Punyashlok Ahilyadevi Holkar Solapur University, Solapur

NAAC Accredited-2015
'B' Grade (CGPA 2.62)

Name of the Faculty: Science & Technology

CHOICE BASED CREDIT SYSTEM

Syllabus: Physical Chemistry

Name of the Course: M.Sc. II (Sem.–III & IV)

(Syllabus to be implemented from w.e.f. June 2021)

M. Sc. II, PHYSICAL CHEMISTRY COURSE SYLLABUS
CHOICE BASED CREDIT SYSTEM (CBCS) (w.e.f. June 2021)

A two-year duration **M. Sc. Physical Chemistry** course syllabus has been prepared as per the CBCS semester system. M. Sc. II, SEM-III & SEM-IV Physical Chemistry syllabus will be implemented from June 2021. The syllabus has been prepared taking into consideration the syllabi of other Universities, SET, NET, UGC guidelines, and the specific inputs of the Expert CommitteeMembers.

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 80 marks for university external examination and 20 marks for internal examination of each semester and two practical's of 80 marks, 20 marks for internal practical of each semester. The distribution of marks is mentioned below

Theory Paper (Semester exam), 16 X80+20marks 1600marks
Practicals (semester end exam.), 8 X80+20marks
800marksTutorials foreachsemester, 4 X25 100marksTotal: 2500marks

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

semester	code	Title of the paper	Semester Examination			L	T	P	Credit
			Theory	IA	Total				
SEM-III		**Hard core**							
	HCT-3.1	Quantum Chemistry	80	20	100	4	--	-	4
	HCT-3.2	Electrochemistry	80	20	100	4		-	4
		Soft core (Any one)	80	20					
	SCT-3.1	Molecular Structure-I	80	20	100	4		-	4
	SCT- 3.2	Biophysical Chemistry	80	20	100	4		-	
		Open elective (Any one)	80	20					
	OET- 3.1	Solid State Chemistry	80	20	100	4		-	4
	OET- 3.2	Radiation and Photochemistry	80	20	100	4		-	
		Seminar/Tutorial/ Industrial Visit/ Field Tour	---	25	25	--	1	--	1
	HCP- 3.1	Practical HCP	40	10	50	-	-	3	2
	HCP- 3.2	Practical HCP	40	10	50	-	-	3	2
	SCP- 3.1/3.2	Practical SCP	40	10	50	-	-	3	2
	OEP- 3.1/3.2	Practical OEP	40	10	50	-	-	3	2
		Total for semester III	**480**	**145**	**625**	**--**	**--**	**---**	**25**
SEM-IV		**Hard core**							
	HCT- 4.1	Statistical Mechanics and Irreversible Thermodynamics	80	20	100	4	--	-	4
	HCT-4.2	Chemical Kinetics	80	20	100	4		-	4
	HCT-4.3	Molecular Structure-II	80	20	100	4		-	4
		Soft Core (Any one)	80	20				-	4
	SCT-4.1	Surface Chemistry	80	20	100	4		-	
	SCT-4.2	Chemistry of Materials	80	20	100	4		-	
		Seminar/Tutorial/ Industrial Visit/ Field Tour	---	25	25	--	1	--	1
	HCP 4.1	Practical HCP	40	10	50	-	-	3	2
	HCP 4.2	Practical HCP	40	10	50	-	-	3	2
	HCMP 4.3	Practical HCP	40	10	50	-	-	3	2
	SCP4.1/4.2	Practical SCP	40	10	50	-	-	3	2
		Total for semester IV	**480**	**145**	**625**	**--**	**--**	**---**	**25**

HCT=Hard Core Theory HCP=Hard Core Practical SCT=Soft Core Theory OET=Open Elective Theory IA=Internal Assessment SCP=Soft Core Practical
L=Lecture T=Tutorials
P=Practical

M. Sc. Part II (Physical Chemistry)

SEMESTER-III

Paper Code HCT-3.1: QuantumChemistry

[60Lectures] [4credits]

Unit – I Formalism ofQuantumMechanics: (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, Hermitian operators, properties of Hermitian operators, Theorems related to commutator operations, Concept of angular momentum, angular momentum operators, Ladderoperators.

