M.Sc. Part II Physical Chemistry

Structure Of The Syllabus

Semester III

CH-310  Quantum Chemistry and Solid state chemistry
CH-311  Nuclear and Radiation Chemistry
CH-312  Advanced Instrumental Methods of analysis
CH-313  Physical chemistry Practical –I

Optional Courses (any one of the following)

CH-314  Polymer Chemistry
CH-315  Special topics in Physical Chemistry

Semester IV

CH-410  Molecular Structure and Spectroscopy
CH-411  Surface and Electrochemistry
CH-412  Physical Chemistry Practical II
CH-413  Physical Chemistry Practical III/Project

Optional Courses (any one of the following)

CH-414 Biophysical Chemistry and Related Techniques
CH-415  Special topics in Nuclear Radiation Chemistry
CH-310 Quantum Chemistry and Solid State Chemistry

Quantum Chemistry

1. Postulates of quantum mechanics, properties of quantum mechanical operators, Eigen functions and Eigen values, Hermitian, linear, ladder, and angular momentum operators. term symbols and selection rules, spin –orbit coupling, regular and inverted multiples (9L)

2. The variation method, theorem and applications, non-degenerate perturbation method (9L)

3. Application of LCAO-MO theory on the basis of Hückel approximation to conjugated aliphatic molecules and monocyclic conjugated polyenes. Hückel (4n+2) rule, calculation of resonance stabilization energy from Schaad and Hess model, antiaromatic molecules. (12L)

Text Books
2. Quantum Chemistry- A.K. Chandra

Solid State Chemistry

1. Properties of metals and semiconductors: band theory, types of solids, intrinsic and extrinsic semiconductors, p-n junctions, optical properties, photoconductivity of crystals (7L)

2. Imperfections and related phenomenon: Defects in solids: point defects line defects, diffusion in solids- mechanism, elastic and plastic deformations (5L)

3. Crystal growth techniques: General principles, growth from solution, growth from melts, growth from vapour (4L)

4. Imperfections and physical properties crystals: Electrical properties, Optical properties: Colour centers in ionic crystals: types, creation, Magnetic properties, Thermal properties and Mechanical properties. (8L)

5. Solid state reactions: reactions of single solids and their kinetic characteristics, gas -solid, solid -solid, addition and double decomposition reactions, photographic process (6L)
Text Books:

1) Introduction of Solids L.V Azaroff , Tata McGraw Hill

2) Principles of the solid state H. V. Keer, Wiley Eastern (1993)


CH-311 Nuclear and Radiation Chemistry

1. Nuclear fission : The discovery, conformation of nuclear fission, types of fission reaction, mass distribution of fission product, emission of neutron in fission, fissile and fissionable nuclides, theory of nuclear fission, critical energy for fission, products of nuclear fission (6L)

2. Nuclear reactors : General aspects of reactor design, thermal, fast and intermediate reactors, reactor fuel materials, reactor moderators and reflects, coolants, control materials, shield, regeneration and breeding of fissile matter, types of research reactors. (6L)

3. Nuclear structure : The liquid drop model, calculation of nuclear binding energies, properties of isobars, missing elements, the nuclear shell model, magic numbers, filling of nucleon shells, the collective and unified models. (7L)

4. Ion beam analysis techniques : Particle induced X-ray emissions- projectile accelerator and target preparation, ionization and X-ray emission detection, analysis and applications. Rutherford back scattering – scattering reaction, surface analysis, depth profiling, channelling effects and applications (5L)


6. Accelerators: Basic components, Cockcroft-Walton accelerator, Van de Graaff accelerator, Linear accelerators, cyclotrons, synchrotrons, (4L)
5. Radiation detectors: Scintillators and their properties inorganic and organic, solid state semiconductor detectors-theory, surface barrier, Li drifted and intrinsic detectors (5)
6. Radiolysis of aqueous solutions: Radiolysis of water, ferric sulphate, ceric sulphate, cupric sulphate solutions (5)
7. Radiation hazards and safety: Natural and manmade sources of radiations, internal and external radiation hazards, safe handling methods, personal dosimetry, reactor safety, the effects of Three miles and Chernobyl accidents, radiation protecting materials. (6)
8. Biological effects of radiations: The interaction of radiations with biological cells, various stages, somatic and genetic effects, maximum permissible dose-ICRP recommendations (5)
9. Hot atom chemistry: Szilard Chalmers process, chemistry of recoil atoms, recoil techniques, models for retention, annealing reactions, annealing mechanisms (5)

