SOLAPUR UNIVERSITY, SOLAPUR
M. Sc.- PHYSICAL CHEMISTRY COURSE SYLLABUS
SEMESTER SYSTEM

A two-year duration **M. Sc.- Physical Chemistry** course syllabus has been prepared as per the semester system. Syllabus for M. Sc. Part I was implemented with effect from June 2011. M. Sc. II syllabus will be implemented from June 2012. The syllabus has been prepared taking into consideration the syllabi of other Universities, SET, NET, UGC guidelines, and the specific inputs of the Expert Committee Members from Shivaji University Kolhapur.

General Structure of the Course:

The course will be of four semesters spread over two academic years. Each semester will have four theory papers of 70 marks for university external examination and 30 marks for internal examination of each semester and two practicals of 70 marks, 30 marks for internal practicals of each semester. The distribution of marks is mentioned below

Theory Paper (Semester exam), 16 X 70+30 marks	1600 marks
Practicals (semester end exam.), 8 X 70+30 marks	800 marks
Seminars for each semester, 4 X 25	100 marks
	Total: 2500 marks

Ratio of marks (Theory: Practical): (73:27)

M. Sc. Part I* Chemistry
(* This course is common for Polymer, Organic and Physical Chemistry courses).

Semester I

Theory Courses:

Paper No.	**Title of Papers**	
CH 101 (I)	Inorganic Chemistry-I	70+30 = (100 marks)
CH 102 (II)	Organic Chemistry-I	70+30 = (100 marks)
CH 103 (III)	Physical Chemistry-I	70+30 = (100 marks)
CH 104 (IV)	Analytical Chemistry-I	70+30 = (100 marks)

Semester II

Paper No.	Title of Papers	
CH 201 (V)	**Inorganic Chemistry-II**	**70+30 = (100 marks)**
CH 202 (VI)	Organic Chemistry-II	70+30 = (100 marks)
CH 203 (VII)	Physical Chemistry-II	70+30 = (100 marks)
CH 204 (VIII)	Analytical Chemistry-II	70+30 = (100 marks)

Practical Course: (Semester end examination) Practicals P - I to IV for semester I and II

Practical Examination will be of 4 days for each semester

P I Chemistry Practicals: Sem-I(70 marks Univ. Exam + 30 Marks Internal Exam)
P II Chemistry Practicals: Sem-I(70 marks Univ. Exam + 30 Marks Internal Exam)
P III Chemistry Practicals: Sem-II (70 marks Univ. Exam + 30 Marks Internal Exam)
P IV Chemistry Practicals: Sem-II (70 marks Univ. Exam + 30 Marks Internal Exam)

M. Sc. Part -II Physical Chemistry: Semester III

Theory Courses:

Paper No.	**Title of Papers**	**Marks**
PCH-301 (IX)	Quantum Chemistry	(70 + 30) =100 marks
PCH-302 (X)	Electrochemistry	(70 + 30) =100 marks
PCH-303: (XI)	Molecular Structure-I	(70 + 30) =100 marks
	(Elective Papers)	
PCH-304 (XII)	(A): Solid State and Nuclear Chemistry	(70 + 30) =100 marks
PCH-304 (XII)	(B): Advanced Chemical Kinetics	(70 + 30) =100 marks
PCH-304 (XII)	(C): Radiation and Photochemistry	(70 + 30) =100 marks

Semester IV

Paper No.	**Title of Papers**	**Marks**
	(Core Papers)	
PCH-401 (XIII):	Statistical Mechanics and Thermodynamics	(70 + 30) =100 marks
PCH-402 (XIV):	Chemical Kinetics	(70 + 30) =100 marks
PCH-403 (XV):	Molecular Structure II	(70 + 30) =100 marks
	(Elective Papers)	
PCH-404 (XVI)	(A): Surface Chemistry	(70 + 30) =100 marks
PCH-404 (XVI)	(B): Chemistry of Materials	(70 + 30) =100 marks
PCH-404 (XVI)	(C): Biophysical Chemistry	(70 + 30) =100 marks

Practical Course: (Semester end examination) Practicals V to VIII

Semester III

P V	Practical experiments + Internal	(70 + 30) =100 marks
P VI	Practical experiments + Internal	(70 + 30) =100 marks

Semester IV

P VII	Practical experiments + Internal	(70 + 30) =100 marks

P VIII Project work/In-plant / Practical experiments 70 marks + Internal 30 marks = 100 marks

Nature of Examination:

Each semester will have theory external examination of four papers of 70 marks each (3 hrs. duration). The practical examination of Semesters I to IV will be conducted at the end of the each Semester. Duly certified copy of laboratory record must be produced at the time of examination.

