S.P.Mandali's
Ramnarain Ruia Autonomous College

Program : M.Sc.

Course: M.Sc. Physical Chemistry
Course code: RPSCHEP

Syllabus for Semester III & IV

(Choice Based Credit System to be implemented from the Academic year 2019-20)

Semester III

Course Code	Unit	Topic	Credits	Lectures
RPSCHEP301	I	Polymer Chemistry-I	4	15
	II	Modern Applications of Surface Chemistry		15
	III	Photo Chemistry-I		15
	IV	Applications of Fluorescence Phenomena		15
RPSCHEP302	I	Advances in Nanomaterials	4	15
	II	Applied electrochemistry		15
	III	Statistical Mechanics		15
	IV	Nuclear Chemistry		15
RPSCHEP303	I	Atomic structure	4	15
	II	Atomic spectroscopy		15
	III	Molecular Structure		15
	IV	Molecular spectroscopy		15
RPSCHEPEC-I 304	I	Electron Spectroscopy and Microscopy	4	15
	II	Hyphenated Techniques		15
	III	Thermal and Radioanalytical Methods		15
	IV	Pulse Polarography		15
RPSCHEPEC-II 304	I	Spectral Methods	4	15
	II	Electro-analytical Methods – I		15
	III	Radio-analytical Methods		15
	IV	Pulse polarography		15
RPSCHEP3P1	Practicals		8	16
RPSCHEP3P2				
RPSCHEP3P3				
RPSCHEP3P4				

Semester IV

Course Code	Unit	Topic	Credits	Lectures
RPSCHEP401	I	Polymer Chemistry-II	4	15
	II	Polymer Chemistry-III		15
	III	Bio-physical Chemistry and Green Chemistry		15
	IV	Photochemistry-II: Kinetics and Applications		15
RPSCHEP402	I	Solid State Chemistry	4	15
	II	Instrumental Methods		15
	III	Lasers and super conductors		15
	IV	Non-equilibrium thermodynamics		15
RPSCHEP403	I	Symmetry in Chemistry	4	15
	II	N.M.R.Spectroscopy-I		15
	III	ESR and Mossbauer Spectroscopy		15
	IV	^{13}C-N.M.R.Spectroscopy		15
RPSCHEPOC-I 404	I	Introduction to Intellectual Property	4	15
	II	Trade Secrets		15
	III	Introduction to Cheminformatics		15
	IV	Applications		15
RPSCHEPOC-II 404	I	Review of Literature	4	15
	II	Data Analysis		15
	III	Methods Of Scientific Research And Writing Scientific Papers		15
	IV	Chemical Safety & Ethical Handling Of Chemicals		15
RPSCHEP4P1	Practicals		8	16
RPSCHEP4P2				
RPSCHEP4P3				
RPSCHEP4P4				

Detail Syllabus

SEMESTER III
Paper-I
Course Code: RPSCHEP301
Credits: 4
Polymer, Surface & Photochemistry

Unit- I	**Polymer Chemistry-I**	**(15 L)**
	1.1 Introduction: Polymer Science, fundamental terms, historical outline, classification based on: the origin (natural, semi-synthetic, synthetic etc.), the structure (linear, branched, network, hyper branched, dendrimer, ladder, cross linked, IPN),the type of atom in the main chain(homo-chain, hetero-chain),the formation (condensation, addition), homopolymers, co polymers (random, alternate, block, graft), the behavior on application of heat (thermoplastic and thermosetting),the form and application (plastics, fiber, Elastomers and resins).	**(5 L)**
	1.2 Molar Mass: Molecular weight averages, fractionation, molecular weight determination by GPC/SEC, end group analysis, viscometry, vapour phase osmometry gradient elution, and molecular weight distribution curve.	**(5 L)**
	1.3 Types of polymerization: condensation, addition (cationic and anionic) and copolymerization (with kinetics), chain transfer reactions.	**(5 L)**
UNIT-II	**Modern Applications of Surface Chemistry**	**(15 L)**
	2.1 Surface active agents and micelle: **2.1.1 Surface active agents** and their classification, hydrophile-lipophile balance **2.1.2 Micellization**: shape and structure of micelles, hydrophobic interaction, critical Micelles concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, micelle catalysis, and reverse micelles. **2.1.3 Emulsions**: Solubilization, micro emulsions, characterization of Micro-emulsions, **2.2 Hydrogen storage by Adsorption:** **2.2.1 Hydrogen storage**: fundamentals Physisorption, temperature and pressure influence, chemisorption, adsorption energy, 'Electrochemical 'adsorption. **2.2.2. Practical adsorption**: storage of hydrogen with carbon materials, activated carbon, graphite graphene, carbon nano structures, fullerene. Carbon nano fibers (CNF) and graphite nano fibers electrochemical storage of hydrogen in carbon materials.	**(8L)** **(7L)**
UNIT-III	**Photo Chemistry-I**	**(15L)**
	3.1 Photo chemical principles: Environmental effect on absorption and emission spectra, properties of excited states, excited state acidity constants, dipole moments and redox properties, Importance of photochemistry, origin of life, **3.2 Photo physical processes in electronically excited molecules:** types of photo-physical pathways, types of radiation less transitions, fluorescence emission, fluorescence and structure. Triplet state and phosphorescence emission, delayed fluorescence–e type and p-type delayed fluorescence. **3.3 Photo chemical reactions**: ketones, olefins conjugated olefins and	