Text Books:

4. Introduction to Nuclear Physics and Chemistry, B.G. Harvey, Prentice hall (1963)

CH-312 Advanced instrumental methods of analysis

1. X-ray methods
   Generation and properties of X-rays, X-ray absorption, Concept of absorptive edge, applications, X-ray absorptive apparatus, radiography and radiotherapy, applications X-ray fluorescence, fundamental principles, instrumentation, wavelength dispersive and energy dispersive, qualitative and quantitative analysis, X-ray emission, fundamental principles, electron microprobe, further advanced techniques, Introduction to STEM, SEM (7L)
2. Luminescence, chemiluminescence, electrochemiluminescence, apparatus, fluorescence, phosphorescence, theory, factors affecting intensity, apparatus, analytical applications.

(8L)

3. Mass spectrometry: Theory, instrumentation-basic components, ionization sources, analyzers, resolution, chemical analysis, advanced techniques—GC/MS, MS/MS introduction

(6L)

4. Neutron Activation Analysis: Principle, target, matrix, cross-section, fluxes, saturation activity, excitation function, Different steps involved in NAA, radiochemical and instrumental NAA, prompt radiation and pulse neutron activation analysis, applications

(10L)

5. Inductively coupled plasma atomic emission spectroscopy: principle, instrumentation, analysis and applications

(6L)

6. Thermal methods of analysis: TGA, DTA, DSC and thermometric titrations—principle, instrumentation, factors affecting TGA curve, applications

(6L)


(5)

8. Coulometry: Current-voltage relationship, coulometric methods, controlled potential coulometry

(5)

9. Voltammetry: Excitation signals, instrumentation, hydrodynamic voltametry, cyclic voltametry, pulse voltametry, applications

(7)

Text Books:


CH-313 - Physical Chemistry Practicals I (Compulsory Course)
1) Thermodynamic data of electrochemical cell by e.m.f. measurements.

2) Simultaneous determination of two ions by polarography.

3) Determination of the equilibrium constant of triiodide ion formation

4) Magnetic susceptibility measurement by Gouy technique.

5) Determination of dipole moment of liquid at various temperatures.

6) Kinetics of iodination of aniline: pH effect and base catalysis.

7) Dissociation constant of an acid-base indicator by spectrophotometry.

8) Actinometry – photolysis of uranyl oxalate

9) Absorption coefficient and half thickness of lead for gamma radiation.

10) Radiation dose measurement by Fricke dosimeter/ceric sulphate dosimeter.

11) Flame Photometric determination of Na, K, Li and Ca (Working curve method)

12) A photometric titration of a mixture of Bi and Cu with EDTA (-745nm)

13) Determination of lead in petrol by atomic absorption technique.

14) To investigate the reaction between potassium persulphate and potassium iodide by colorimetry.

15) To determine the chain linkage in poly (vinyl alcohol) from viscosity measurements.

16) Calibration of Gamma ray spectrometer and determination of energy of given radioisotope

CH-314 Polymer Chemistry
1. Basic concepts of polymer science, classification of polymers as biological - nonbiological, linear branched network, condensation, addition homo- and hetero-chain, thermoplastic - thermosetting, History of Macromolecular Science, molecular forces and chemical bonding in polymers. 

(5L)


(5L)

3. Copolymerization - Kinetics of copolymerization, the copolymer equation, monomer reactivity ratios, instantaneous composition of polymer. 

(6L)

4. Morphology and rheology of polymers - configuration of polymer chains crystal structure, crystallization processes, viscous flow, rubber elasticity, viscoelasticity, the glassy state and glass transition, mechanical properties of crystalline polymers. 

(8L)

5. Polymer structure and physical properties - The crystalline melting point $T_m$ - the glass transition temperature ($T_g$) - properties involving small and large deformations- polymer requirements and polymer utilization. 