Practical Examination of M. Sc. II

The practical examination will be of 3 days for each semester. There will be 70 marks external practical examination while 30 marks internal examination. The distribution of marks for each Practical paper -V, VI, VII and VIII will be of 70 marks. Project work / In-plant training / Review Report of 70 marks will be included in P-VIII Whereas distribution of marks for P VIII will be Project work / In-plant training / Review Report + Practical experiments = 70**

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** The valuation to be done by both external and Internal examiners at the time of P V-VII practical examination. Valuation of Seminars is to be done in Semester III by Departmental Faculty involved in Physical Chemistry.

Nature of question paper (for M. Sc. I and II):

Time: 03 hours Maxi Marks 70

Instructions

1. Attempt 05 questions.
2. Section I (question 1) is compulsory
3. Attempt any two questions from section II and any two questions from section III.
4. Answers to all 05 questions (from section I, II, III) should be written in the one and the same answer book.
5. All questions carry equal marks.
6. Figures to the right indicate full marks.
7. Use of log tables and calculators is allowed.

Question Paper
Section I

Q 1. Answer the following (14 sub-questions) Marks 14 (1 x 14)

Multiple choice / fill in the blanks / define the term / True-False, predict the product, provide the reagent and conditions etc.

Sub-questions (i) to (xiv)

Section II

Q 2. a) - --- -- - - - - - - - Marks 07
b) - - - - - - - - - - - - Marks 07

Q 3. a) - --- -- - - - - - - - Marks 07
b) - - - - - - - - - - - - Marks 07

Q 4. a) - --- -- - - - - - - - Marks 07
b) - - - - - - - - - - - - Marks 07

Section III

Q 5. a) - --- -- - - - - - - - Marks 05
b) - - - - - - - - - - - - Marks 05
c) - - - - - - - - - - - - Marks 04

Q 6. a) - --- -- - - - - - - - Marks 05
b) - - - - - - - - - - - - Marks 05
c) - - - - - - - - - - - - Marks 04

Q 7. Write short notes on (any three) Marks 14
a) - - - - - - - - - - - -
b) - - - - - - - - - - - -
c) - - - - - - - - - - - -
d) - - - - - - - - - - - -

N.B. In sections II and III, the sub-questions (a, b, and c) in a given question should be from different topics of the syllabus.

At least 25 % questions should be problem oriented, where-ever possible, in view to train students for the SET/NET/GATE and other competitive examinations. These questions should test the understanding of candidate rather than the memory. The question paper should cover all the Units included in the syllabus of the respective paper and the weightage of the questions should correspond to the number of lectures allotted to the respective Units / Topics.

M. Sc. Part II (Physical Chemistry)
SEMESTER-III
Paper No. PCH 301: Quantum Chemistry

Unit – I Formalism of Quantum Mechanics: (12)

Failure of classical physics. Postulates of Quantum Mechanics, Eigen function and Eigen values. Acceptability of wave functions, Normalized and orthogonal wave functions. Operators and operator algebra. Principles of superposition, Schmidt Orthogonalisation. Hermition operators. Theorems related to commutator operations, Stern-Gerlach experiment and spin of electron. Spin eigen function. Concept of angular momentum, angular momentum operators. Ladder operators.

Unit – II Quantum Mechanics of some simple systems: (15)

Practical in a box; One / two / Three dimensional Box. Degeneracy in multidimensional box. Tunneling effect, Rigid rotator, Linear harmonic oscillator, the formal solutions, energy levels, degeneracy, properties of wave functions and selection rules. **The hydrogen and hydrogen like atoms:** Schrodinger equation for hydrogen atom (in polar coordinates) and its complete solution. The radial distribution function and its significance, shapes of atomic orbitals. Application to hydrogen like atoms and molecules (e.g H_2^+, He^+, Li^{2+} etc)

Unit – III. Hückel molecular Orbital Theory (10)

Secular equation and secular determinants, Assumptions and formalism of Hückel molecular Orbital Theory, origin of aromatic stability and calculation of delocalization energy. Brief introduction to hetero-nuclear systems. Use of symmetry based linear combination to simplify the problem of Hückel theory calculations for larger aromatic molecules (like butadiene).

