer science
- 3. Bilmayer: Polymer Science
- 4. N.B.Hanny: Solid state chemistry
- 5. S. Glastone: Physical chemistry
- 6. J.O.M..Bokries& A.K.N. Reddy: Modern Electrochemistry Vol I & II
- 7. J.D.Lee: Inorganic Chemistry.
- 8. N.N.Greenwood: Chemistry of Elements
- 9. D. Patranabis: Sensor and Tranducers.

### IND EO4 Environmental Chemistry

### Unit I:Water pollution and wastewater management

Introduction, use and conservation of water resources, water qualitymanagement, rainwater harvesting, water management in agriculture rain fed systems, irrigated systems, industries. Water pollution: Definition, types of water pollution (Physical, Chemical, biological and physiological), water pollutants.Ground water pollution and its protection, Surface, river, sea and lake water pollution, effect of excess nutrients and oil on water pollution, Sea water for agriculture, remedial measures for water pollution.

# 15 Hrs

15 Hrs

15 Hrs

### 15 Hrs.

### 15 Hrs.

**Industrial waste treatment:** Characteristics and types of industrial waste, principles of industrial waste treatment and disposal, protection of biosphere and surface water form industrial pollution.

### **Unit 2 Soil Pollution**

Introduction, industrial, agricultural, radioactive, sewage, domestic, chemical and metallic wastes, soil pollution by mining, by sediments and biological agents, Effect of heavy metals, diseases caused by soil pollution and impact of soil pollution on airquality

### **Control of soil pollution:**

Control of sewage, domestic and industrial waste, eco-farming and ecotechnology, biotechnology, integrated nutrient, pest, genetic resource and water management, land use systems

### **Unit 3: Air pollution**

Definition, composition and reactions occurring in atmosphere, Sources of air pollution, units of measuring air pollutants. Classification and effect of air pollution; oxides of nitrogen, Sulphur and carbon, Hydrocarbons, organic and inorganic particulates and ozone as pollutants, WHO Standards, Indoor air pollution, occupational air pollution, outdoor air pollution, Air pollution episodes; Bhopal gas, Seveso, Chernobyltragedies.

### Noise pollution:

Sources of Noise, Units and Measurements of Noise, Characterization of Noise from Construction, Mining, Transportation and Industrial Activities, Airport Noise, Auditory Effects, Non-Auditory Effects, Control of Noise Pollution.

### Unit 4:

### **Removal of Heavy toxic metals:**

Chromium, mercury, lead, cadmium, arsenic, analytical methods of determination of small amounts of metal pollutants, copper recovery, treatment of waste water to remove heavy metals, recovery techniques.

### **Polymer Recycling:**

Environment and polymer industry, recycling of polymer wastes

### **Reference:**

1. F. A. Henglein: Chemical safety Management and Engineering (Pergamon).

2. B. K. Sharma EnvironmentChemistry,

3. M. K. Hill; Understanding Environmental Pollution A Primer, Cambridge University Press,2004.

4. I. L. Pepper, C. P. Gerba, M. L. Brusseau, Environmental &

PollutionScience, Elsevier, 2006.

5. G. M. Masters, Introduction to Environmental Engineering and Science, Pearson, 2004.

6. Antony Milne, "Noise Pollution: Impact and Counter Measures", David & Charles PLC, 1979.

7. Peterson And E.Gross Jr., "Hand Book Of Noise Measurement", 5 Th Edition, 1963

### Paper- IND E05-Pharmaceutical Chemistry

### Unit – I

**Drug Design:** Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioavtivity, resonance, inductive effect, isosterism, non-isosterism, special considerations. Theroies of drug activity: occupuancy theory, rate theory, induced fit theory. Quantiative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded).

### Unit – II

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

### Unit – III

### 15 Hrs

**Cardiovascular Drugs:** Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular ooutput. Direct acting arteriolar dilators. Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol. Local Antiinfective Drugs: Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ehtionamide, ethambutal, fluconazole, griseofulvin, chlroquinprimoquin.

### 15 Hrs

### Unit – IV

**Psychoactive Drugs-** The Chemotherapy of Mind: Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazipines, buspirone, neurochemistry, of mental diseases. Antipsychotic drugs-the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimthadione, barbiturates, thiopental sodium, glutethimide. Antibiotics: Cell wall biosynthesis, inhibitors,  $\beta$ -lactum rings, antibiotics inhibiting protein synthesis. Synthesis of penicillin G, penicillin V, ampicillin, amoxicillin, chloramphenicol, Cephalosporin, tetracycline and streptomycin.

