SOLAPUR UNIVERSITY, SOLAPUR

M. Sc. –II- PHYSICAL CHEMISTRY

SYLLABUS

(CHOICE BASED CREDIT SYSTEM)

(w.e.f. June-2016-17)

The syllabus of M.Sc. - Physical Chemistry course of two years duration has been prepared as per the Choice based credit system (C.B.C.S.). M. Sc. II syllabus is to be implemented from June 2016. The syllabus of M. Sc. Part I was implemented with effect from June 2015. The syllabus has been prepared taking into consideration the UGC guidelines, SET, NET examination syllabus, the syllabus of other universities and the specific inputs of the Expert Committee Members.

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 each for University External Examination and 30 marks each for Internal Examination and two practical courses of 70 marks each for University External Examination and 30 marks each for Internal practical course. The distribution of marks is as mentioned below.

Theory Paper (Semester Exam),	16 X (70+30) marks	1600 marks
Practical's (Semester End Exam.),	8 X (70+30) marks	800 marks
Seminars for each Semester,	4 X (25 Marks)	100 marks
		Total: 2500 marks

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

Semester I

Theory Courses: Paper No.	Title of Papers	Ext. + Int. = Total
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	Ext. + Int. = Total
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 Practical: Sem-I (70 marks Univ. Exam + 30 Marks Internal Exam)

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

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

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

Semester III

Paper No.	Title of Papers	External Marks	Internal Marks	Total Marks	Total Credit
PCH-301 (IX)	Quantum Chemistry	70	30	100	4
PCH-302 (X)	Electrochemistry	70	30	100	4
PCH-303: (XI)	Molecular Structure-I	70	30	100	4
PCH-304 (XII) A* **CBCS**	Solid State and Nuclear Chemistry	70	30	100	4
PCH-304 (XII) B **Elective**	Advanced Chemical Kinetics	70	30	100	4
PCH-304 (XII) C **Elective**	Radiation and Photochemistry	70	30	100	4
Practical course	Paper-V Paper-VI	70 70	30 30	100 100	4 4
Seminar		--	25	25	1

*PCH-304 (XII) A, course in Physical Chemistry is offered under CBCS to the students in Chemistry of specialization other than Physical Chemistry.

Semester IV

Paper No.	Title of Papers	External Marks	Internal Marks	Total Marks	Total Credit
PCH-401 (XIII)	Statistical Mechanics and Thermodynamics	70	30	100	4
PCH-402 (XIV)	Chemical Kinetics	70	30	100	4
PCH-403 (XV)	Molecular Structure II	70	30	100	4
PCH-404 (XVI) A **Elective**	Surface Chemistry	70	30	100	4
PCH-404 (XVI) B **Elective**	Chemistry of Materials	70	30	100	4
PCH-404 (XVI) C **Elective**	Biophysical Chemistry	70	30	100	4

Practical course	Paper-VII Paper-VIII*	70 70	30 30	100 100	4 4
Seminar		--	25	25	1

* VIII Project work/In-plant / Practical experiments

Summary:

Course	No. of Papers	Total marks	Examination Pattern		Total Credits
			UA	IA	
Core	14	1400	980	420	56
Elective	06 (any two)	200	140	60	08
Practical Course	08	800	560	240	32
Seminars	04	100	-	100	04
TOTAL		**2500**	**1680**	**820**	**100**

Nature of Examination: Each semester will have theory University external examination of four papers of 70 marks each (2 and 1/2 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 University 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 = (Project Report 50 Mark + Experiment 20 Mark) 70 Mark

** 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 by Departmental Faculty involved in Physical Chemistry.

Solapur University, Solapur
Nature of question paper (for M. Sc. I and II)

Time: 02.30 hours Max. Marks 70

Instructions:

1. Attempt any five 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 questions 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 are 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 [60 Lectures] [4 credits]

Unit – I Formalism of Quantum Mechanics: (15)

Failure of classical mechanics. Postulates of Quantum Mechanics, Eigen function and Eigen values. Acceptability of wave functions, Normalized and orthogonal wave functions. Operators and operator algebra, Schmidt Orthogonalisation. Hermition operators. Theorems related to commutator operations, 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 (15)

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 (15)

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, 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 Levine, Prentice Hall.

6) Theoretical Chemistry by S. Glasstone, Van Nostrand.

7) Physical Chemistry by Alberty.

8) Quantum Chemistry by R. K. Prasad, New Age International.

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.

12) Modern Quantum Chemistry, N. S. Ostlund & A Szabo, McGraw Hill.

13) Density Functional Theory of atoms and molecules, R. G. Parr and W. Yang, Oxford Press.

14) Semiempirical MO Theory, J. Pople and D. L. Beveridge.

Paper No. PCH- 302: Electrochemistry [60 Lectures] [4 credits]

Unit – I Electrolytic conductance: (15)

Debye – Huckel theory of inter – ionic attraction, ionic atmosphere, time of relaxation, relaxation and electrophoretic 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. Qualitative and quantitative verification of Debye-Huckel limiting law, ion association, Bjerrum theory, problems.

Unit - II Ion solvent interactions: (15) 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 etc.).

Unit- III Electrolysis: (15)

Decomposition potentials: calculations and determinations. Polarization: types of polarization, overvoltage, hydrogen and oxygen overvoltage, Laws of electrolysis, role of electrolysis in electrometallurgy. Electroforming: process, advantages and disadvantages, Electrotyping: technique, description, electrotyping in printing and in art.

Unit – IV : Electrode reactions. (15)

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, Tata McGraw Hill Ind. Pvt. Ltd.

2) Modern electrochemistry Vol I & II by J. O. M. Bockris and A. K. N. Reddy.

3) Physical chemistry by S. Glasstone, Tata McGraw Hill Pvt. Ltd.

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.

9) Electroforming: A comprehensive survey of theory, practice and commercial applications by P. Spiro, London 1971.

10) Electrotyping by McMillan Walter George

11) Electrotyping and Stereotyping by B. Harris and S. Alexander.

Paper No. PCH –303: Molecular Structure – I [60 Lectures] [4 credits]

Unit – I Symmetry properties of molecules and group theory: (15)

Symmetry elements, symmetry operations and point groups. Properties of group, symmetry operations as a group, multiplication table. Classes of symmetry operations, basis, representative and matrix representations of operations. Reducible and irreducible representations, orthogonality theorem, Properties of irreducible representations. Constructions of character table for point groups. Explanations for the complete character table for a point group. Representations of vibrational modes of vibrations. Application of group theory in understanding IR and Raman spectral transition, geometry and bonding in co-ordination complexes.

Unit-II: Introduction to spectroscopy and Rotational Spectra (15)

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 rotational constant B for real spectrum eg CO, HCl, NO etc. Instrumentation, source, waveguide and detectors.

Unit- III Infrared spectroscopy and Raman Spectroscopy: (15)

Infrared spectroscopy :Diatomic molecules : Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero point energy. 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 principle.

Unit – IV Electronic Spectroscopy of atoms and molecules: (15)

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.

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. Raman, 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, McGraw Hill.

10) Atomic and Molecular Spectroscopy, M.L. Gupta, New Age International Pub., 2001.

11) Molecular Structure and Spectroscopy, G. Aruldas, Prentice Hall, 2001.

12) Physical Methods in Chemistry, R. S. Drago, Saunders College.

13) Basic principles of Spectroscopy, R. Chang, McGraw Hill.

14) Introduction to photoelectron Spectroscopy, P. K. Ghosh, Jonh Wiley.

15) Modern Spectroscopy, J. M. Hollas, Jphn Wiley.

16) Group theory and its chemical applications, P. K. Bhattacharaya, Himalaya Pub. House, 1999.

17) Symmetry and Group theory for chemists, H. N. Dass,

Paper : PCH-304 (Elective) (A): Solid State and Nuclear Chemistry [60 Lectures][4 credits]

Unit I: The solid state : (15) 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 – Bragg's single crystal and powder diffraction method. Fourier synthesis, structure factor and electron density, determination of structure of naphthalene by electron density map.

Unit II : Solid State Reactions (15)

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

Unit III : Preparation of materials: (15)

Purification: Crystallization, sublimation and zone refining. Preparation of single crystal: Theory of nucleation, crystal growth, methods of preparation of single crystal, single crystal growth from solution, growth from melt. Doped organic and inorganic crystalline materials for device application. Nano materials: Basic principle of methods used for nano material preparations, organic and inorganic nano materials for devices.

Unit IV: Nuclear Chemistry: (15)

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 detectors: Gas detectors, scintillation detectors, semi conductor detectors, neutron detectors and their applications.

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. V. 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. Wiley-Eastern Ltd. 4th Edn.

15) Solid state chemistry by Jyoti Kumar, Sonali pub, New Dehli.

16) Solid state Chemistry and its applications, A. R.West, Plenum.

17) New Directions in solid state chemistry, C. N. R. Rao and J. Gopanlkrishnan, Cambridge University Press,1997.

18) Solid state Chemistry: An Introduction, 3rd Ed., L. E. Smart and E. A. Moore, Taylor and Francis, 2005.

19) Introduction to solids, L. V. Azaroff, Tata McGraw Hill., 1977.

Paper : PCH : 304 (Elective) (B): Advanced Chemical Kinetics [60 Lectures] [4 credits]

Unit-I: Reaction rates: (15)
Protonation and hydrolysis equilibria, determination of active reactant species form kinetic data, interpretation of hydrogen ion effect with example.

Unit-II: Electron transfer reaction: (15)
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: (15) 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 : (15) 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 B Jonson, 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 (Elective)C: Radiation and Photochemistry [60 Lectures] [4 credits]

Unit-I : Radiation Chemistry: (15)

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

Unit-II Lasers and Lasers in Chemistry: (15)

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: (15)

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 : (15)

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

[60 Lectures] [4 credits]

Unit –I : Modern Theoretical principals: **(15)** 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.

Unit-II: Phase space, Stirling's approximation : **(15)**
Configuration and weights, the most probable configuration. Statistical Equilibrium. Postulates of equal probabilities. Ensembles. Ensemble average and time average of property. The classical Boltzmann Distribution law. Principle of the equi-partition 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: **(15)**
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 temperatures.

Unit –IV : Thermodynamics of irreversible processes. **(15)**
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. Saxen's 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 Prigogine.

5) Thermodynamics of Steady State by Denbeigh

6) Advanced Physical Chemistry by S.N.Blinder, The Macmilan Company,1967.

7) Thermodynamics 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.

11) An Introduction to Statistical Thermodynamics, M. Dole, Dover, New York, 1986.

12) Thermodynamics of Irreverisible Processes, R. Hasse, Addison Wiley.

13)Non Equilibrium Thermodynamics: Principles and Applications, C. Kalidas and M.V. Sangaranarayan, MacMillan Ind. Pvt., Ltd. 2002.

14) An Introduction to Statistical Thermodynamics, R. P. H. Gasser and W. G. Richards, World Scientific Pub. Co. Pvt. Ltd., 1995.

Paper No. PCH-402 : Chemical Kinetics [60 Lectures] [4 credits]

Unit – I : Theories of reaction rates: (15)

Equilibrium and rate of reaction, Partition functions and activated complex, Transition state theory (Thermodynamic and partition 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: (15)

Kinetics of complex reactions: Opposing reactions, derivation of rate law for first order opposed by first order, second order opposed by first order, sequential reactions: expression for the rate law, maximum concentration of intermediate, time for maximum concentration of intermediate. Kinetics of parallel reactions and their rate law, ratio of products and examples, Numerical problems.

Unit-III: Chain reactions: (15)

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 (semi-empirical treatment), saddle point, reaction co-ordinate, example of tunneling effect, reaction $H+H_2$.

Unit – III: Homogeneous catalysis: (15)

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 [60 Lectures] [4 credits]

Unit – I : The Electric Properties of molecule (15)

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: (15)

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: (15)

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, significance 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 : (A) 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 instrumentation, applications. Bonding parameters from 'g' and coupling constants.

(B) Mossbauer Spectroscopy: (05)

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 Mossbauer 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.

11) Molecular Spectroscopy by G. M. Barrow, McGraw Hill.

12) Atomic and Molecular Spectroscopy, M.L. Gupta, New Age International Pub., 2001.

13) Molecular Structure and Spectroscopy, G. Aruldas, Prentice Hall, 2001.

14) Physical Methods in Chemistry, R. S. Drago, Saunders College.

15) Basic principles of Spectroscopy, R. Chang, McGraw Hill.