	aromatic compounds, photosynthesis	
UNIT-IV	**Applications of Fluorescence Phenomena**	**(15L)**
	4.1 Fluorescence sensing: Mechanism of sensing; sensing techniques based on Coalitional quenching, energy transfer, electron transfer; examples of pH sensors glucose sensors and protein sensors. **4.2 Novel fluorophores**: Quantum dots, lanthanides and long-lifetime Metal-ligand complexes. **4.3 Radiative decay engineering**: metal enhanced fluorescence **4.4 DNA technology**–sequencing.	**(05L)** **(05L)** **(03L)** **(02L)**

Reference books:

1.	P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition,NarosaPublishingHouse,2005.
2.	C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York,2010.
3.	Joel R. Fried, Polymer Science and Technology, Prentice-Hall of India Pvt. Ltd., 2000.
4.	V.R.Gowarikar,H. V. Viswanathan and J. Sreedhar, Polymer Science. New Age International Pvt. Ltd., New Delhi, 1990.
5.	M. J. Rosen. Surfactants and Interfacial Phenomena (3rd edn.), John Wiley (2004).
6.	Y. Moroi, Micelles: Theoretical and Applied Aspects, (1992) Plenum Press, New York
7.	Tushar K. Ghosh, Energy Resources and Systems: Volume 2, Springer Link:Bücher,Springer,2011.
8.	R. Str¨obel a, J. Garche b, P.T. Moseley c, L. J¨orissen b, G. Wolfd. "Review Hydrogen storage by carbon materials." Journal of Power Sources (WWW.Sciencedirect.com) 159 (June 2006): 781–801.
9.	C. H. De Puy, O. L. Chapman, Molecular reactions and photo chemistry, Prentice hall of India PVT. LTD. 1988.
10.	K.K.Rohatgi-Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher,1978.
11.	B. Valeur, Molecular Fluorescence: Principles and Applications, Wiley-VCH (2001).
12	J.R.Lakowicz, Principles of Fluorescence Spectroscopy,Springer(2006). Reference Book

Semester III
Paper II
Course Code: RPSCHEP302
Credits: 4
Nanochemistry, Applied Electrochemistry, Statistical Mechanics & Nuclear Chemistry

UNIT-I	Advances in Nanochemistry	(15L)
	1.1: Types of nanomaterials e.g. nanotubes, nanorods, solid spheres, core-shell nanoparticles, mesoporous materials, General preparative methods for various nanomaterials **1.2 I mportant properties on nanomaterials:** optical properties of metal and semiconductor nanomaterials, magnetic properties **1.3 Some special nanomaterials:** **1. Carbon nanotubes-** Types, synthesis using various methods, growth mechanism, electronic structure. **2. Porous Silicon**- Preparation and mechanism of porous silicon formation, factors affecting porous structure, properties of porous silicon. **3. Aerogels**- types of aerogels, properties and applications of aerogels **1.4 Application of nanomaterials** in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defence. **1.5 Environmental effects of nanotechnology**	
UNIT-II	**Applied Electrochemistry**	**(15L)**
	1.1 Electroplating: electroplating of metals, factors affecting throwing power of an electroplating bath, mechanism of electrodeposition, typical electroplating processes, applications of electroplating metal (Sn, Ni, Cr, Cu, Cd, Zn, Ag and Au) **1.2 Electrochemical corrosion of metals**- Classification of corrosion processes, conditions for the occurrence of corrosion process, kinetic theory of corrosion and its application to pure metals, methods of corrosion protection, corrosion of technical metals **1.3 Batteries**- Working principle, cell reactions and cell performances of Lithium batteries (primary and secondary), Lithium based conducting polymer batteries, solid state and molten solvent batteries, silver-anode primary batteries, high temperature solid-state batteries, ambient temperature thermal batteries. **1.4 Fuel Cells**- Classification, H2-O2 fuel cell, choice of electrolyte, advantages, disadvantages, electrodes and electrocatalysis, phosphoric acid fuel cells, methanol fuel cells, solid polymer electrolyte fuel cells, solid oxide fuel cells, diaphragm fuel cells, biochemical fuel cells	
UNIT- III	**Statistical Mechanics**	**(15L)**
	3.1.Thermodynamic probability: Combinatorial problems, Strilling approximation**,** Lagranges method, macro and microstates, ensembles, Boltzmann distribution law. **3.2 Partition functions**: Translational, rotational, vibrational, electronic and nuclear partition functions, Expressions for the thermodynamic functions in terms of partition function -Internal energy, heat capacity, the Helmholtz and Gibbs functions, Enthalpy, entropy and equilibrium constants. Sackur –Tetrode equation for the entropy of a mono atomic gas. Molecular partition function.	