Unit – IV: Advanced quantum chemistry (11)

Schrödinger wave equation and Hamiltonian for Multi-electron systems. An introduction to *ab initio* and semi-empirical approximate methods: Variation principle, Perturbation theory, Self–consistent field (SCF) theory, Hertree-Fock (HF) method, Restricted and unrestricted HF methods, Basis sets, Slater and Gaussian type atomic orbitals (STO's and GTO's).

REFERENCE BOOKS

1) Introductory Quantum Chemistry by A. K. Chandra. Tata McGraw-Hill.1988.
2) Basic Physical Chemistry by W. J. Moore, Prentice Hall, 1986.
3) Physical Chemistry, by P. W. Atkins, ELBS, 1986.
4) Quantum Chemistry, W. Kauzmann, Academic press.
5) Quantum Chemistry by Hanns.
6) Theoretical Chemistry by S. Glasstone,Van Nostrand.
7) Physical Chemistry by Alberty.
8) Quantum Chemistry by Prasad.
9) Physical Chemistry: A molecular Approach – Donald A. McQuarrie and John D. Simon, Viva Books, New Delhi, 1998.
10) Quantum Chemistry – Donald A. McQuarrie, Viva Books, New Delhi, 2003.
11) Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists - S. Glasstone, D. Van Nostrand Company, Inc., 1944.

Paper No. PCH- 302: Electrochemistry.

Unit – I Electrolytic conductance: (16)

Debye – Huckel theory of inter – ionic attraction, ionic atmosphere, time of relaxation, relaxation and electro–phoretic effects, Debye-Huckel –Onsagar equation and its validity for dilute solutions and at appreciably concentrated solutions. Debye- Falkenhagen and Wein effects. Abnormal ionic conductance of hydroxyl and hydrogen ions – Grotthuss mechanism. Activity coefficients: forms of activity coefficients and their interrelationship. Debye-Huckel limiting law and its applications to concentrated solutions. Debye-Huckel Bronsted equations. Quantitative and qualitative verification of Debye-Huckel limiting law, ion association. Bjerrum theory, problems.

Unit - II Ion solvent interactions and electrolysis: (16)

The Born Model and expression for the free energy of ion solvent interactions. Thermodynamic parameters for the ion solvent interactions. Calculations of heats of hydration of ions and the concept of hydration number (Van Arkel, de Boer's and Bernal-Fowler method).

Electrolysis: Decomposition potentials: calculations and determinations. Polarization: types of polarization, overvoltage, hydrogen and oxygen overvoltage, applications of electrolysis in electrorefining, electroplating and electrotyping.

Unit – III : Electrode reactions. (16)

Tafel equations, kinetics of discharge of hydrogen ions. Diffusion overpotentials, theory of diffusion overpotential and its importance.

Fuel cells: significance of fuel cells: hydrogen – oxygen, phosphoric acid, molten carbonate, solid polymer electrolytes, hydrocarbon – air, natural gas and carbon monoxide- air fuel cells.

Corrosion: concept and importance, classification, mechanism and kinetics of corrosion, Pourbaix diagrams, methods of corrosion prevention.

Electrical double layer concept, Electrokinetic and electro-capillary phenomena, electro-capillary curve. Electro-osmosis, electrophoresis. Streaming and Sedimentation potentials, Zeta potentials and its determination by electrophoresis, Influence of ions on Zeta potential.

REFERENCE BOOKS:

1) An Introduction to Electrochemistry by S. Glasstone
2) Modern electrochemistry Vol I & II by J. O. M. Bockris and A. K. N. Reddy.
3) Physical chemistry by S. Glasstone
4) Electrolytic Solutions by R. A. Robinson and R. H. Stokes
5) Physical Chemistry by P. W. Atkins. ELBS.
6) Theoretical electrochemistry by L. I. Antropov, MIR Publishers.
7) Chemical and electrochemical energy systems by R. Narayan and B. Viswanathan, Universities press
8) Handbook of fuel cell technology by Maget HJR, prentice-Hall, New Jersey.

Paper No. PCH –303: Molecular Structure – I

Unit – I Symmetry properties of molecules and group theory: (11)

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 of vibrations. Application of group theory in understanding IR and Raman spectral transition, geometry and bonding in co-ordination complexes.

Unit-II: Introduction of spectroscopy and Rotational Spectra (10)

Characterization of electromagnetic radiation. The quantification 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. Selection rules. The intensities of spectral lines. The effect of isotopic substitution. Polyatomic molecules. The Stark effect. Calculations of B for real spectrum eg NO. Instrumentation, source, waveguide and detectors.

Unit- III Infrared spectroscopy and Raman Spectroscopy: (11)

Diatomic molecules : 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. Selection rules. Analysis of one real spectrum.

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. Selection rules. Mutual exclusion effect.

Unit – IV Electronic Spectroscopy : (10)

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 polyatonic molecules. Chemical analysis by electronic spectroscopy. (d-d), (p-p*) and (p-n*) transitions. Photochemical mechanism of vision.

Unit – V Photoelectron Spectroscopy (PES): (6)

Basics of photoelectron spectroscopy, Phtoelectron spectroscopy of atoms and diatomic molecules. PES of polyatomic molecules like NH_3, H_2O, etc. Core electron PES; X-ray photoelectron spectroscopy (ESCA) applications

REFERENCE BOOKS :

1) Fundamental of molecular spectroscopy by C. N. Banwell Tata McGrew Hill.
2) Physical Chemistry by P. W. Atkins, ELBS,1986
3) Symmetry, Orbitals and spectra by M. Orchin & H. Jaffe, Willey, interscience.
4) Chemical applications of group theory by F. A. Cotton Willey, interscience.
5) Symmetry in chemistry by H. Jaffe and M. Orchin, Jhon willey.
6) Group theory and its applications to chemistry by K. V. Ramen, Tata McGrew Hill.
7) Molecular Structure and Molecular Spectra by G. Herzberg, Van Nostrand.
8) Molecular Spectroscopy by I. N. Levine, Willey interscience.
9) Molecular Spectroscopy by G. M. Barrow.

Paper : PCH-304 (A): Solid State and nuclear Chemistry (elective)

Unit I: The solid state : (12)

Types of solids, crystal structure, crystal symmetry, symmetry element, crystal defects and non-stoichiometry, miller indices, lattice constants, Bravis lattice, and crystal structure determination by X-ray diffraction – single crystal rotation and powder diffraction method. Fourier synthesis, structure factor and electron density, analysis by X-ray diffraction of proteins.

Unit II : Solid State Reactions and preparation of materials: (14)

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

Purification and crystal growth, zone refining, growth from solution, growth from melt. Preparation of organic semiconductors for device applications, high surface area materials, zeolites and related structures

Unit III : Elements of radiation Chemistry : (10)

Interaction of radiation with matter, passage of neutrons through matter, interaction of γ radiation with matter, units for measuring radiation absorption, radiation energy and radiation dosimetry- fricke dosimeter, ceric sulphate dosimeter. Radiolysis of water, Radiolysis of some aqueous solutions (ferrous sulphate, cupric sulphate solution).

Unit IV: Nuclear Chemistry: (12)

Nuclear Reactors: Nuclear fission as a source of energy, the four factor formula. Classification of reactors, Reactor power, critical size of a thermal reactor, research, power and the breeder reactors, energy from nuclear fission reaction, India's nuclear energy programme.

Nuclear radiation detector: scintillation detectors, semi conductor detectors, neutron detectors and their applications. Resonance fluorescence, line width and Doppler broadening, nuclear resonance fluorescence due to recoilless emission of gamma radiation, chemical shift, quadrapole splitting, applications in the study of tin and iron.

REFFERENCE BOOKS :

1) Principals of solid state, H. V. Keer, Wiley Eastern.
2) Solid state chemistry, N. B. Hannay
3) Solid state chemistry, D. K. Chakrabarty, New Age International
4) An Introduction to Crystallography : F. G. Philips
5) Crystal Structure Analysis : M.J. Buerger
6) The Structure and properties of materials: Vol.III Electronic properties by John Wulff.
7) Electronic processes in materials: L. U. Azroff and J. J. Brophy
8) Chemistry of imperfect crystal : F. A. Krogen
9) Elements of X-ray Diffraction by B. D. Cullity, Addison Weily.
10) Source book on atomic energy- S. Glasstone; (D.Van Nostrand Company)
11) Chemical Application of radioisotopes- H.J.M.Bowen; Buttler and Tanner Ltd.
12) Introduction of Nuclear and Radiochemistry G. Friedlaunder, T. W. kennedy and J. M. Miller John Willey and sons 2nd Edn.
13) Nuclear Chemistry and its applications; M. Haissinsky, Addison Welsley publi. Co.
14) Essentials of Nuclear Chemistry- H. J. Arnikar; New Age International publisher Ltd. Willer- Eastern Ltd. 4th Edn.
16) Solid state chemistry by Jyoti Kumar, Sonali pub, New Dehli.

Paper : PCH : 304 B: Advanced Chemical Kinetics (Elective)

Unit-I: Reaction rates: (12)

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

Unit-II: Electron transfer reaction: (12)

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: (12)

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 oxidations : (12)

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.

REFFERENCE 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 chromim (VI) oxidation of organic substrates By Asim K. Das, Coordination Chemistry Reviews, Vol 248, p 81-89 (2004).
4) Some aspects of election 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 : PCH :304 C: Radiation and Photochemistry (Elective)

Unit-I : Radiation Chemistry: (12)

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

Unit-II Lasers and Lasers in Chemistry: (12)

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: (12)

Electrochemistry of excited states, life time measurements, flash photolysis, energy dissipation by radiative and non radiative processes, properties of excited states, structure, dipolemoment, 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 : (12)

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

SEMESTER – IV

Paper-PCH-401 : Statistical Mechanics and Irreversible Thermodynamics

Unit –I : Modern Theoretical principals: (12)

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, Caratheodory's theory. 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: Phase space,Stirlings approximation : (13)

Configuration and weights, the most probable configuration. Statistical Equilibrium. Postulates of equal probalilities. Ensembles. Ensemble average and time average of property. The classical Boltzmann Distribution law. Principle of the equipartition of energy, Quantum Statistics : Bose-Einstein, Fermi-Dirac and Maxwell – Boltzmann statistics, comparison of three statistics, Fermi- Dirac systems. Thermodynamics of electromagnetic radiations using BE statistics, Calculation of thermodynamic properties for boson and fermion gases using quantum statistics. Fermi energy. Electron gas in metals.

Unit – III : Molecular partition function: (13)

Expressions for transnational, rotational, vibrational and electronic partition functions, relation between the partition function and thermodynamic properties. Free energy functions, ortho and para hydrogen, use of spectroscopic and structural data to calculate thermodynamics functions. Molecular and statistical interpretation of entropy, third law of thermodynamics and equilibrium constant.

Heat capacity of solids, Einstein and Debye specific heat theories. Characteristic temperature.

Unit –IV : Thermodynamics of irreversible processes. (10)

Conservation 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. Entropy production in closed and open systems. Entropy production due to heat flow. Chemical potentials. Generalized fluxes, forces and their transformation. Phenomenological equations and coefficients, concepts of reciprocity relations and Onsager theorem of microscopic reversibility. Diffusion, electromotive force and other reactions involving cross relations e.g. thermoelectric and electrokinetic effects. Saxens relations. Oscillatory reactions.

RECOMMENDED BOOKS :

1) Elements of statistical thermodynamics – L.K.Nash,Addison Wesley
2) Statistical thermodynamics by B.J.McCelland, Chapman and Hall.
3) A Introduction to Statistical Thermodynamics by T.L. Hill Addison- Wesley
4) An Introduction to Thermodynamics of Irreversible Processes by Iila Prigofine.
5) Thermodynamics of steady state by Denbeigh
6) Advanced physical Chemistry by S.N.Blinder, The Macmilan Company,1967.
7) Themodynamics by R.C. Srivatsava, S.Saha and A.K.Jain,Prentice-hall, India.
8) Theoretical Chemistry by S.Glasstone. D. Van Nostrand Company, Inc., 1944.
9) Thermodynamics: A Core Course- R. C. Srivastava, S. K. Saha and A. K. Jain, Prentice-Hall of India, IInd edition, 2004.
10) Statistical Mechanics – Donald A. McQuarrie, 2000.