(6L)

6. Analytical chemistry of polymers - physical and chemical analysis: IR, NMR and EPR spectroscopy, XRD analysis, thermal analysis - TGA, DTA, microscopy, physical testing. 

(8L)


(8L)

8. Polymer processing - Plastic technology - molding, other processing techniques fibre technology - textile and fabric properties, spinning fibre after treatments, elastomer technology- natural rubber, vulcanization, reinforcement, carbon blocks. 

(5L)
9. Radiation induced polymerization - kinetics and mechanism of polymerization in the liquid and solid phases, effect of irradiation on polymers - degradation and cross-linking, block copolymerization. 

10. Conducting polymers - Basics, synthesis, conduction mechanism, applications. 

Text Books:

4) Polymer Chemistry - An introduction, Seymour-Carraher, Marcel Dekker Inc, New York

CH-315 Special Topics in Physical Chemistry

1. Chemical sensors
Different types of sensors, semi conducting oxide sensors, electrochemical sensors, biosensors e.g. glucose, testing of sensors, Lab-on-a-chip. (8L)

Reference.

2. Ionic equilibria and pH calculations
Solution of an equilibrium problem, general approach to problem solving, mass balance, the proton condition, charge balance; solving simultaneous equations, Weak acid problem: exact solution, approximations on the equations, Weak acid problem: approximate solution, Graphical representations – the distribution diagram, the logarithmic concentration diagram. Construction of a logarithmic concentration diagram, calculations using a logarithmic diagram, pH of a weak base, pH of salts of a weak acid strong base and strong acid weak base, Polyprotic acids – stepwise dissociation, distribution diagram, logarithmic concentration diagram, pH calculations. 

Reference.

3. Nanoscience: Materials and Technology

Low dimensional structures – quantum wires and dots, excitons, nanotube, porous silicon and other special nanomaterials. (4 L)
Properties of nanoparticles: Mechanical, thermal, optical, magnetic and electrical. (4 L)
Applications: LED, SET, GMR, display panels, sensors, medicine (4 L)


1. Quantum Dots - L.Jacak, P. Hawrylak. A. Waojsspringer (1977)
4. Semiconductor quantum dots – L.Bajaj and S.W. Kotch

4. Smart Materials

Definition of smart materials (SM), Design of intelligent materials, actively smart and passively smart materials and their characteristics.
e.g. - smart ceramics, oxides, smart polymers and gels, shape memory alloys, electrorheological fluids, ferrofluides, smart windows, smart sensors, smart electroceramics. Magnetostrictive materials, biomineralisation and biosensing. Integration to smart clothes, smart rooms. (8L)
References:
2. Intelligent materials – Craig A. Rogers, Scientific American, 1995, p.122
3. Smart structures and materials by B. Culshaw (Artech House, Norwood, MA 1998)
5. MRS Bulletin, April 1993, P 27
6. Intelligent Gels Y. Osada and S. B. Ross – Murphy- Scientific American May 1993 p.82

5. Phase Studies : 10 L

Temperature – Composition diagrams, lever rule, phase rule, counting components, experimental procedures, liquid – liquid, liquid-solid diagrams, eutectics, technologically important eutectics, ultra-purity, controlled purity, role of added salt, supercritical liquids and applications.

Ref. :1. Thermodynamics, statististical thermodynamics and kinetics
Thomas Engel, Philip Reid 1st Edn.
2. Physical chemistry- Ira Levin 1st Edn

6. Catalysis
Introduction with definitions of various terms involved in catalysis.
Acid-base catalysis in dilute aqueous solutions, general and specific acid-base catalysis.
Organometallic catalysis, reactions of transition metal complexes. Catalysis by enzymes,
Michachis-Menten kinetics, enzyme activities. (10L)

Reference
1. Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance saturation. Shielding of magnetic nuclei, chemical shift and its measurements. Factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant “J” Classification (ABX, AMX, ABC, A2 B2) spin decoupling, basic ideas about.