	3.3 Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. **3**.4. Debye and Einstein theory of specific heat of solids	
UNIT—IV	**Nuclear Chemistry**	**(15L)**
	4.1 Charged particle accelerator- linear accelerator, cyclotron, Betatron, Synchrotron **4.2 Nuclear forces-** characteristics and Meson field theory of nuclear forces **4.3 Nuclear Models-**Liquid drop model**,** Fermi Gas Model, Shell Model, Collective Model, Optical Model. **4.4 Applications of Nuclear radiations- g**eological applications of radioactivity, age of minerals and rocks, age of earth and solar system, medical, industrial and Agricultural applications of radiochemistry, positron emission topography, Radio-immune assay.	

References:	
1.	Sulabha K. Kulkarni, Nanotechnology: Principles and Practices, Capital publishing company (2007)
2.	Lesley E. Smart and Elaine A. Moore, Solid State Chemistry- An introduction, 3rd Ed., Taylor and Francis, (2005), Chapter 11
3.	Atkins P. W, Physical Chemistry, Oxford University Press,6th edition,1998
4.	Laidler K.J. and Meiser J.H., Physical Chemistry, 2ndedition, CBS publishers & distributors,1999.
5.	John M. Seddon & Julian D. Gale, Thermodynamics and Statistical mechanics, Tutorial Chemistry Texts series,Vol.10,Royal Society of Chemistry,2001.
6.	D. A. McQuarrie, Statistical Mechanics, (1976) Harper and Row Publishers, New York.
7.	Silbey RJ & Alberty RA,Physical Chemistry,3rd edition, John Wiley and sons, Inc.2002.
8.	B. K. Agarwal and M. Eisner, Statistical Mechanics,(1988)Wiley Eastern, New Delhi.
9.	G. Friedlander, J. W. Kennedy, Nuclear and Radio Chemistry.Third. John Wiley and sons,1981.
10.	H. J. Arnikar, Essentials of Nuclear Chemistry. Wiley Eastern Ltd., 1989.

SEMESTER-III
Paper-III

Course Code: RPSCHEP303
Credits: 4
Atomic and Molecular: Structure and spectroscopy

UNIT-I	**Atomic structure**	**(15L)**
	1.1: Introduction to approximate methods in Quantum Mechanics- **1.1.1** Variation Theorem, linear and nonlinear variation functions. **1.1.2** Perturbation Theory, Non degenerate Perturbation Theory, first order wave function correction, first order and second order energy correction. **1.1.3** Application of variation and perturbation theory to ground state of Helium Atom. **1.2: Multi –electron atoms**: Anti-symmetry and Pauli principle, Slater determinants, Hartree. Fock and configuration interaction wave functions, Slater type orbitals, Gaussian orbitals, orbi plot, basic sets, and density function theory.	
UNIT-II	**Atomic spectroscopy**	**(15L)**
	2.1 Angular momentum, orbital and spin, total angular momentum, total angular momentum (J) of many electron atoms, Russell Saunders (L-S) coupling and J-J coupling	**(04L)**
	2.2 Term symbols, term symbols for multi electron atoms like He, Li, Be, B etc.	**(04L)**
	2.3 Exchange of interactions and multiplicity of states.	**(02L)**
	2.4 Anomalous Zeeman Effect and Paschen Back effect.	**(02L)**
	2.5 Atomic spectra and selection rules, energy level diagram of atomic sodium.	**(03L)**
UNIT-III	**Molecular Structure**	**(15L)**
	3.1 The Born–Oppenheimer approximation	
	3.2 LCAO method-molecular orbital formation	**(01L)**
	3.3 Calculation of energy of hydrogen molecule ion using	**(01L)**
	3.3.1 Valence bond method	**(05L)**
	3.3.2 Heitler-London treatment	
	3.3.3 Improvements in Heitler-London treatment	
	3.4 Electronic structure of polyatomic molecules	**(08L)**
	3.4.1 Valence bond method for BeH_2, H_2O, NH_3, BH_3 ,CH_4.	
	3.4.2 Huckel molecular orbital's Theory for–ethylene, Allyl system, cyclo-propenyl system and cyclo-butadiene.	
UNIT-IV	**Molecular spectroscopy**	**(15L)**
	4.1. Rotational spectroscopy: Einstein coefficients, classification of poly atomic Molecules spherical top, symmetric top and asymmetric top molecules, rotational Spectra of polyatomic molecules Stark modulated microwave Spectrometer.	**(03L)**
	4.2 Raman Spectroscopy-Classical theory of molecular polarizability, pure rotational, vibrational and vibration-rotation spectra of diatomic and polyatomic molecules polarization and depolarization of Raman lines correlation between IR and Raman spectroscopy Instrumentation.	**(05L)**
	4.3 Electronic Spectra of molecules: Term symbols for linear molecules, selection rules characteristics of electronic transitions-Franck-Condon principle, types of electronic transitions-d-d, vibronic, charge transfer, π-π^*,n-π^*transitions, fate of electronically excited states, fluorescence, phosphorescence, dissociation and pre-dissociation	**(07L)**