Paper No. PCH-402 : Chemical Kinetics

Unit – I : Theories of reaction rates: (16)

Equilibrium and rate of reaction, Partion functions and activated complex, Transition state theory (Thermodynamic and partion function approach), Reaction between polyatomic molecules, calculation of activation parameters of a reaction. Collision theory, energy factor, orientation factor, rate of reaction, Lindemann's mechanism of unimolecular reaction, weakness of the collision theory.

Unit – II : Chemical kinetics: (16)

Kinetics of complex reactions (Equilibrium, parallel and consecutive reactions) Rate laws. Chain reactions. General aspects of chain reactions, chain length, reaction between H_2-Br_2, H_2-Cl_2, H_2-I_2 and their comparison, thermal decomposition of acetaldehyde, Kinetics of branching chain reactions & explosion limits.

Potential energy surfaces: construction of multidimensional potential energy surfaces (semiempirical treatment), saddle point, reaction co-ordinate, example of tunneling effect, reaction $H + H_2$.

Unit – III: Homogeneous catalysis: (16)

Kinetics of homogeneous catalysis, general catalytic mechanism, equilibrium and steady-state treatment, activation energies for catalyzed reactions. General acid-base catalysis, mechanisms of acid-base catalysis (Arrhenius and van't Hoff intermediates), catalytic activity and acid base sterngth,Acidity functions, autocatalysis and oscillatory reactions.

Mechanism of enzyme catalyzed reactions and rate law for single substrate, Lineweaver-Burk plot, effect of pH and temperature.

REFERENCE BOOKS :

1) Chemical Kinetics by K.J.Laidler.
2) Kinetics and Mechanism by A.A. Frost and R.G. Pearson.
3) Chemical kinetics and reaction dynamics by Santosh K. Upadhyay, Anamaya Publishers.
4) Theory of chemical reaction rates by K.J.Laidler, McGrew Hill,New York,1969.
5) Physical Chemistry by W.J.Moores
6) Physical Chemistry by P.W. Alkins
7) Principles of physical chemistry by Puri, Sharma and Pathania, Vishal Pub. Co.

Paper No.PCH-403 – Molecular Structure-II

Unit – I : The Electric Properties of molecule (10)

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. Dipole moment and ionic character, Bond moment, Group moment, vector addition of moments, bond angles, The energies due to dipole-dipole, dipole-induced dipole and induced dipole-induced dipole interaction. Lennard-Jones potential.

Unit – II :The Magnetic properties of Molecules: (10)

Diamagnetism and paramagnetism. Volume and mass susceptibilities. Lengevins classical theory of diamagnetism and paramangenetism. Atomic and ionic susceptibility. Pascal constants, Curie- Weiss law. Van Vleck general equation of magnetic susceptibility. Determination of magnetic susceptibility, Gouy method. Ferro and ferri magnetism, application to coordination complexes and complex ions of transition metals.

Unit – III: Nuclear Magnetic Resonance Spectroscopy: (10)

The nature of spinning particles, interaction between spin and a magnetic field. Population of energy levels and signal to noise ratio, The larmor precession, relaxation times, the meaning of resonance, selection rules and the resonance condition. NMR experiment and instrumentation, singnificance of shielding constants and chemical shift, the origin and effect of spin – spin coupling, factors affecting chemical shift, chemical analysis by NMR. Simple and complex splitting patterns. Fourier Transform and FT NMR. Exchange phenomena, ^{13}C NMR spectroscopy, double resonance and nuclear-overhauser effect (NOE).

Unit - IV : Electron Spin Resonance Spectroscopy: (10)

Basic Principles, Zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities, selection rules and McConnell relationship, measurement techniques and instrumentatinon, applications. Bonding parameters from 'g' and coupling constants.

Unit – V : Mossbauer Spectroscopy: (8)

Basic principle of Mossbauer spectroscopy, Doppler effect, isomer effect, hyperfine structure, quadrupole splitting, instrumentation and applications of Mossbauer spectroscopy especially of iron and tin compounds, Problems related to Mossbaur spectra.

REFERENCE BOOKS :

1) Fundamentals of molecular spectroscopy by C.N.Banwell.
2) Physical chemistry by P.W.Atkins. ELBS. 1986
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.Carrington and A.D.McLachlan. Harper and Row.
7) Electron Spin Resonance, Elemenatry theory and practical applications by J.E.Wetz and J.R.Boulton, McGrew Hill.
8) Introduction to Magnetochemistry by Earnst Shaw. Academic Press
9) Electrical and optical properties of molecular behavior by M. Davies, pergman press.
10) Polar molecules by P.Debye, Dover publications.