Instrument, NMR studies of nuclei other than proton $^{13}$C, $^{19}$F and $^{31}$P, FT NMR, advantages of FT NMR, use of NMR in medical diagnostics. (10L)

2. Electron Spin Resonance Spectroscopy

Basic principles, Zero field splitting and Kramers degeneracy, factors affecting the “g” value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications. (10L)

3. Nuclear quadrupole resonance spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, and applications. (3L)

4. Photoacoustic Spectroscopy

Basic principles of photoacoustic spectroscopy (PAS), PAS gases and condensed system, chemical and surface, applications. (3L)

5. X-Ray diffraction

Index reflections, Identifications of unit cell from systematic absences in diffraction pattern. Structure of simple lattices and X-Ray intensities Structure factor and its relation to intensity and electron density, phase problems in XRD (10L)

6. Electron Diffraction

Scattering intensity Vs Scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules, low energy electron diffraction and structure of surfaces. (10L)

7. Neutron Diffraction analysis
8. Magnetic susceptibility

Pascal constant, Diamagnetic susceptibility, paramagnetic susceptibility, Langevin Equation, Van Vlecks formula, Ferro, Ferri and Antiferromagnetism,

Measurement of Magnetic susceptibility by Faraday and Gouy Techniques. (10L)

References
1. Modern Spectroscopy J.M. Hollas, (John Wiley)
2. Spectroscopy (Atomic and Molecular) Gurdeep Chatwal, Sham Anand (Himalaya Publishing house)
4. Introduction to Magnetic resonance A. Carrington and A.D Maclachalan, Harper & Row
5. Spectroscopy B.K. Sharma
6. NMR, NQR, & Mossbauer spectroscopy in Inorganic chemistry R.V. Parish, Ellis Harr wood
7. Physical methods in Chemistry R.S Drago, Saunders college
11. Introduction to Magento chemistry Alen Earnshaw, Acad Press (1968)
12. Magneto chemistry Sanyal and Dutta

CH - 411 – Surface and Electrochemistry

Surface Chemistry

1. Adsorption at liquid surfaces, Gibbs equation and its verification, Gibbs Monolayers, insoluble films on liquid substrates, states of monomolecular Films, Wetting, flotation, detergency. (6 L)
   Ref. 1,6
2. Adsorption forces, thermodynamics of physical adsorption, heat of adsorption and its determination, measurement of adsorption by different methods, chemisorption and its mechanism. (6 L)
Ref. 1,2,5,6

Ref. 1, 6

4. Porous solids – Definition, pore size distribution, methods to determine pore size, hysteresis of adsorption, theories of hysteresis, Adsorption behaviors of porous materials, (4 L)
Ref. 3,4,6

5. Catalysis - Introduction and basic concepts – Industrial heterogeneous catalysis. Definitions – catalyst, catalyst activity, catalyst selectivity, negative catalyst, heterohomogeneous catalysis, sites, turnover number, functionality, naming of catalyst and catalyst structures, catalyst deactivation. Zeolites – their structure and application as molecular sieves, catalyst and carriers of radioactive wastes (8 L)
Ref. 7,4,5

References:
Electrochemistry


(10L)
Ref. 1, 2

2. Electrodics – Standard electrode potentials, different chemical and physical processes at the electrode surfaces, electrode-electrolyte interface, double layer and phase boundaries, Butler-Volmer equation, Tafel equation.

(10L)
Ref 1, 2

3. Applications -
   a. Fuel cells and batteries – primary and secondary power cells, fuel cells, Li ion battery, evaluation of performance of electrochemical systems, energy density, shelf life, and Faradic efficiency.
   b. Corrosion and corrosion prevention- Thermodynamics and kinetics of corrosion, methods of prevention to corrosion.
   c. Electrosynthesis – use of electrodes in synthesis of organic compounds

(10L)
References
1. Physical chemistry - Peter Atkins, Julio de Paula , 7th Edition
Oxford University Press.
5. Electrochemical techniques in corrosion science and engineering
6. Lectures on electrochemical corrosion  M.Pourbaix, Plenum NY (1973)

d.
CH-412 Physical Chemistry Practical II (Compulsory)