16) Introduction to photoelectron Spectroscopy, P. K. Ghosh, Jonh Wiley.

17) Modern Spectroscopy, J. M. Hollas, Jphn Wiley.

Paper No.PCH – 404 (Elective) (A): Surface Chemistry [60 Lectures] [4 credits]

Unit-I : Adsorption and surface phenomenon: (15)

Introduction, types of adsorption and isotherms, Langmuir and B.E.T. adsorption isotherms, BET instrumentation, measurement of surface area of solids, Catalysis: types, heterogenesis catalysis, turnover number, activity and selectivity. Surface activity, surfactants and their classification, surface excess concentration, surface pressure, concept of positive and negative adsorption, Derivation of Gibb's adsorption equation, significance and experimental verification, micelle and reverse micelle ,Kraft Temperature methods for the determination of critical micelle concentration, energetics of micelization and applications .

Unit II : Liquid-Gas interfaces (15)

Types of interfaces, Surface and interfacial tension, Young and Laplace equation for vapor pressure at curved , plane and spherical interfaces , Kelvin equation for Vapor Pressure inside and outside the liquid droplet, methods of determination of surface tension.

Unit III: Liquid-Liquid interfaces: (15)

Surface spreading, spreading coefficient, cohesion and adhesion energy, surface energy and spreading coefficient, Langmuir–Adam surface pressure balance, formation of insoluble monomolecular films, Langmuir-Blodget films, physical states of film, π-A isotherm and its comparison with P-V isotherm, derivation $\pi A = kT$ equation, gaseous, liquid expanded and condensed films. Emulsion, identification of emulsion, types of emulsion, emulsion stability, emulsifier, theories of emulsification, preparation of nanoparticles by using reprecipitation and emulsion method.

Unit IV : Solid –Liquid and Solid-Solid interfaces (15)

Contact angle and wetting of solids, methods of determination of contact angle, contact angle hysteresis, detergency, surface energy of solids, adhesion and adsorption, sintering and sintering mechanism, Tammann temperature and its importance, surface structure and surface composition solid lubricants

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 colloids and surface chemstry by D.J.Shaw.
5. Solid state chemistry Chakraborty
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.

9) Physical chemistry Gurdeep Raj

Paper No.PCH-404 (Elective) (B) : Chemistry of materials [60 Lectures] [4 credits]

Unit I : Glasses, Ceramics, Composite and Nanomaterials: (15)

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: (15)

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: (15)

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

Unit IV : (A)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.

(B) Materials of Solid State Devices: (7)

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 (Elective) (C): Biophysical Chemistry [60 Lectures] [4 credits]

Unit – I : Chemistry and Biology : (15)

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

Unit - II : Physical aspects of biopolymers: (15)

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: (15)

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

Unit – IV : Mechano-chemical processes: (15)

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 [120 Lectures][8 credits]

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 electrolytes 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:

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

Thermometry:

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

Amperometry:

1. To determine unknown concentration of Iodine using amperometry.

Latent heat of Fusion:

1. Determination of latent heat of fusion of a given solid.

*** Any other relevant experiment may be added.**

Semester IV P- VII to P – VIII [120 Lectures] [8 credits]**

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.

5. Analysis of rotational-vibrational spectra of simple molecules.

Fluorimetry:

1. Estimation of quinine as quinine sulfate from medicinal tablets.

Thermochemistry:

1. Determination of heats of dilution and integral heat of solutions.

*** Any other relevant experiment may be added.**

****Project or industrial in plant training or literature review articles:**

In the final semester, students have to carry out project either at college laboratory or university laboratory or in any recognized R & D laboratory (Public/Private/Government) or Industry or Institute of national repute across the country under the guidance of scientist or a post-graduate faculty member. Alternatively the student can undertake the literature review of the articles.

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, Tata McGraw Hill.

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. Selected Experiments in physical Chemistry, N. G. Mukherrjee, J. N. Ghosh and Sons.

10. Experiments in Physical Chemistry, J. C. Ghosh, Bharati Bhavan.

11. Practical Physical Chemistry, B. Vishwanathan and P. S. Raghvan, Viva Books, 2005.

12. A Laboratory manual of experiments in physical chemistry, C. D. Brennan & C. F. H. Tipper, McGraw Hill, 1967.