Paper No.PCH – 404 A : Surface chemistry (Elective)

Unit-I : Adsorption and surface phenomenon: (12)

Solid surface, thypes of adsorption and isotherm, Langmuir and B.E.T.adsorption isotherm, BET equipment, calcualation of surface area of solids, Cataluysis: heterogenesis, activity and selectivity, surface activity, surfactants and calssification, micelle formation, surface active agents, surface excess concentration, surface pressure, concept of positive and negative adsorption, Gibb's adsorption equation: derivation, significance and experimental verification.

Unit II : Liquid-Gas interfaces (12)

Types of interfaces, Surface and interfacial tension, Young and Laplace equation for vapor pressure, plane and spherical interfaces (soup bubble and water droplet), Kelvin equation for Vapor Pressure inside and outside the liquid droplet, methods of determination of surface tension, surface tension across curved surfaces

Unit III: Liquid-Liqid interfaces: (14)

surface spreading, spreading coefficient, cohesion and adhesion energy, surface energy and spreading coefficient, Lagmiur–adam surface pressure balance, formation of insoluble monomolecular films, physical states of film, pi-A isotherm and its comparision with P-V isotherm, derivation Pi-A= kT equation, gaesous, liquid expanded and condensed films.

Liquid-liquid (Oil-water) Emulsion, identification of emulsion, emulsion stability, emulsifier, theories of emulsification, microemulsion and nanoparticle preparation with examples and applications

Unit IV : Solid –Liquid and Solid-Solid interfaces (10)

contact angle, contact angle hystereis, wetting and detergency, surface energy of solids, adhesion and adsorption, sintering and sintering mechanism, Tammann temperature and its importance, surface structure and surface composition.

REFERENCE BOOKS :

1. Physical chemistry of surfaces: A.W.Adamson.
2. Theory of adsorption and catalysis by Alrfed Clark,
3. Chemisorption by B.M.W. Trapnell and H.O. Hayward.
4. Introduction to colloide and surface chemstry by D.J.Shaw.
5. Theories of chemical reaction rates A.J.K. Laidler
6. Surface chemistry by J.J. Bikermann
7. Colloidal and Surface chemistry by Satake, Hayashi and Sethi, Discovery Pub. House
8. Surface chemistry by K. R. Desai, Oxford Book Co.

Paper No.PCH-404(B) : Chemistry of materials (Elective)

Unit I : Glasses, Ceramics, Composite and Nanomaterials: (12)
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: (12)
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: (8)
Molecular shape, structure and configuration, crystallinity, stress- strain behavior, thermal behavior, polymer types and their applications, conducting and ferro- electric polymers.

Unit IV : Thin films and Langmuir- Blodgett Films : (8)
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.

Unit V : Materials of Solid State Devices: (8)
Rectifiers, transistors, capacitors IV-V compounds, low demensional quantum structure; optical properties.

REFERENCE 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 No:PCH-404 C: Biophysical Chemistry (Elective)

Unit – I : Chemistry and Biology : (12)

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

Unit - II : Physical aspects of biopolymers: (12)

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: (12)

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

Unit – IV : Mechano-chemical processes: (12)

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

REFERENCE 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.

PRACTICAL COURSE

Semester-III
P- V to P - VI

Potentiometry

1. Determination of standard electrode potential (E^o) value of Ag / AgI electrode and the solubility product of AgI and PbI_2.
2. determination of dissociation constants of dibasic acid potentiometrically.

Conductometry

1. To determine equivalent conductance at infinite dilution of strong electrolyles and weak acid by using Kohlrausch Law and dissociation constant for weak acid conductometrically.
2. Kinetic study of hydrolysis of ethyl acetate in presence of OH-ions.

pH – Metry

1. determination of hydrolysis constant and degree of hydroysis of aniline hydrochloride pHmetrically.
2. Determination of acid- base dissociation constants of amino acids.

Polarography

1. To determine half wave potential of a given ion using half height method, differential method and wave equation method
2. Determination of unknown concentration of Cd+2/Zn+2 ion in the given solution by standard addition method.