1. Hydrolysis constant of aniline hydrochloride by distribution coefficient method.
2. Determination of the dimerization constant of an organic acid in benzene.
3. Differential potentiometric titration.
4. Amperometric titration with platinum microelectrode.
5. Determination of the stability constant of a complex by spectrophotometry.
6. Determination of the heat of ionization of phenol/weak acid.
7. Studies on a clock reaction: determination of the energy of activation
   a. Reactions such as bromate-bromide reaction, iodate-iodide reaction,
   b. Formaldehyde-bisulphite reaction etc.
8. Magnetic susceptibility measurements by the Faraday technique.
9. Analysis of fruit juice for vitamin C by HPLC technique.
10. Determination of half-life of two isotopes in a mixture.
11. Study of characteristics of GM counter.
12. Effect of salt on the distribution of acetic acid between water ethyl acetate.
13. To study the effect of addition of a salt on the solubility of an acid in water.
14. Determination of concentration of sulfuric acid, acetic acid and copper sulphate
    by conductometric titration with sodium hydroxide.
15. Determine the formula and stability constant of a metal ion complex (Lead Oxalate) by polarography.
16. Analysis of tertiary mixture by gas chromatography.

CH-413 - Project or Additional Practicals (Compulsory)

1. Solubility of a sparingly soluble salt by conductometry.
2. Coulometric estimation of arsenite by bromine.
3. Dead stop end point titration.
4. Activity coefficient of electrolyte by emf measurements.
5. Titration of polybasic acid with sodium hydroxide by pH-metry.
6. Formation constant of a complex by pH-metry
7. Kinetics of the reaction between 2,4-dinitrochlorobenzene and piperidine.
8. Dipole moment of a liquid at various temperatures.
9. Latent heat of fusion by solubility measurement at various temperatures.
10. Determination of solubility diagram for a three component liquid system.
11. Radiolysis of aqueous iodate solution and determination of G values.
12. Molecular weight of a polymer by end group estimation.
13. Determination of the formula of complexes such as silver–ammonia complex by titration, cuprammonium ion complex by distribution coefficient measurement. Determine the transport number of silver and nitrate ions in aqueous solution from the cell potential of the concentration cell with junction potential.

15. Recording of TGA curve of CuSO₄ and NaCl and hence to find the percentage composition of the mixture.

**Reference.**

1. Findlay’s Practical Chemistry, S.P. Levitt (Editor), Longman Group Ltd.
7. Practical Physical Chemistry, D.V. Jahagirdar

**CH-414 Biophysical Techniques**

1. Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living system. (6)
2. Statistical mechanics of biopolymers, chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimensions for various chain structures. (8)
4. Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical systems.
5. Structure and functions of cell membrane, ion transport through cell membrane. Irreversible thermodynamic treatment of membrane transport Nerve conduction
6. Enzyme kinetics and enzyme inhibitory reactions and their implications, Oscillatory reactions. (6)
9. Membrane equilibria: membrane systems, miscelles, bilayers structure and function. (3)

References:

CH-415 Special topics in Nuclear Radiation Chemistry

1. Applications of radioisotopes in nuclear medicine and pharmaceuticals: general applications of radiopharmaceuticals, use of nuclear properties of indicator nuclides. In vivo diagnostic procedures, in vitro diagnostic testing therapeutic use of radiations. Use of radiation for food preservation and sterilization. (10L)

2. The origin of chemical elements, cosmology, premordial nucleosynthesis, stellar evolution and stellar nucleosynthesis, solar neutrino problem, Synthesis of Be, B, Li in cosmos. (8L)

3. Management of radioactive waste: liquids, solids and gases (6L)

4. Separation of isotopes: General methods of isotope separation, separation of isotopes with special reference to heavy hydrogen, Lithium, Boron, Uranium. (7L)

5. Radiolysis of organic systems: Alkanes, aromatic hydrocarbons, alcohols (7L)

6. Techniques in nuclear chemistry: Targets for nuclear reaction, studies measurement of beam energies and intensities, target chemistry, preparation of samples for activity measurement, carriers. (7L)

7. Radiolysis kinetics: Empirical rate studies, molecular kinetics, non-homogeneous kinetics, effect of solute concentrations on the molecular yields from water, radical scavenging, chain reactions, pulse radiolysis (7L)

8. Radiometric titrations: Principle techniques and titrations based on precipitate formation, complex formation and neutralization reactions (8L)

Text Books:


