

Department of Chemistry
M. Phil. Curriculum in Physical Chemistry

Students wishing to study for the M. Phil. Degree in Physical Chemistry must take Courses PC 601H and PC 602H as compulsory courses. In addition he/she should take two other courses from the remaining courses. Each course carries a credit of half unit, and there will be a 3-hours examination of 50 marks.

1. **PC 601H Advanced Spectroscopy**
2. **PC 602H Advanced Chemical Kinetics**
3. **PC 603H Solid Surfaces and Heterogeneous Catalysis**
4. **PC 604H Advanced Electrochemistry**
5. **PC 605H Advanced Photochemistry**
6. **PC 606H Advanced Polymer Chemistry**
7. **PC 607H Chemistry of Materials**
8. **PC 608H Structures of Liquids and Solutions**
9. **PC 609H Advanced Electrochemical Techniques**
10. **PC 610 H Biophysical Chemistry**

PC 601H Advanced Spectroscopy

Learning Objectives

The learning objectives of this course are to

- (i) Impart knowledge on molecular symmetry, group multiplication table, and character table, the relation between molecular symmetry and infra-red and Raman activities.
- (ii) Acquaint with advanced concepts of Raman and electronic spectroscopy.
- (iii) Give details on Mossbauer spectroscopy and its application.
- (iv) Provide advanced knowledge on ESR and NMR techniques, including details of ^{13}C NMR and their interpretation.
- (v) Demonstrate skills and abilities needed for analysis of spectra.

- 1. Principles of Molecular Spectroscopy:** Rotational, Vibrational and Electronic Transitions; MW, IR and UV ground and excited state of molecules. Intensity and Width of Spectral lines.
- 2. Advanced Treatment of Raman Spectroscopy.** -Visible Spectrometer; Dispersive and FT Spectrometers. Determination of bond length in
- 3.** Polarization of Raman scattered light. Raman investigation of phase transitions. Resonance Raman Scattering. Structure determination using IR and Raman Spectroscopy. Surface Enhanced Raman Scattering. Non-Linear Raman phenomenon. Stimulated Raman scattering. Multiphoton Spectroscopy.
- 4. Electronic Spectra of Diatomic Molecules.** Electronic angular momentum of diatomic molecules. Spectroscopic term symbols for molecules. Photoelectron spectroscopy.
- 5. Mossbauer Spectroscopy:** Nuclear properties and nuclear gamma resonance, Doppler Effect, Mossbauer parameters and theory. The application of isomer shift and quadruple splitting measurements in tin and iron complexes.
- 6. Nuclear Magnetic Resonance Spectroscopy:** General theory of high resolution of NMR, Pulse and Fourier transformation methods, Experimental techniques, Double resonance methods, Lanthanide shift reagents, The relation between structure and chemical shifts, spin-spin coupling (general, vicinal and long range), The effect of molecular conformational motions. ^{13}C & ^{31}P spectra.
- 7. Electron Spin Resonance Spectroscopy:** Quantization of angular momentum, relation between magnetic moment and angular momentum, g factor, fine structure of E.S.R., hyperfine structure, instrumentation and applications of E.S.R.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Gather knowledge on molecular symmetry, group multiplication table, character table, infra-red (IR) and Raman activities.
- (ii) Explain the understanding principle of Molecular, Raman, Photoelectron, Mossbauer, NMR and ESR Spectroscopic techniques.

- (iii) Acquaint with Mossbauer Spectroscopy, NMR and ESR Spectroscopy and their interpretations.
- (iv) Know the structure of compounds using IR, Raman and NMR spectroscopy.
- (v) Realize the cause of hyperfine and super hyperfine splitting in ESR spectrum, calculation of g value and understand anisotropy in g and A values.

Books recommended

1. F. A. Cotton, Chemical Application of Group theory, Wiley New York 1963.
2. C. N. Barnwell, Fundamental of Molecular Spectroscopy.
3. G. M. Brown, Introduction to Molecular Spectroscopy.
4. John A. Weil, J. R. Bolton, and John E. Wertz, Electron Paramagnetic Resonance, John Willy & Sons Inc.
5. Recently published papers on the above topics in different journals.
6. Physical Chemistry by Peter-Atkins, 8th Edition.

PC 602H Advanced Chemical Kinetics

Learning Objectives

The learning objectives of this course are to

- (i) Provide advanced concept of chemical kinetics of non stationary systems and acquire knowledge on explosion, ignition, combustion and stationary flames.
- (ii) Impart knowledge on theories of reaction rates like, transition state theory (TST), theories of Lindemann and Hinshelwood, RRK & RRKM theories.
- (iii) Give idea about potential energy surface (PES), models for chemical reactions in solution and theory of diffusion and activation controlled reactions.
- (iv) Know the concepts of acid-base catalysis, micellar catalysis, linear free energy relation, Hammett equation, substituent and correlation effects.
- (v) Gather knowledge about molecular dynamic calculations and state to state kinetics and know the experimental techniques for studying the kinetics of fast reactions.

Course Content

1. **Theories of Reaction Rates:** Transition State Theory; potential energy surface; basic postulates and derivation; Statistical treatment of transition state theory. Unimolecular reactions. Formation of energized species. Sum and density of states. Theories of Lindemann and Hinshelwood. Statistical energy-dependent rate constant. RRK and RRKM theories.
2. **Complex Reactions:** Characterization, kinetic behaviors, kinetic behavior of non-stationary systems. Mechanism of reactions from kinetic behaviour. Thermal explosion, chemically sensitized explosion, branching chain explosion, explosion limit. Reaction of hydrogen and oxygen. Ignition and combustion. Stationary flames. Combustion of hydrocarbons.

- 3. Reactions in Solutions:** Models for chemical reactions in solution; factors determining reactions rates in solution; diffusion and activation controlled reactions. Acid-base catalysis. Substituent and correlation effects. Hammett equation. The Brønsted relation; linear free energy relations. Micellar Catalysis.
- 4. Reaction Dynamics:** Molecular-dynamical calculations. The reaction $H + H_2$; the reaction $Br + H_2$. Features of potential energy surfaces; attractive and repulsive surfaces. Molecular beams. State-to-state kinetics.
- 5. Experimental Techniques for Studying Kinetics of Fast Reactions:** Flow Method, Flash Photolysis, Relaxation Techniques, Relative Method.

Learning Outcomes

Upon completion of this course the students will be able to

- Understand advanced concept of chemical kinetics of non stationary systems explosion, ignition, combustion and stationary flames.
- Discuss different theories of reaction rates, such as, transition state theory (TST), theories of Lindemann and Hinshelwood, RRK & RRKM theories.
- Demonstrate knowledge of potential energy surface (PES), models for chemical reactions in solution and theory of diffusion and activation controlled reactions.
- Describe the kinetics of acid-base catalysis, micellar catalysis, linear free energy relation, Hammett equation, and substituent and correlation effects.
- Explain state to state kinetics, kinetics of fast reactions, attractive and repulsive surfaces, molecular dynamical calculations for the reactions between atoms and molecules.

Books Recommended

- The foundation of Chemical Kinetics, Sidney W. Benson, McGraw-Hill, New York.
- Kinetics and Mechanism, A. A. Frost and R. G. Pearson, John Wiley & Sons, NY, 2nd Edition, 1961.
- Chemical Kinetics, K. J. Laidler, Pearson Education, Singapore (3rd Edn), 1987.
- Chemical Kinetics and Dynamics, J. I. Steinfeld, J. F. Francisco and W. L. Hase, Prentice Hall.
- Chemical Kinetics, Kenneth A. Connors.
- Selected articles from recent journals.

PC 603 H Solid Surfaces and Heterogeneous Catalysis

Learning Objectives

The learning objectives of this course are to

- Give modern concepts on physicochemical characteristics of solid surfaces, adsorption and energetic involved.
- Impart advanced knowledge on catalysis and preparation, characterization and industrial applications of catalysts.

- (iii) Provide knowledge on adsorption thermodynamics, kinetics of catalytic reactions and their mechanism.
- (iv) Give idea on basic principle, operation and applications of different modern techniques for characterization of solid surfaces.

Course Content

- 1. Nature of Solid Surfaces:** Steps, terraces, kinks, dislocations, and defects. Contamination. Cleaning of surfaces.
- 2. Adsorption Energetics:** Isotherms, isobars and enthalpy changes.
- 3. Experimental Techniques:** Adsorption measurements. Studies on physical properties of adsorbents, surface area, pore structure of polycrystalline adsorbents, work function, electrical conductivity, and magnetic properties. Desorption studies.
- 4. Kinetics of Adsorption:** Elovich equation, Lagergren equation, Tempkin equation. Mobility of adsorbed species on surfaces.
- 5. Heterogeneous Catalysis:** General description of heterogeneous catalysis, Classification of heterogeneous catalysts, preparation and modification of catalysts, and some applications. Transition state theory of heterogeneous reactions, specificity and selectivity in catalysis, catalytic activity and chemisorption.
- 6. Mechanism of Catalytic Reactions:** Chemisorption processes on solid surfaces. The Langmuir-Hindshelwood mechanism, the Eley-Rideal mechanism and general considerations in the determination of heterogeneous reaction mechanism. Catalysis by transition metals : hydrogenation, dehydrogenation, hydrogenolysis, the volcano curve. Oxidation on oxide surfaces. Hydrocarbon conversion, Reforming catalysts.
- 7. Industrial Processes Based on Solid Catalysts:** Hydrogenation of vegetable oils. Ammonia and nitric acid production. Methanol synthesis. Synthesis gas conversion. Ethylene oxide production. Sulphuric acid production. Linear polyethylene production. Catalytic cracking. Synthetic gasoline production.
- 8. Studies of Solid Surfaces and Adsorbed Species:** Ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), Low energy electron diffraction (LEED), Auger electron spectroscopy (AES), Field emission microscopy (FEM), Field ion microscopy (FIM), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Vibrational spectroscopy of adsorbed species: FTIR, EELS. Temperature programmed desorption spectroscopy.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the physicochemical characteristics of solid surfaces.
- (ii) Know the methods of preparation, characterization and industrial applications of catalysts.

- (iii) Demonstrate knowledge on adsorption thermodynamics, kinetics of catalytic reactions and their mechanism.
- (iv) Apply knowledge on basic principle, operation and applications of different modern techniques for characterization of solid surfaces.

Books Recommended

1. Physical Chemistry of Surfaces, Adamson, Wiley, New York.
2. Physical Chemistry, P. W. Atkins, Oxford University Press, Oxford.
3. Catalytic at surfaces, Ian Campbell (1988), Chapman and Hall.
4. Surface Chemistry, Elaine M. McLash, Oxford University Press, 2001
5. An Introduction to Chemisorption and Catalysis by Metals, R. P. H. Gasser, Clarendon, Oxford.
6. Heterogeneous Catalysis: Principles and Applications, G. C. Bond, Clarendon, Oxford (2nd Edn).
7. Heterogeneous Catalysis, S. J. Thomson and G. Webb, Oliver and Boyd, Edinburgh.
8. Introduction to Zeolite Science and Practice, Studies in Surface Science and Catalysis (Vol. 58), H. Van Bekkum,, E. M. Flanigen and J. C. Jansen (Editors), Elsevier, Amsterdam.
9. Solid State Chemistry and its applications, A. R. West, John Wiley & Sons (Asia), Singapore.
10. Selected articles from recent journals.

PC 604 H Advanced Electrochemistry

Learning Objectives

The learning objectives of this course are to

- (i) Explain the mechanism of formation of electrical double layer and their models.
- (ii) Provide knowledge on conducting polymers and modification of electrode surface.
- (iii) Impart knowledge on electrosynthesis and electrocatalysis.
- (iv) Know the under potential and over potential deposition (UPD & OPD) at electrode surfaces and their nucleation growth kinetics.
- (v) Gather knowledge on corrosion and passivation, basic electrodictics of corrosion and typical applications of electrochemistry.

Course Content

- 1. Electrified Interface and Electrode Kinetics:** Formation of electrical double layer. Models of electrified interfaces. Over-potentials, exchange current density, symmetry factor, β , Electrode kinetics, Butler-Volmer equation and its modifications.
- 2. Modified Electrodes:** Modification of metallic and semi-conducting electrodes by using electrochemical (EC) and self-assembly (SA) techniques.
- 3. General properties of electronically conducting organic polymers:** Ionically doped organic polymers as semiconductors. The structure of poly-pyrrole / solution interface. Apparent catalysis by redox couples introduced into polymers attached to electrodes.
- 4. Electro-Synthesis & Dynamic Electrochemistry:** Cell design, new electrode materials, and electro-crystallization, under potential (UPD) and over potential deposition (OPD) of metals. Factors that affect crystal growth. Nucleation and initial growth kinetics. Passivation and nature of the passive layer, structure of the passive film and depassivation.
- 5. Corrosion and Passivation:** Mechanism of corrosion of ultra pure metals. Thermodynamics and stability of metals. Potential-pH diagram uses and abuses. The corrosion current and potentials. Basic electrochemistry of corrosion in absence of oxide films. Inhibiting corrosion.
- 6. Typical Applications of Electrochemistry:** The electrolysis of seawater. The electrochemical transport system. Recent advances in portable batteries and rechargeable batteries. The fixing of carbon dioxide. The electrochemical treatment of wastes. The super electrolyzes.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Explain the formation, mechanism and different models of electrified interfaces.
- (ii) Develop modified electrodes of metallic and semiconducting materials using various methods.
- (iii) Apply knowledge of electroanalytical techniques in various applications such as, electrolysis, electrocatalysis, industrial and environmental electrochemistry.
- (iv) Understand electrocrystallization, nucleation and growth kinetics under potential and over potential deposition (UPD & OPD).
- (v) Know basic electrochemistry of corrosion, corrosion current, corrosion potential, passivation and inhibition of corrosion.

Books Recommended

1. Modern Electrochemistry- John O' M Bockris and K N Reddy (Plenum Press, New York).
2. Laboratory Techniques in Electroanalytical Chemistry- Peter T. Kissinger & William R. Heineman (Marcel Dekker Inc. N Y).
3. Chemistry Experiments for Instrumental Methods- Donald T. Sayer, William R. Heineman & Janice M. Beebe (John Wiley & Sons).
4. Electrochemical Methods: Fundamentals and Applications - A. J. Bard and L. R. Faulkner (Wiley, New York).
5. Electrochemistry at Solid Electrodes- R. N. Adams (Marcel Dekker , New York).
6. Selected Articles from Recent Journals.

PC 605 H Advanced Photochemistry

Learning Objectives

The learning objectives of this course are to

- (i) Give general concepts on photochemical and radiochemical processes and use of various light sources in photochemistry.
- (ii) Impart knowledge on different photophysical and photochemical processes and related terminologies.
- (iii) Demonstrate a detailed knowledge on photoactive materials and their applications; such as photoelectrochemical solar cells, photovoltaic cells etc.
- (iv) Give knowledge on different advanced oxidation processes for treatment of water and photodegradation of dyes and other organic substances.
- (v) Introduce different advanced techniques for study of photochemical behavior; such as flash photolysis, matrix isolation etc.

Course Content

- 1. General consideration:** Pathways of dark reactions and photochemical reactions. Photochemistry and radiation chemistry. Dosimeters. Current trends in photochemistry.
- 2. Techniques in Photochemistry.** Light sources. Lasers: basic principle of laser action; various types of lasers; tunable lasers. Actinometry. Quantum yield measurement.
- 3. Photochemical Kinetics:** Excited species and their fates. Jablonsky diagram. Unimolecular and bimolecular processes. Collisional quenching: Stern-Volmer equation and plot.
- 4. Photoelectrochemistry:** Photocathodes and photoanodes. Rate-determining step in photoelectrochemical reactions. Dye sensitized photoelectrochemical processes.

- 5. Photodegradation:** Degradation of dyes and other organic substances in aqueous system. Roles of mediators, hydrogen peroxide and ozone. Advanced oxidation process in water treatment.
- 6. Frontiers of Photochemistry:** Pico- and femto- second photolysis. Solar energy storage. Photo-electrochemical hydrogen generation from water. Photochemistry of vision. Photosynthesis.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the differences between dark and photochemical reactions; realize the principle and application of different light sources.
- (ii) Describe different photophysical and photochemical processes and detailed on fluorescence, phosphorescence and related phenomena.
- (iii) Realise photoactive materials and their applications; such as photoelectrochemical solar cells, photovoltaic cells etc.
- (iv) Apply knowledge of different advanced oxidation processes for treatment of water and photodegradation of dyes and other organic substances.
- (v) Use different advanced techniques for study of photochemical behavior; such as flash photolysis, matrix isolation etc.

Books Recommended

1. Photochemistry- J.G. Culvert & J. N. Atkins (John Wiley & Sons)
2. Principles and applications of Photochemistry - R P Wayne (Oxford University Press)
3. Chemistry and Light - P Suppan (Royal Society of Chemistry)
4. Modern Electrochemistry- John O' M Bockris and K N Reddy (Plenum press, NY)
5. Fundamentals of Photochemistry - K.K. Rohatgi-Mukharjee (revised edition, Wiley Eastern Ltd., Calcutta).
6. Principles of Radiation Chemistry - J. H. O' Donnel & D F Sangster (Edward Arnold)
7. Selected Articles from Recent Journals.

PC606 H Polymer Chemistry

Learning Objectives

The learning objectives of this course are to

- (i) Provide basic understandings on different kinds of polymerization techniques and mechanisms
- (ii) Give idea about commercially important and functional polymers in industry and research.
- (iii) Make aware of advanced techniques of characterization, commercial utilizations of polymers and their environmental impact.
- (iv) Impart knowledge on polymer modification and processing.

Course Content

- 1. Kinetics of Polymerization :** Kinetics of addition polymerization, (free radical chain polymerization), molecular-weight control and kinetic chain length, effect of chain transfer and chain transfer agents, autoacceleration. kinetics of step polymerization, crosslinking (Carother's equation, gelation and statistical approach). kinetics of cationic and anionic polymerization.
- 2. Polymerization Techniques:** Bulk (mass) polymerization, solution polymerization, emulsion Polymerization, heterogeneous polymerization.
- 3. Reaction of Synthetic Polymers :** Enzymatic degradation, oxidation, high-temperature degradation, hydrolysis of side-group structures, graft polymer formation, lithography and microlithography of polymer (radiation chemistry of polymer). Polymer in solution : criteria for polymer solubility, thermodynamics of polymer solubility.
- 4. Structure and Properties of Polymers:** Configuration and conformation of polymer, secondary valency forces, nature of chain packing, molecular weight distribution.
- 5. Crystalline and Amorphous State of the Polymer :** Melting of polymer and crystalline melting point, T_m , factors affecting crystallinity and T_m , amorphous polymer and glass transition temperature T_g , experimental determination of T_g , detection of T_g , factors affecting T_g .
- 6. Rheology and Mechanical Properties of Polymer :** Rheological behaviour of polymer, phenomena of viscous flow, kinetic theory and thermodynamics of rubber elasticity, molecular theory of viscoelasticity and five regions of viscoelastic behaviour, linear viscoelastic behaviour of amorphous polymer, creep, stress-strain behaviour of elastomer.
- 7. Polymer Processing :** Plastic technology, molding, extrusion, other processing technique, additives and compounding, elastomer technology, vulcanization and reinforcement.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Gather detailed knowledge on kinetics and mechanism involved in polymerization reactions.
- (ii) Acquire insight into different techniques and reactors used in polymer synthesis, and the industrial processes involved.
- (iii) Characterize polymers and discuss their structural, thermal, and mechanical properties.
- (iv) Apply knowledge on sortation, and disposal of polymers.

Books Recommended

1. Contemporary Polymer Chemistry, 3rd edition. H R Allcock, F W Lampe and J E Mark.
2. Polymers : Chemistry & Physics of Modern Materials, 2nd edition J M G Cowie
3. Introduction to Polymers, 2nd edition R J Young and P A Lovell

4. Textbook of Polymer Science, 3rd edition F W Billmeyer, Jr
5. Polymer Science and Technology, J R Fried

PC 607 H Chemistry of Materials

Learning Objectives

The learning objectives of this course are to

- (i) Provide with a basic understanding of the various materials used in engineering applications.
- (ii) Acquire knowledge on basics of material science, structure and property relationships for polymers, metals, ceramics, nanomaterials and advanced materials.
- (iii) Describe phase equilibria of materials and the microstructure involved during phase changes.
- (iv) Design and synthesis of new materials including composites.

Course Content

- 1. Materials:** Classification of Materials, Materials of the Future, Modern Materials' Needs.
- 2. Properties of Materials:** Mechanical, Thermal, Magnetic, and Optical Properties. Concept of Stress and Strain, Elastic Deformation, Plastic Deformation, Property Variability and Design/Safety Factors, Slip, Creep, and Viscoelastic Deformation; Heat Capacity, Thermal Expansion, Thermal Conductivity, and Thermal Stresses; Optical Properties of Metals and Non-Metals and Application of Optical Phenomena: Luminescence, Photoconductivity, LASER.
- 3. Phase Diagrams and Microstructure in Materials:** Equilibrium Phase Diagrams, Binary Isomorphous Systems, Development of Microstructure in Isomorphous Alloys, Mechanical Properties of Isomorphous Alloys, Binary Eutectic Systems, Development of Microstructure in Eutectic Alloys, Equilibrium Diagrams Having Intermediate Phases or Compounds, Eutectic and Peritectic Reactions, Congruent Phase Transformation, The Iron-Iron Carbide Phase Diagram, Development of Microstructure in Iron-carbon Alloys; Superalloys.
- 4. Composite Materials:** Particle-Reinforced Composites: Large-Particle Composites, Dispersion-Strengthened Composites. Fiber-Reinforced Composites: Influence of Fiber Length, Influence of Fiber Orientation and Concentration, The Fiber Phase, The Matrix Phase, Polymer-Matrix Composites, Metal-Matrix Composites, Ceramic-Matrix

Composites, Carbon-Carbon Composites, Hybrid Composites, Structural Composites: Laminar Composites, Sandwich Panels.

5. **Nanomaterials:** Bulk Behavior of Nanomaterials, Methods for the Synthesis of Nanomaterials, Chemical Application of Nanomaterials, Kinetics of Chemical Reactions in Nanosystems.
6. **Advanced Materials:** Fullerenes and Carbon Nanotube, Optical Fibers in Communications, Polymer Electrolytes.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Describe processing, structure, property and performance of material.
- (ii) Explain the basic properties and characteristics of metals, polymers and ceramics, etc.
- (iii) Realize basic concepts of phase equilibria of materials and understand the changes in microstructures involved during phase changes and transformation.
- (iv) Demonstrate the basic aspects of nanomaterials and advanced materials and their applications, such as electronic materials, optical materials, and magnetic materials.
- (v) Design new materials including composite materials and select the proper materials for application in multidisciplinary areas.

Recommended Books

1. William D. Callister, D. G. Rethwisch, Materials Science and Engineering: An Introduction, 9th Edition, Wiley, 2002.
2. J.F. Shackelford, Introduction to Materials Science for Engineers, 6th Edition, Prentice Hall, 2004.
3. Donald R. Askeland, Pradeep Phulé, The Science and Engineering of Materials, 4th Edition, PWS Publishing Company, 2002.
4. Smith, William F., Foundations of Materials Science and Engineering, 3rd Edition, McGraw-Hill, New York, 2004.
5. Guozhong Cao, Nanostructures and Nanomaterials: Synthesis, Properties & Applications, Imperial College Press, 2004.
6. Christof M. Niemeyer, Chad A. Mirkin (Editors) Nanobiotechnology : Concepts, Applications and Perspectives, John Wiley & Sons, 2004.
7. Andreas Hirsch, Michael Brettreich, Fred Wudl, Fullerenes: Chemistry and Reactions, John Wiley & Sons, 2005.
8. Recent publications from Journals on relevant topics

PC 608 H Structures of Liquids and Solutions

Learning Objectives

The learning objectives of this course are to

- (i) Understand recent concepts and acceptable models of structure of liquid state.
- (ii) Understanding of possible intermolecular forces among the molecules of liquids.
- (iii) Illustrate the important physical properties of liquids, such as: viscosity, surface thermodynamic properties, dielectric constant, etc. and their measurement techniques.
- (iv) Discuss the physicochemical properties of liquid crystals and ionic liquids.

Course Content

- 1. Theories and concepts of liquid state:** Cluster theory, Cybotatic state theory, X-rays and the solid like state theory of liquids, cell concepts. Distribution of molecules in liquids, Monte Carlo method of molecular distribution.
- 2. Intermolecular forces in liquids:** Nature of intermolecular forces in liquid, Different types of forces, Molecular attraction-repulsion, forces between molecules, dipole-dipole forces, dipole induced dipole forces, London dispersion forces, hydrogen bonding, the repulsive energy, the total potential energy of a pair of molecules.
- 3. Viscous flow of liquids:** flow as a rate process, viscosity and holes in liquids, free energy of activation for viscous flow and energy of vaporisation, calculation of viscosity using statistical mechanics, viscosity of mixtures.
- 4. Nature and thermodynamics of liquid surfaces:** Surface thermodynamic quantities and the temperature dependence of surface free energy, the total surface energy, change of vapor pressure for a curved surface, effect of curvature pressure and other variables on surface tension.
- 5. Liquid crystals:** Structures and properties; methods of characterization; materials applications.
- 6. Experimental techniques for investigations of the structures of liquids:** Measurements of viscosity, surface tension, density, refractive index, dipole moment, dielectric properties.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Illustrate different modern theories and models of liquid.
- (ii) Demonstrate on different possible intermolecular forces among the molecules of liquids.
- (iii) Explain important properties of liquids, such as; viscosity, surface thermodynamic properties, dielectric constant, etc. and their theoretical basis of measurements.
- (iv) Synthesize and use liquid crystals and ionic liquids for different purposes based on their physicochemical properties.

Books Recommended

1. J. D. Hirschfeder, C. F. Curties and R. B. Bird. Molecular theory of gases and liquids, Chapman 7 Hall, London
2. J. S. Rowshion and E. L. Swinton, Liquids and liquid mixture, Butterworth, London.
3. H. X. Green Molecular theory of Fluids, North-Holian Amsterdam
4. J. A. Pryde, The liquid state Hutehinson & Co Ltd. London.
5. A. Bondi, Physical properties of molecular crystals liquids and glasses, John Wiley 7 sons and N. Y.
6. I. Prigogine, The Molecular theory of Solution, Interscience, N. Y.
7. The Structure and Properties of Solution, Dissscusion of Faraday Society, No. **43**, 1967, Chemical Society, London.
8. K. J. Laidler, S. Glasstone and H. Eyring, The Theory of Rate Process, Mc Graw-Hill Book Company Inc. N. Y.
9. J. T. Dayics and E.K. Rideal, Interfacial Phenomenon, Academic Press, N.Y.
10. A.W. Adamson, Physical Properties of Surface, Interscience Publishers, N.Y.
11. Recent papers publish in different journals on the above topics.

PC 609 H Electrochemical Techniques

Learning Objectives

The learning objectives of this course are to

- (i) Know the reversible and irreversible electrode reactions, mass transport and diffusion control processes at the electrode surface under static and dynamic conditions.
- (ii) Provide knowledge on Potentiostat / Galvanostat, types of cells and electrodes, buffers and electrolytes used in modern electro analysis.
- (iii) Give idea about different voltammetric techniques like normal pulse, differential pulse and square wave voltammetry, anodic and cathodic stripping voltammetry, mass transport analysis at the electrode surface.
- (iv) Impart knowledge on the development of potentiometric sensors and biosensors for specific chemical and biochemical analysis.

Course Content

1. **Background:** Fundamental Concepts of Electroanalytical Chemistry. Electrode reactions, diagnosis of reversible and irreversible electron transfer reactions. Mass transport and diffusion control processes at the electrode surface: static and dynamic conditions.
2. **Instrumentation:** Potentiostat/Galvanostat, Operational amplifiers and FET for i-v signal processing, High speed data acquisition system
3. **Electrochemical Cells and Electrodes :** (a) Types of cells: Three –electrode cells of different designs, Membrane cells, Flow-through cells for on - line analysis, Micro cells, (b) Electrodes of new generation : SDME, Hg and Au film electrodes on glassy carbon and platinum, graphite electrodes, Micro and Nano- fiber electrodes of carbon, gold and

platinum (construction, theory and applications), Buffers and electrolytes in modern electroanalysis.

- 4. Voltammetric Methods with Pulse Techniques:** Fundamentals of (a) Controlled Potential Techniques, (b) Controlled Current Techniques. Principle of electrochemical pulsing : normal pulse, differential pulse, square waves. Potential Sweep Pulse Voltammetric Methods of Electroanalysis.
- 5. Stripping Voltammetric Analysis with Pulse Techniques:** Stripping voltammetric analysis at trace and ultratrace levels using DPASV, DPCSV, AdSV and PSA.
- 6. Mass Transport Analysis at the Electrode Surface:** Amperometry, Chronoamperometry, Chronocoulometry, Chronopotentiometry, Chronoabsorbimetry (Methodology, Principle and Applications).
- 7. Ion-specific Analysis:** Potentiometric Sensors and Bio-Sensors. Potentiometric sensors for ions: (a) Transducers, (b) Principle of: (i) Crystalline and non-crystalline membrane sensors, (ii) Metallic sensors for cations, construction of electrodes, selection of electrolytes, solvents, analytical function and limitations.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Explain the the reversible and irreversible electrode reactions, mass transport and diffusion control processes at the electrode surface under static and dynamic conditions.
- (ii) Gain knowledge on Potentiostat / Galvanostat, types of cells and electrodes, buffers and electrolytes used in modern electroanalysis.
- (iii) Understand about different voltammetric techniques like normal pulse, differential pulse and square wave voltammetry, anodic and cathodic stripping voltammetry, mass transport analysis at the electrode surface.
- (iv) Develop potentiometric sensors and biosensors for specific chemical and biochemical analysis.

Books Recommended

1. Electrochemical Methods: Fundamentals and Application, 2nd Edition, allen J. Bard and Larry R. Faulkner.
2. Electroanalysis, Christopher M. A. Brett.
3. Analytical Electrochemistry, Second Edition, Joseph Wang, John Wiley & Sons, IWC, Publication.
4. Laboratory Techniques in Electroanalytical Chemistry, 2nd Edition, Peter T. Kissinger and William R. Heineman, Marcel Dekker, 1996.
5. Analytical Chemistry, Gary D. Christian.
6. Principle of Instrumental Analysis, 5th Edition, Douglas A. Skoog, Fjames Holler and Timothy A. Nieman.
7. Modern Analytical Chemistry, David Harvey, McGraw-Hill Higher Education.

PC 610 H Advanced Biophysical Chemistry

Learning Objectives

The learning objectives of this course are to

- (i) Deal with enzyme kinetics, enzyme inhibition, allosteric interactions in biological system.
- (ii) Compare thermodynamics and standard states of physical science with those of biological system, and understand bioenergetics involving ATP.
- (iii) Describe biological membrane, models for studying membrane, diffusion through membrane, Donnan effect.
- (iv) Understand the structure of protein (macromolecules), ligand-macromolecule binding equilibrium, solubility of proteins, dissociation of amino acids.

Course Content

1. **Enzyme Kinetics:** Basic equations, Enzyme-Substrate interactions, Multisubstrate systems, Enzyme inhibition, Allosteric interactions, Effect of pH on enzyme kinetics.
2. **Bioenergetics:** Introduction, Bioenergetic systems, Mechanism of collection and utilization of energy, Coupling mechanism, Substrate level phosphorylation, phosphorylation, Oxidative chain phosphorylation, Self regulation of energy production, Biochemist's standard state, ATP-the carrier of energy, Some limitations of thermodynamics.
3. **Biological Membrane:** Structure and function of biological membranes, Diffusion-Simple diffusion, Facilitated diffusion, Active transport, Donnan effect, Donnan equilibria involving protein bearing multiple charges, Membrane equilibrium.
4. **Biological Macromolecules:** Structure and stability of proteins, Protein binding, Binding equilibria, Equilibrium dialysis, dynamic dialysis, hydrophobic interaction, Denaturation of proteins, Protein binding and pharmacodynamics, Complexation and drug action, Metal complexation in biological systems, Thermodynamic treatment of stability constants, Solubility of proteins: salting-in and salting-out effects.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the enzyme kinetics, allosteric interaction of enzymes, enzyme inhibition and the factors affecting this kinetics.
- (ii) Compare thermodynamics with bioenergetics and understand the ATP as energy carrier and some limitations of thermodynamics.
- (iii) Understand the structure and function of biological membrane, models for studying membrane, diffusion through membrane, Donnan effect the and the associated models developed for this interaction.
- (iv) Explain the structure of protein (macromolecules), ligand-macromolecule binding equilibrium, solubility of proteins, dissociation of amino acids.

Books Recommended

1. Physical Pharmacy: Physical Chemical Principle in Pharmaceutical Sciences, A. Martin and J. Swarbrick. LEA & FEBIGER Publication, Philadelphia.
2. Physical Chemistry with Applications to Biological Systems. Raymond Chang. MacMillan Publication Co. Inc.
3. Biochemistry, Richard A. Harvey and Pamela C. Champe, 4th edition, Lippincott William& Wilkins, New York.
4. Biochemistry, Abraham Ctarow and Bernard Schepartz., W. B. Sanders Co.
5. Artificial Cells - Cell Engineering and Therapy, S. Prakash.
6. Biophysical Chemistry Part III: The Behaviour of Biological Macromolecules, C. R. Cantor and P. R. Schimmel.
7. Harper's Biochemistry, R. K. Murphy, D. K. Granner, P. A. Mayes and V. W. Rodwell.
8. Analytical Electrochemistry, J. Wang.
9. Biochemistry, A. Catarow and B. Schepartz.
10. Recent Publications in the Journals.