Chemical Kinetics

1. To determine the order of reaction between acetone and iodine catalyzed by acid.

Cryoscopy

1. To determine molecular weight and state of benzoic acid in benzene.
2. determination of mean activity coefficient of sulphate by freezing point depression method.

Spectrophotometry

1. To determine pKa value of methyl red indicator at room temperature.
2. Determination of indicator constant and isosbestic point of an indicator (bromocresol purple).
3. Determination of stability constant of ferric thiocyanate complex by Ostwald method.

Moving boundary Method

To determine transport of H+ions by using Moving boundary method.

Thermometry:

Determination of normality of given HCl & CuSO4 by thermometric titration.

Amperometry

To determine unknown concentration of Iodine using amperometry.

Latent heat of Fusion

Determination of latent hear of fusion of a given solid.

Reference books:

1. Practical physical chemistry by Friendly and kitchner-logmann, Green and Co.
2. Senior Practical physical chemistry by B.D. Khosala and V.S. Gerg-R chand and Co.
3. Systematic experimental physical chemistry by Rajboj and Chondhekar-Anjali pub.
4. Advanced Practical physical chemistry by JB Yadhav – Goel pub.
5. Experimental physical chemistry by Das and Behra
6. Practical physical chemistry by Athawale and Mathur
7. Experimental physical chemistry by Daniel, Mathews and Williams.
8. A textbook of qualitative and quantitative inorganic analysis by AI Vogl.

Semester IV
P- VII to P - VIII

Potentiometry

1. To determine instability constant & stiochiometry of silver ammonia complex potentimetrically.
2. Determination of Thermodynamic Parameters for electrochemical reactions. (To determine ΔG^o, ΔH^o and ΔS^o for the formation of 1 mole cadmium in 1 wt.% amalgam at 25^0C and activity coefficient of solution).

Conductometry

1. Determination of the critical micelle concentration of sodium lauryl sulphate in aqueous solution.
2. To determine the hydrolysis constant and degree of hydrolysis of aniline hydrochloride.

pH – Metry

1. To determine the dissociation constants of dibasic acids pHmetrically.

Polarography

1. To determine half wave potential of a given ion using half height method, differential method and wave equation method
2. Determination of unknown concentration of Cd^{+2}/Zn^{+2} ion in the given solution by standard addition method.

Chemical Kinetics

1. Study of the effect of ionic strength on the reaction between persulphate and iodide by visual method.

Cryoscopy

1. To determine molecular weight and state of acetic acid in benzene.
2. Study of composition of complex formed between mercuric iodide amd potassium iodide.

Spectrophotometry

1. To determine stoichiometry & stability constant of ferric- Sulphosalicylic acid/salicylic acid complex by Job's Method and mole ratio method spectrophotometrically.
2. To determine equilibrium constant of reaction $KI+I_2=KI_3$ spectrophotometrically.
3. Determination of concentration of Cr and Mn simultaneously spectrophotometrically.

Spectroscopy:

1. Characterization of the complexes by electronic and IR spectral data.
2. Analysis of an ESR spectrum of an organic/inorganic radicals.
3. Interpretation of TGA curve.
4. Interpretation of X-ray diffractogram.

Fluorimetry:

Estimation of quinine as quinine sulfate from medicinal tablets.

Thermochemistry

Determination of heats of dilution and integral heat of solutions.

Reference books:

1. Practical physical chemistry by Friendly and kitchner-logmann, Green and Co.
2. Senior Practical physical chemistry by B.D. Khosala and V.S. Gerg-R chand and Co.
3. Systematic experimental physical chemistry by Rajboj and Chondhekar-Anjali pub.
4. Advanced Practical physical chemistry by JB Yadhav – Goel pub.
5. Experimental physical chemistry by Das and Behra
6. Practical physical chemistry by Athawale and Mathur
7. Experimental physical chemistry by Daniel, Mathews and Williams.
8. A textbook of qualitative and quantitative inorganic analysis by AI Vogl.
9

Project work / In-plant training / Review Report and Seminar

The student will develop utilities such as analytical spectra, simulation programmes that will supplement laboratory exercises. For this variety of small research project designed by the teacher based on the interest of the student and capabilities should be worked out.

Seminars:

The students will have to give at least one seminar in each semester in their subject of specialization. For this submission of synopsis of seminar delivered by every student is compulsory.