References	
1.	Atkins P.W, Physical Chemistry, Oxford University Press,6th edition,1998.
2.	William Kemp, Organic spectroscopy,3rd Edition,ELBS,1996.
3.	R. K. Prasad, Quantum Chemistry,3rd Ed., New Age International Publishers,2006.
4.	D.A.McQuarrie, Quantum Chemistry, Viva Books Private Limited, New Delhi, first Indian ed.,2003.
5.	A.K.Chandra,IntroductoryQuantumChemistry,4McGrawH edition(1994),Tata ill,NewDelhi
6.	I.N. Levine, Quantum Chemistry,5 Edition (2000), Pearson Educ. Inc., New Delhi.
7.	James E. House, Fundamentals of Quantum Chemistry, Second Ed.,Academic Press,2005.
8.	C.N.Banwell and E.M.McCash,Fundamentals of Molecular Spectroscopy,4thEd.,Tata-McGraw-Hill,1994.
9.	M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers,2001.
10.	H.S.Randhawa, Modern Molecular Spectroscopy,McMillanIndiaLtd.,2003
11.	G.Aruldas, Molecular Structure and Spectroscopy,Prentice-HallofIndia,2001.
12.	J.Michael Hollas, Modern Spectroscopy, 4thEd., John Wiley and Sons,2004.
13.	Donald L. Pavia, Gary M. Lampman and George S. Kriz, Introduction to Spectroscopy,3rded., Thomson, Brooks/Cole,2001.
14.	F.A.Cotton,Chemical Applications of Group Theory,3rdEd., John Wiley and Sons(Asia) Pte. Ltm, 1999.

SEMESTER-III
Paper IV
Course Code: RPSCHEPEC- 304
Credits: 4
Advanced Instrumental Techniques

UNIT-I	**Electron Spectroscopy and Microscopy**	**(15L)**
	1.1 Electron Spectroscopy**:** principles, instrumentation and applications of the following ESCA (XPS), AUGER, UPS. **1.2** Chemiluminescence method **1.3** Nuclear Quadrupole Resonance (NQR), ENDOR, ELDOR, EWDOR	
UNIT-II	**Hyphenated Techniques**	**(15L)**
	2.1 Introduction, need for hyphenation, possible hyphenations. **2.2** Interfacing devices and applications of the following- GC-MS, GC-IR, MS-MS, HPLC-MS, ICP-MS, Spectro-electrochemistry and radio chromatography	
UNIT-III	**Thermal and Radioanalytical methods**	**(15L)**
	3.1 Enthalpimetric methods **3.2** Thermometric titrations **3.3** Evolved Gas Analysis **3.4** Radiometric titrations and Applications **3.5** Auto, X-ray and Gamma Radiography	
UNIT-IV	**Pulse polarography**	**(15L)**
	4.1 Normal Pulse Polarography (NPP), Differential Pulse Polarography (DPP). Double Differential Pulse Polarography (DDPP) **4.2** Sinusoidal AC Polarography, Square wave polarography **4.3** Applications of electrochemical methods in Organic synthesis	

References

1. Skoog DA, West DM, Fundamentals of Analytical Chemistry, Thomson Asia Pvt. Ltd., 8th Ed, (2004).
2. Skoog, Holler, Nieman, Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd., 5th Ed, (2004)
3. Willard Merrit and Settle, Instrumental Methods of Analysis
4. Robert D. Braun, Introduction to Instrumental Analysis (IndiaReprint2006)
5. Nuclear Ch emistry by Arnikar
6. J.W. Dood, K.Tonge, Thermal Methods, Analytical Chemistry, Open Learning
7. A. J. Bard and Faulkner, Electrochemical Methods, 2ndEd, John Wileyand Sons (Asia) Pvt. Ltd., 2004.

Practical

SEMESTER-III

Credits: 8

Paper Code	No.	Experiment
RPSCHEP3P1	1.	To determine the formula of copper (II) ammonia complex by partition method.
	2.	To determine the transport no. of copper (II) ions by Hittorf's method.
	3.	To determine the isoelectric point of gelatin by viscosity measurement.
	4.	To determine the molar conductance of a weak electrolyte at infinite dilution hence to determine its dissociation constant conductometrically.
RPSCHEP3P2	1.	To construct the phase diagram for a two component system forming a simple eutectic.
	2.	To determine the partial molal volume of ethanol.
	3.	To titrate potassium ferrocyanide with zinc sulphate and hence to determine the formula of the complex conductometrically.
	4.	To determine the equilibrium constant for the reaction $CaSO_{4\,(s)} + 2Ag^{+1}{}_{(aq)} \rightarrow Ag_2SO_{4(s)} + Ca^{2+}{}_{(aq)}$
RPSCHEP3P3	1.	Determination of the energy of activation and other thermodynamic parameters of activation for the acid catalyzed hydrolysis of methyl acetate.
	2.	To determine the formula of the zinc (II) ferrocyanide complex by titration of Zn(II) sulphate with potassium ferrocyanide potentiometrically.
	3.	To determine the E^0 of the quinhydrone electrode potentiometrically.
	4.	To estimate the amount of hydrochloric acid and acetic acid in a mixture by titration with an alkali using a pH meter.
	5.	To determine hydrolysis constant and degree of hydrolysis of ammonium chloride and hence to estimate the dissociation constant of the base pH-metrically
RPSCHEP3P4	1.	To determine the molar mass of a non-volatile solute by cryoscopic method.
	2.	To study complex formation between nickel (II) with 1.10-phenanthroline.
	3.	To determine the ionization constant of bromophenol blue
	4.	To determine the dissociation constant of methyl red.

1. The candidate is expected to submit a journal certified by the Head of the Department/institution at the time of the practical examination.

2. A candidate will not be allowed to appear for the practical examination unless he / she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.

3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

List of reference Books for Practicals:

1. B.Vishwanathan and P. S. Raghavan, Practical Physical Chemistry, Viva

   Books Private Limited, 2005.
2. A. M. James and F. E. Prichard, Practical Physical Chemistry, 3rd ed., Longman,1974.

3. B.P.Lewitt(ed.),Findlay'sPracticalPhysicalChemistry,9thed.,1973.
4. C.D.BrennanandC.F.H.Tipper,ALaboratoryManualofExperimentsin PhysicalChemistry,McGraw-Hill,1967.

5. F. Daniel & Others, Experimental Physical Chemistry,1965, Kogakasha Co Ltd.

SEMESTER –IV
Paper-I
RPSCHEP401
Credits: 4

Chemistry: Polymer, Green, Biophysical, Photochemistry

UNIT-I	**Polymer Chemistry-II**	**(15L)**
	1.1 Polymers in solid state – Transitions (glass transition and crystalline melting temperature), crystalline behavior, factors affecting crystallinity, polymer blends and Alloys. **1.2 Identification and characterization of polymers**: Chemical analysis- End group analysis; Physical analysis by Spectral methods: IR, UV, Raman, NMR, X-ray diffraction analysis, Microscopic methods: SEM, TEM, Thermal analysis-TGA,DTA, DSC. **1.3 Properties of polymers**: Thermal (glass transition temperature, and its determination),mechanical(deformationandfracture)effectsinpolymers,viscoelasticity surface (surface tension, hardness, friction, abrasion), physical (Impact strength, Tensile strength, solubility) of polymers, weather ability, rheology and mechanical models, mechanical behavior, Rubber elasticity, **1.4 Polymer degradation and stabilization**: Oxidative, thermal, radiation, Biodegradation.	
Unit II	**Polymer Chemistry-III**	**(15L)**
To be reduced?	**2.1Techniquesofpolymerization**:Bulk polymerization,solution polymerization,suspension Ion polymerization, emulsion polymerizations, **2.2Thermodynamics of polymersolutions**: Solubility parameter, thermodynamics of mixing**,** theta temperature **2.3 Polymer technology**: **2.3.1** Polymer auxiliaries, plasticizers, heat Stabilizers, colorants, flame retardants. F**illers, reinforcements.** **2.3.2** Elastomers: Introduction, Processing, Rubber Types, Vulcanization, Properties. Reclaiming. **2.3.3** Fibers: Introduction, production, Fiber spinning, Textile fibers, Industrial fibers, recycling. **2.3.4** Films sheets: Introduction and processing techniques (injection and blow moulding extrusion),Recyling of plastics. **2.4 Properties and applications of some commercially important polymers**. Carbon chain polymers- Polyolefins, ABS group, elastomers, vinyl polymers, acrylic polymers, heterochain polymers- polyethers, polycarbonates, polysaccharides, polyamides fluoropolymers, Resins (epoxy, alkyd, phenol-formaldehyde and urea-formaldehyde), Silicones, polyphosphazenes, sulphur containing polymers.	
UNIT-III	**Bio-physical Chemistry and Green Chemistry**	**(15L)**
To shift Green Chem in polymer unit	**3.1 Biophysical Chemistry** **3.1.1 Introduction to Complex Biomolecules:** Proteins, enzymes, DNA, RNA, polysaccharides andlipids.chirality and pH dependence of biomolecules. **3.1.2 Biosensors** : Enzyme based, Electrochemical, immunosensor, fluorescence, optical, Piezoelectric Biosensors **3.1.3 Electrophoresis (Technique for bio-molecular study) :**Principle and factors affecting electro-phoreticmobility, zone electrophoresis–Paper electrophoresis,cellules acetate electrophoresis, Gel electrophoresis. capillary Electrophoresis, Application of electrophoresis. **3.2 Green Chemistry:** **3.2.1** Recapitulation of principles of green chemistry, Waste minimization techniques. **3.2.2** Catalysis and Green Chemistry: Phase transfer catalysts, biocatalyst, Photo Catalysis. **3.2.3** Organic solvents, solvent free system, supercritical fluid, ionic liquid, their	**(15L)** **(07L)**

	characteristics, use as catalyst and solvents. **3.2.4** Alternative energy sources for initiation and execution of chemical reaction: Microwave and sonochemistry.	
UNIT-IV	**Photochemistry-II: Kinetics and Applications**	**(15L)**
	4.1 Photophysical Kinetics of Bimolecular processes: Collisions in solutions, Kinetics of Collisional Quenching and Stern-Volmer equation and deviations from Stern-Volmer equation. **4.2** Concentration dependence on quenching and excimer formation. **4.3** Quenching by added substances- charge transfer mechanism and energy transfer mechanism. **4.4** Solar cells: Photovoltaic and photo-galvanic cells, photoelectron chemistry; Prospects of solar energy conversion and storage, organic solar cell.	

Reference Books:

1.	P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition,NarosaPublishingHouse,2005.
2.	C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8th edition, CRC Press, New York,2010.
3.	JoelR.Fried,Polymer Science and Technology, Prentice-Hall of India Pvt. Ltd., 2000
4.	V.R.Gowarikar, H.V.Viswanathan and J.Sreedhar,Polymer Science.New Age International Pvt.Ltd., New Delhi,1990.
5.	U.N Dash,.AText Book of Biophysical Chemistry,Macmillan India Ltd
6.	Gurtu and Gurtu, Biophysical Chemistry, Pragati Prakashan.
7.	MikeLancaster, Green Chemistry An Introductory Text, Royal Society of Chemistry.
8.	K.K.Rohatgi-Mukherjee. Fundamentals of Photochemistry.Reprint 2002. New AgeInternationalPublisher,1978.

Semester-IV

Paper-II

RPSCHEP402

Credits: 4

Solid State Chemistry, network and irreversible thermodynamics

UNIT-I	**Solid State Chemistry**	**(15L)**
	1.1 Bonding and Structure: Classification of solids based on nature of forces (ionic, metallic, van der Waal's, hydrogen bonded), crystal structures. **1.2** Symmetry and choice of unit cell, Bravais lattice, Miller indices, Point groups and space groups, Close packing. Packing efficiency of a unit cell. **1.3** Crystalline solids, ionic radii, radius ratio rule, lattice energy, lattice energy, crystal structure determination by powder diffraction, and single crystal X-ray diffraction **1.4** Defects in Crystal: point defects, plane defects, line defects.	
UNIT-II	**Instrumental Methods**	**(15L)**
	2.1 X-Ray Diffraction: Introduction to XRD, Diffraction of waves by crystal, particle and solid. Generation of X Rays (K shell knockout), Bragg condition, Bragg method, Miller indices, Methods of diffraction, Laue method, Debye-Scherrer method of X ray structural analysis of crystals, Advantages of these methods, Index reflections, Identification of unit cells from systematic absences in diffraction pattern, Uses of powder XRD. **2.2 Electron and Neutron Diffraction** **2.2.1 Electron diffraction**: Diffraction patterns for single crystal, polycrystalline and amorphous material. Difference between X-ray and electrons, experimental technique. Applications of electron diffraction **2.2.2 Neutron diffraction**: Properties of neutron, Principle of neutron scattering, comparison with X-rays. Advantages of neutron scattering, scattering of neutrons by solids and liquids.	
Unit III	**Lasers and super conductors**	**(15L)**
	3.1 Lasers in chemistry **3.1.1** General principles of LASER action-Population Inversion, cavity and mode Characteristics, Q-switching, Model-locking. **3.1.2** Practical lasers- Solid state lasers-Ruby, neodymium, gas lasers-He-Ne, Ar, Kr, Carbon dioxide, Chemical and exciplex Lasers,Dye lasers LED and Semiconductor Lasers**.** **3.1.3** Applications of Lasers in chemistry**:** Spectroscopy at high photon fluxes, collimated beams, Precision specified transitions, Isotope separation, Study of fast reactions using pulsed techniques**.** **3.2 Super conducting solid materials** Band theory of electrical conductivity, Bardeen-Cooper-Schriffer Theory of super conductivity,the superconducting state, High critical temperature super conductors, magnetic properties of superconductors.	**(10L)** **(05L)**
Unit IV	**Non-equilibrium thermodynamics**	**(15L)**
	Non-equilibrium thermodynamics : **4.1** Features of non-equilibrium thermodynamics, second law of thermodynamics, uncompensated heat and its relation to thermodynamics function. **4.2** Entropy production and its rate. Entropy production in heat transfer process and during mixing	**(02L)** **(04L)**

	of gases.Entropy production and efficiency of galvanic cell. **4.3** Onsagers theory: Reciprocal relation, principle of microscopic reversibility. Coupled and uncoupled reactions and their condition. **4.4** Transport phenomena across membranes. Electro kinetic effect and thermo mechanical effects.	**(05L)** **(04L)**

References	
1.	Keer H.V, Principles of the Solid State, first reprint, Wiley Eastern Limited, 1994.
2.	R.S. Drago, Physical Methods for Chemists, 2nd edition, Saunders College Publishing (1992)
3.	A.R.West,Solid State Chemistry and its Applications,John Wiley and Sons (Asia) Pvt.Ltd.,
4.	L.E.Smart and E.A.Moore, Solid State Chemistry–An Introduction,3rdEd., Taylor and Francis, 2005.
5.	P.W, Physical Chemistry, Oxford University Press, 6th edition, 1998.
6.	E.D.Kaufmann, Advanced Concepts in Physical Chemistry, McGraw-Hill,1966.
7.	C.Kalidas and M.V.Sangaranarayan, Non-Equilibrium Thermodynamics, Principles and Applications, McMillanIndia Ltd.,2002.
8.	S. Glasstone, Theoretical Chemistry, Affiliated East–West Press Pvt. Ltd., New Delhi, 1973.

Paper-III
RPSCHEP403
Credits: 4
Symmetry & Spectroscopy

UNIT-I	Symmetry in Chemistry	(15L)
	1.1 Recapitulation: point groups, character tables	**(02L)**
	1.2 Reduction formula, application of reduction formula to vibrational modes of water molecule	**(02L)**
	1.3 Application in vibrational spectroscopy, selection rules for IR spectroscopy for molecules such as H_2O, CO_2, HF, H_2	**(03L)**
	1.4. Application to Raman spectra, selection rules, comparison of IR and Raman selection rules, general approach to vibrational spectroscopy.	**(02L)**
	1.5. Symmetry in chemical bonding: symmetry adapted linear combination of molecular orbitals, H^{2+},H_2, LiH, BeH_2, BH_3, CH_4, molecular orbital energy, and bond order	**(06L)**
UNIT-II	**N.M.R.Spectroscopy-I**	**(15L)**
	2.1 A review of one dimensional NMR spectroscopy.	**(01L)**
	2.2 Spin-relaxation. Nuclear Overhauser Effect (NOE).polarization transfer.	**(03L)**
	2.3 Two-dimensional NMR. Correlated spectroscopy(COSY)	**(03L)**
	2.4 Nuclear Overhauser effect Spectroscopy(NOESY)	**(02L)**
	2.5 Hetero nuclear correlation Spectroscopy(HETCOR)	**(02L)**
	2.6 Solid-state NMR	**(02L)**
	2.7 Magnetic Resonance Imaging(MRI)	**(02L)**
UNIT-III	**ESR and Mossbauer Spectroscopy**	**(15L)**
	3.1Electron spin Resonance Spectroscopy-	**(10L)**
	3.1.1 Basic principle, hyperfine splitting(isotropic systems);	
	3.2.2 G-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy);	
	3.3.3 An isotropic effects (the g-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes.	
	3.4.4 Fundamentals and hyper fine splitting, application to study of free radicals spin densities McConnell relationship Zero field splitting.	
	3.2 Mossbauer Spectroscopy: Principles, Recoille emission and absorption of γ-rays, experimental methods, isomer shift, hyperfine structure (quadrupole interaction), magnetic hyperfine interaction, applications.	**(05L)**
UNIT-IV	**^{13}C-N.M.R.Spectroscopy**	**(15L)**
	4.1 Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. proton noise decoupling technique advantages and disadvantages, off-resonance technique.	**(05L)** **(03L)** **(03L)**
	4.2 Chemical shifts of solvents, factors affecting chemical shifts, analogy with ^{1}HNMR.	**(02L)**
	4.3 Calculations of chemical shift of hydrocarbons, effect of substituent's on chemical shifts, different types of carbons (alkene, alkyne and allene).	
	4.4 Chemical shift of aromatic carbons and effect of substituent.	
	4.5 Chemical shifts of carbonyl, nitrile, and oxime carbons.	**(02L)**