### **REFERENCE BOOKS**:

1. Introduction to medicinal chemistry, A Gringuage, Wiley- VCH.

2. Wilson 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 Volume 1 (Chap. 9 and Chap.14), Ed.M.E. Wolff, John Wiley.

5. Goodman and Gilman's Pharmacological Basis of Therapeutics, Mc Graw-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.

### Paper- IND E06- Chemistry of Industrially Important Materials

### Unit – I

### 15 Hrs

**Industrial Materials:** Glasses, Ceramics, Composites and Nonmaterial'sGlasssy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Refractories, characterizations, properties and applications. Microscopic composites; dispersion-strengthened and particle-reinforced fibre- reinforced composites, macroscopic composites. Nanocrystalline phase, preparation phase, preparation procedures, special properties, applications. Thin Films and Langmuir-Blodgett Films: Preparation techniques, evaporation/sputtering, chemical processes, MOCVD, sol- gel etc., Langmuir-Blodgett(LB) film, growth techniques, photolithography properties and applications of thin and L-B films. Liquid crystals: Mesomorphic behaviour, thermotropic liquid crystals,

positional order, bond orientational order, nematic and smectic mesophases, smectic nematic transition and clearing temperature-homeotropic, planer and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic B phasesopoptical properties of liquid crystals, Dielectric susceptibility and dielectric constants. Lytropic phases and their description of ordering in liquid crystals.

### Unit-II

Polymeric Materials: Moleculr shape, structure and configuration, crystallinity, stressstrain behaviour, thermal behaviour, polymer types and their applications, conducting and ferroelectric polymers. Ionic Conductors: Types of ionic conductors, mechanism of ionic conduction, interstitial jumps(Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

### Unit – III

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

### Unit – IV

Materials for Solid State Devices: Rectifiers, transistors, capacitors-IV-V compounds, lowdimensional quantum structures; optical properties. Organic Solids, Fullerenes, Molecular Devices: Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes-dopped, fullerenes as superconductors. Molecular rectifiers and transistors, photosynthetic artificial devices, optical storage memory and switches- sensors. Nonlinear optical materials; nonlinear optical effects, second and third order- molecular hyperpolarisability and second order electric susceptibility, materials for second and third harmonic generation.

### **REFERENCE BOOKS:**

- 1. Solid State Physics, N.W.Ashcroft and N.D.Mermin, Saunders College.
- 2. Material Science and Engineering, AnIntroduction, W.D.Callister, Wiley.
- 3. Principles of the Solid State, H.V.Keer, Wiley Eastern.

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15 Hrs

- 4. Materials Science ,J.C.Anerson,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.

### M.Sc. Part-II, Semester – IV (Practical VII/VIII) Physical Chemistry Practicals

1. Potentiometry: Todetermine Solubility of PbI2 with Ag/AgI electrode by using potentiometry.

2. Potentiometry:Todeterminethedissociationconstantoftribasicacid(H<sub>3</sub>PO<sub>4</sub>) potentimetrically

3. Conductometry: To determine the critical micelle concentration of sodium laurylsulphate in aqueous solution conductmetrically.

- 4. Fluorometry: To estimate the Quinine sulphate in given sample byFlurometry.
- 5. pH metry: To determine hydrolysis constant of aniline hydrochloride by pHmetry

6. pH – metry: To determine isoelectronic point and dissociation constant of aminoacid (Glycine) by pHmetry

7. Spectrophotometry: To determine stability constant of Ferric thiocynate complex byFrank Ostwald methodspectrophotometrically

8. Polarography: To determine unknown concentrations of Cd <sup>+2</sup> ionin given solution by standard additionmethod

## **Organic Chemistry Practicals**

- 1. Identification and separation of ternary organic mixtures by physical and chemical methods.
- 2. Preparation of benzanilide from benzophenone by use of Beckmann'srearrangement
- 3. Preparation of p- Bromo aniline fromacetanilide
- 4. Estimation of Vit –C
- 5. Estimation Sulfur from SulfurFungicide
- 6. Preparation of Anthranilic acid
- 7. Preparation of p-iodoazobenzene.