Unit – II Quantum Mechanics of somesimplesystems: (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 He^{+}, Li^{2+}etc)

Unit – III. Hückel molecularOrbitalTheory (15)

Secular equations and secular determinants, Assumptions and formalism of Hückel molecular Orbital Theory, origin of aromatic stability and calculation of delocalization energy. HMO calculations for organic molecules,(e.g. ethylene, cyclopropyl, allyl, butadiene, cyclobutadiene, trimethylene methane etc.), free valence index and prediction of chemical reactivity,Use of symmetry based linear combination to simplify the problem of Hückel theory calculations for larger aromatic molecules (like butadiene).

Unit – IV: Advancedquantumchemistry (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 andGTO's).

REFERENCE BOOKS

1) Introductory Quantum Chemistry by A. K. Chandra. TataMcGraw-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, Academicpress.

5) Quantum Chemistry by Levine, PrenticeHall.

6) Theoretical Chemistry by S. Glasstone, VanNostrand.

7) Physical Chemistry byAlberty.

8) Quantum Chemistry by R. K. Prasad, New AgeInternational.

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, statisticalmechanics, and molecular spectra for chemists - S. Glasstone, D. Van Nostrand Company, Inc., 1944.

12) Modern Quantum Chemistry, N. S. Ostlund&ASzabo, McGrawHill.

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 Code HCT-3.2 :Electrochemistry

[60Lectures] [4credits]

Unit – IElectrolyticconductance: (15)

Debye – Hückel theory of inter – ionic attraction, ionic atmosphere, time of relaxation, relaxation and electrophoretic effects, Debye-Hückel –Onsagar (DHO)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-Hückel limiting law and its applications to concentrated solutions. Debye-HückelBronsted equations. Qualitative and quantitative verification of Debye-Hückel limiting law, ion association, Bjerrum theory,problems.

Unit - II Ionsolventinteractions: (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 methodetc.).

Unit-IIIElectrolysis: (15)

Decomposition potentials: calculationsand 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, MIRPublishers.

7) Chemical and electrochemical energy systems by R. Narayan and B.Viswanathan, Universitiespress

8) Handbook of fuel cell technology by Maget HJR, prentice-Hall, NewJersey.

9) Electroforming: A comprehensive survey of theory, practice and commercial applications by P. Spiro, London1971.

10) Electrotyping by McMillan WalterGeorge

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

Paper Code SCT-3.1 : Molecular Structure – I

[60 Lectures] [4 credits]

Unit–ISymmetrypropertiesofmoleculesandgrouptheory: (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. Application of group theory in understanding IR and Raman spectral transition, geometry and bonding in co-ordinationcomplexes.

Unit-II: Introduction to spectroscopy andRotational Spectroscopy (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 e.g. CO, HCl, NO etc. Instrumentation, source, waveguide anddetectors.

Unit- III Infrared spectroscopy andRamanSpectroscopy: (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 andcombinationfrequencies. The influence of rotations and molecular spin on the spectra of polyatomic molecules. Analysis by Infraredtechniques.

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 exclusionprinciple.

Unit – IV Electronic Spectroscopy of atomsand 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 polyatomicmolecules.

REFERENCE BOOKS :

1) Fundamental of molecular spectroscopy by C. N. Banwell Tata McGrewHill.

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, Jhonwilley.

6) Group theory and its applications to chemistry by K. V. Raman, Tata McGrewHill.

7) Molecular Structure and Molecular Spectra by G. Herzberg, VanNostrand.

8) Molecular Spectroscopy by I. N. Levine, Willeyinterscience.

9) Molecular Spectroscopy by G. M. Barrow, McGrawHill.

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, SaundersCollege.

13) Basic principles of Spectroscopy, R. Chang, McGrawHill.

14) Introduction to photoelectron Spectroscopy, P. K. Ghosh, JonhWiley.

15) Modern Spectroscopy, J. M. Hollas, JphnWiley.

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

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

Paper Code -SCT-3.2: Biophysical Chemistry

[60 Lectures] [4 credits]

Unit – I : Chemistry andBiology: (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 aspectsofbiopolymers: (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 : PhotobiologicalProcess: (15)

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

Unit – IV :Mechano-chemicalprocesses: (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, LongmarEssex

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

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

5) Principals of biochemistry, A.L. Lechinger, worthpublisher

6) Biochemistry, J.DavidRawn, NeilPatterson

7) Hydrophobic interactions byBen-Naim,Plenum.

Paper : OET-3.1 : Solid State Chemistry

[60Lectures] [4 credits]

Unit I: The SolidState: (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. Debye-Sherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-Ray intensities, structure factor and its relation to intensity and electrondensity,

Unit II : SolidStateReactions (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 : Preparationofmaterials: (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.

Unit IV :Synthesis and Characterization of Nanomaterials (15)

General Introduction to Nanomaterials, Nanoscience and nanotechnology, History. Chemical Methods: Metal nanoparticles: Reduction method, Semiconducting or composite nanomaterials: Hydrothermal and Solvothermal method,Sol-gel,Arrested Precipitation, and other methods include Langmuir-Blodgett, Micelles-Microemulsions. Characterization Tools: Electron Microscopy (TEM & SEM), Probe Microscopy (STM & AFM), Diffraction Technique (XRD), UV-Visible-NIR spectroscopy, BET.

REFFERENCE BOOKS :

1) Principals of solid state, H. V. Keer, WileyEastern.

2) Solid state chemistry, N. B.Hannay

3) Solid state chemistry, D. K. Chakrabarty, New AgeInternational

4) An Introduction to Crystallography : F. G.Philips

5) Crystal Structure Analysis : M.J.Buerger

6) New Directions in Solid State Chemistry (Second Eds.), C.N.R.Rao and G. Gopalkrishnan, Cambridge Oxford Press.

7) A basic course in crystallography, JAK Tareen, TRN Kutty, Universities press.

8) Essentials of crystallography, M.A. Wahab, Narosa Publications.

9) Synthesis of Inorgnic Materials: Ulrich Schubert, Nicola Hüsing.

10) Solid State Chemistry: Lasley E. Smart, Elaine A. Moore.

11) Introduction to Solid State Physics: Charles Kittel

12) Wilcox : Preparation and Properties of Solid State Materials: Vol I & II, Dekker

13) Hagenmuller, Preparative Methods in Solis State Chemistry

14) Lohn Wulff, The Structure and Properties of Materials Vol. IV, Electronic Properties (Wily Eastern)

15) Chemistry of Imprefect Crystals (Holland) E.A. Kroger

16) Solid State Chemistry A. R. West,

17) The Structure and properties of materials: Vol.III Electronic properties by JohnWulff.

18) Electronic processes in materials: L. V. Azroff and J. J.Brophy

19) Chemistry of imperfect crystal : F. A.Krogen

20) Elements of X-ray Diffraction by B. D. Cullity, AddisonWeily.

21) Solid state chemistry by Jyoti Kumar, Sonali pub, NewDehli.

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

23) Solid state Chemistry: An Introduction, 3rd Ed., L. E. Smart and E. A. Moore,

Taylor and Francis,2005.

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

25) LudovicoCademartiri and GeoffreyA.Ozin,Concepts of Nano chemistry,Wiley–VCHVerlagGmbH&co,2009

26) C.Bréchignac,P.Houdy,MarcelLahmani, Nano materials and Nano chemistry, Springer,2007

27) C.N.R.Rao,Achim Müller,Anthony K. Cheetham, Nano materials Chemistry ,John Wiley & Sons, 2007

28) Geoffrey A. Ozin,André C. Arsenault,LudovicoCademartiri, Nano chemistry: A Chemical Approach to Nano materials, Royal Society of Chemistry (GreatBritain)2, illustrated, Royal Society of Chemistry,2009

Paper : OET-3.2: Radiation and Photochemistry

[60Lectures] [4 credits]

Unit-I :RadiationChemistry: (15)

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

Unit-II Lasers and LasersinChemistry: (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 : Basicsofphotochemistry: (15)

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

Unit-IV :Micellaneous Photochemicalreactions: (15)

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

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& KerryK.Karukstis.

6) Photochemistry, R.P.Kundall, A Gilbert, ThomsonNelson

SEMESTER – IV

Paper Code- HCT-4.1 : Statistical Mechanics and Irreversible Thermodynamics

[60Lectures] [4 credits]

Unit –I : ModernTheoreticalprincipals: (15)

Exact and inexact differential expressions in two variables. Total differentials. Techniques of partial differentiations. Transformation of variables. Maxima and mimima. Integrating Factors, Pfaff 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: Statistical Thermodynamics: (15)

Configuration and weights, the most probable configuration. Statistical Equilibrium. Postulates of equalprobabilities.Ensembles. Phase space, Stirling'sapproximationEnsemble 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 : Molecularpartition function: (15)

Expressions for transnational, rotational, vibrational and electronic partition functions, relation between the partition function andthermodynamicproperties. 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 ofirreversibleprocesses. (15)

Conservation of mass in closed and open systems. Conservation of energy in closed and open systems.Law ofincreasing entropy.Non- adiabatic process and clausius inequality,steadystate.Thermodynamicequationsofmotion.Entropyproductionin

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, AddisonWesley

2) Statistical thermodynamics by B.J. McCelland, Chapman andHall.

3) A Introduction to Statistical Thermodynamics by T.L. Hill, Addison-Wesley

4) An Introduction to Thermodynamics of Irreversible Processes by IilaPrigogine.

5) Thermodynamics of Steady State by Denbeigh

6) Advanced Physical Chemistry by S.N.Blinder, The MacmilanCompany,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, AddisonWiley.

13)Non Equilibrium Thermodynamics: Principles and Applications, C. Kalidasand 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 Code- HCT-4.2: Chemical Kinetics

[60Lectures] [4credits]

Unit – I : Theories ofreaction 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 collisiontheory.

Unit – II :Chemicalkinetics: (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:Chainreactions: (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:Homogeneouscatalysis: (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 andtemperature.

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,NewYork,1969.

5) Physical Chemistry byW.J.Moores

6) Physical Chemistry by P.W.Alkins

7) Principles of Physical Chemistry by Puri, Sharma and Pathania, Vishal Pub.Co.

Paper Code: HCT-4.3: MolecularStructure-II

[60Lectures] [4credits]

Unit – I : The Electric Propertiesofmolecule (15)

Electric dipole moment of molecule, polarization of a dielectric, polarizability of molecules, Clausius-Mossottiequation. 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 propertiesofMolecules: (15)

Diamagnetism and paramagnetism. Volume andmass 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 MagneticResonanceSpectroscopy: (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 SpinResonanceSpectroscopy: (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 couplingconstants.

(B)MossbauerSpectroscopy: (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 byC.N.Banwell.

2) Physical chemistry by P.W.Atkins. ELBS.1986

3) Introduction to molecular spectroscopy byG.M.Barrow.

4) Molecular spectroscopy by I.N.Levins, Wileyinterscience.

5) Nuclear magnetic Resonance by J.D.Roberts, McgrewHill.

6) Introduction to Magnetic resonance by A.Carrington and A.D.McLachlan. Harper andRow.

7) Electron Spin Resonance, Elemenatry theory and practical applications by J.E.Wetz and J.R.Boulton, McGrewHill.

8) Introduction to Magnetochemistry by Earnst Shaw. AcademicPress

9) Electrical and optical properties of molecular behavior by M. Davies, pergmanpress.

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

11) Molecular Spectroscopy by G. M. Barrow, McGrawHill.

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, SaundersCollege.

15) Basic principles of Spectroscopy, R. Chang, McGrawHill.

16) Introduction to photoelectron Spectroscopy, P. K. Ghosh, JonhWiley.

17) Modern Spectroscopy, J. M. Hollas, JphnWiley.

18) Advanced physical chemistry by Gurudeep Raj. Goel publication

Paper Code No. SCT – 4.1 : Surface Chemistry

[60Lectures] [4 credits]

Unit-I : Adsorption andsurfacephenomenon: (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-Gasinterfaces (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-Liquidinterfaces: (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 andSolid-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 solidlubricants

REFERENCE BOOKS :

1. Physical chemistry of surfaces:A.W.Adamson.

2. Theory of adsorption and catalysis by AlrfedClark,

3. Chemisorption by B.M.W. Trapnell and H.O.Hayward.

4. Introduction to colloids and surface chemstry byD.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 BookCo.

9) Physical chemistry Gurdeep Raj

Paper Code: SCT-4.2 : Chemistry of Materials

[60Lectures] [4 credits]

Unit I : Glasses, Ceramics, CompositeandNanomaterials: (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, andapplications.

Unit II : HighTcMaterials: (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:PolymericMaterials: (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- BlodgettFilms: (8)

Preparation techniques: evaporation/ sputtering, chemical processes, MOCVD, sol – gel etc. Langmuir- Blodgett (LB) film, growth techniques, photolithography, properties and application of thin and LBfilms.

(B) Materials of SolidStateDevices: (7)

Rectifiers, transistors, capacitors IV-V compounds, low demensional quantum structure; opticalproperties.

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, ChemieVerlag

PRACTICAL COURSE Semester-III

HCP- 3.1 to OEP- 3.2

[120Lectures] [8 credits]

Potentiometry

1. Determination of standard electrode potential (E_o) value of Ag / AgI electrode and the solubility product of AgI andPbI_2.

2. Determination of dissociation constants of dibasic acidpotentiometrically.

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 ofOH^-ions.

pH – Metry

1. Determination of hydrolysis constant and degree of hydroysis ofaniline hydrochloridepHmetrically.

2. Determination of acid- base dissociation constants of aminoacids.

Polarography

1. To determine half wave potential of a given ion using half height method, differential method and wave equationmethod

2. Determination of unknown concentration of Cd^{+2}/Zn^{+2} ion in the given solution by standard additionmethod.

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 inbenzene.

2. determination of mean activity coefficient of sulphate by freezing point depression method.

Spectrophotometry

1. To determine pKa value of methyl red indicator at roomtemperature.

2. Determination of indicator constant and isosbestic point of an indicator (bromocresol purple).

3. Determination of stability constant of ferric thiocyanate complex by Ostwaldmethod.

Moving boundary Method:

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

Thermometry:

1. Determination of normality of given HCl& $CuSO_4$ 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 beadded.**

PRACTICAL COURSE Semester-IV

HCP- 4.1 to HCMP – 4.3**

[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 ofsolution).

Conductometry

1. Determination of the critical micelle concentration of sodium lauryl sulphate in aqueoussolution.

2. To determine the hydrolysis constant and degree of hydrolysis ofaniline 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 equationmethod

2. Determination of unknown concentration of Cd^{+2}/Zn^{+2} ion in the given solution by standard additionmethod.

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 inbenzene.

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 simultaneouslyspectrophotometrically.

Spectroscopy:

1. Characterization of the complexes by electronic and IR spectraldata.

2. Analysis of an ESR spectrum of an organic/inorganicradicals.

3. Interpretation of TGAcurve.

4. Interpretation of X-ray diffractogram.

5. Analysis of rotational-vibrational spectra of simplemolecules.

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 beadded.**

****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 andCo.
2. Senior Practical physical chemistry by B.D. Khosala and V.S. Gerg-R chand andCo.
3. Systematic experimental physical chemistry by Rajboj and Chondhekar-Anjalipub.
4. Advanced Practical physical chemistry by JB Yadhav – Goelpub.
5. Experimental physical chemistry by Das and Behra, Tata McGrawHill.
6. Practical physical chemistry by Athawale andMathur
7. Experimental physical chemistry by Daniel, Mathews andWilliams.
8. A textbook of qualitative and quantitative inorganic analysis by AIVogl.
9. Selected Experiments in physical Chemistry, N. G. Mukherrjee, J. N. Ghosh andSons.
10. Experiments in Physical Chemistry, J. C. Ghosh, BharatiBhavan.
11. Practical Physical Chemistry, B. Vishwanathan and P. S. Raghvan, VivaBooks, 2005.
12. A Laboratory manual of experiments in physical chemistry, C. D. Brennan & C.F. H. Tipper, McGraw Hill, 1967.