### **Inorganic Chemistry Practicals**

- - ii) Magnesiumcomplexometrically.
- 2. Analyse the given sample of pyrolusite ore, determine the percentage of, i) Silica gravimetrically.
  - ii) Ironvolumetrically.

iii) Manganesevolumetrically.

- 3. Analyse the given sample of Bronze metal alloy, determine the percentageof,
  - i) Tin as tin oxide gravimetrically. ii) Lead as lead sulfategravimetrically. iii) Copper Iodometrically iv) Zinc complexometrically.
- 4. Find out the amount / percentage of **Iron** per gram of soap samplecolorimetrically

- 5. To prepare **potash alum** & find out the percentage of **Aluminium**in thealum.
- 6. Find out the percentage of '**Magnesium**' in a given sample of Talcumpowder complexometrically.
- 7. Determine the concentration in mg/lit of sulphate ion in the given sample of water nephelometrically.

# Department of Industrial Chemistry Prorgamme Outcome

The main objective of the course is to provide students with the general criteria useful for an industrial chemical process planning and with the fundamental concepts that must be taken into account in designing a plant. To this aim, some industrial chemical processes are described and analyzed in terms of thermodynamic and kinetic aspects and are also highlighted the most important technology. Problems associated with the cost, sustainability and safety of an industrial process are also discussed.

### Shivaji University, Kolhapur

Industrial chemistry is the link between the research and industrial-scale chemical engineering. Industrial chemists make use of their broad understanding of chemistry and environmental sustainability in areas like pharmaceutical companies, polymer manufacturing, petrochemical processing, food science, and manufacturing industries.

Industrial chemists can be found in the most unexpected places. They could be challenging the norm at the cutting edge of research, or taking responsibility for successful operations of some of Australia's largest companies in the chemical industry. In a general sense, industrial chemists are involved in:

**Safety and efficiency** – industrial chemists are constantly striving to improve the safety and efficiency of making important chemicals and materials.

**Product development and innovation** – industrial chemists create new chemical 'recipes' that meet identified needs. They will scrutinise the chemical composition of substances and then study the chemical changes which occur under different conditions and apply this to their end result.

Process optimization - an industrial chemist plays a part in optimising production to

produce large amounts of a substance as cheaply as possible – but, unlike with engineers, they do so by making the 'chemistry' better and more efficient.

**Environmental monitoring and control** – industrial chemists work on the management and control of the environment during industrial processes, to ensure everything is being done to minimise the impact and work towards a clean and safe future.

**Production plant design** - in the construction of a new production plant, industrial chemists work in teams with other engineers like chemical engineers or control engineers to ensure the optimal outcomes.

### Ideas, design, testing - making a product as good as it can be

Industrial chemistry is part of the long chain in the design and manufacturing process. Industrial chemists deal with the ideas, the design, the testing, and prototyping of new industrial products. In order to design something entirely new to help solve the major problems of the world their essential skills are, in-depth knowledge and application of chemistry and creativity with chemicals.

Whereas a chemical engineer deals with the whole process of changing raw materials into a useful, marketable product, an industrial chemist would look specifically at the nitty gritty science stuff, scrutinising the chemical components and designing a 'method' for the product then work out the best way to make it. The industrial chemist precedes the chemical engineer in the process of bringing something to market.

Basically, if you want to know exactly where a product comes from, you should ask an industrial chemist.

### Where do industrial chemists work?

Industrial chemists work in many different industries – including petrochemicals, polymers, plastics food, cosmetics, pharmaceuticals, minerals and new materials.

You could find an industrial chemist wearing a number of different career titles including, research scientist, development chemist, technical representative, plant manager, development chemist, production process manager, operations manager, fuel development chemist, research scientist, production process manager or operations manager. You might

also find an industrial chemist working in marketing or management in the chemical industry.

### **Outcomes of Programme:**

The Industrial Chemistry Department has also identified specific objectives and outcomes for both the Masters and Ph.D. Graduate programs.

### M.S. in Industyrial Chemistry

1. Students should have an advanced level understanding of at least three of the following areas of Chemistry - Analytical, Inorganic, Organic, and Physical Chemistry. They should have a graduate level understanding of their major area(s) of research.

2. Students should broaden their professional foundations through activities such as teaching, internships, and fellowships

3. Students should be able to communicate scientific results in writing and in oral presentation.

4. Students should acquire the basic tools needed to carry out independent chemical research. Students should become proficient in their specialized area of chemistry and successfully complete an advanced research project.