References	
1.	K.Veera Reddy, Symmetry and Spectroscopy of molecules,2nded,new age International publishers.
2.	F.A.Cotton, Chemical applications ofGroup Theory, Wiley Student Ed., 2006, JohnWiley and Sons,(Asia) Pvt.Ltd
3.	S.Swarnalakshmi, T.saroja, R.M.Ezhilarisi, A simple approach to Group theory in chemistry, 2008, Universities Press (India) Pvt. Ltd.
4.	R.L.Carter, Molecular symmetry and Group theory, Wiley Student Ed.,1996,John Wiley and Sons, (Asia) Pvt.Ltd.
5.	C.N.Banwell and E.M.McCash, Fundamentals of Molecular Spectroscopy, 4thEd., Tata-McGraw-Hill,1994.
6.	M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers,2001.
7.	H.S.Randhawa, Modern Molecular Spectroscopy, McMillan India Ltd.,2003
8.	G.Aruldas, Molecular Structure and Spectroscopy, Prentice-HallofIndia,2001.
9.	J.MichaelHollas, Modern Spectroscopy ,4thEd.,John Wiley and Sons,2004.
10.	Donald L. Pavia, Gary M. Lampman and George S. Kriz, Introduction to Spectroscopy,3rded.,Thomson,Brooks/Cole,2001.
11.	R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, Pitman, London, 1983.
12.	R.Drago,Physical Methods for Chemists, Saunders ,Philadelphia,1992.

SEMESTER-IV
Paper-IV
Course Code: RPSCHEPOC-I 404
Credits: 4
INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS

UNIT-I		**(15L)**
	Introduction to Intellectual Property: Historical Perspective, Different types of IP, Importance of protecting IP **Patents:** Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India. **Industrial Designs:** Definition, How to obtain, features, International design registration. **Copyrights:** Introduction, How to obtain, Differences from Patents. **Trade Marks:** Introduction, How to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc. **Geographical Indications:** Definition, rules for registration, prevention of illegal exploitation, importance to India.	
UNIT-II		**(15L)**
	Trade Secrets: Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection. **IP Infringement issue and enforcement:** Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. **Economic Value of Intellectual Property:** Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer. **Different International agreements:** **(a) World Trade Organization (WTO):** (i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement (ii) General Agreement on Trade Related Services (GATS) Madrid Protocol. (iii) Berne Convention (iv) Budapest Treaty **(b) Paris Convention** **WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.	
UNIT-III	**Introduction to Chem-informatics:**	**(15L)**
	History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation. **Representation of molecules and chemical reactions:** Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits, Different electronic effects, Reaction classification. **Searching Chemical Structures:** Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.	
UNIT-IV	**Applications**	**(15L)**
	Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Chem-informatics in Drug Design.	

References	
1.	Andrew R. Leach & Valerie J. Gillet (2007) An Introduction to Cheminformatics. Springer: The Netherlands.
2.	Gasteiger, J. & Engel, T. (2003) Cheminformatics: A textbook. Wiley–VCH
3.	Gupta, S. P. QSAR and Molecular Modeling. Springer-Anamaya Pub.: New Delhi.

SEMESTER-IV
Course Code: RPSCHEPOC-II 404
Credits: 4

PAPER – IV: RESEARCH METHODOLOGY

UNIT-I		**(15L)**
	Review of Literature: Primary, Secondary and Tertiary sources. **Journals:** Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text- books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples. **Digital:** Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, Chem-Industry, Wiki-databases, Chem-Spider, Science Direct, Sci-Finder, Scopus. **Information Technology and Library Resources:** The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	
Unit II	**DATA ANALYSIS**	**(15L)**
	The Investigative Approach: Making and recording Measurements, SI units and their use, Scientific methods and design of experiments. **Analysis and Presentation of Data:** Descriptive statistics, choosing and using statistical tests, Chemo metrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, and its abuse, basic aspects of multiple linear regression analysis.	
Unit III	**METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS**	**(15L)**
	Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation. **Writing Scientific Papers:** Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.	
Unit IV	**CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS**	**(15L)**
	Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressure, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.	

REFERENCES:

1. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), Practical skills in Chemistry, 2nd Ed., Prentice Hall, Harlow.
2. Hibbert, D. B. & Gooding, J. J. (2006) Data Analysis for Chemistry Oxford University Press.
3. Topping, J., (1984) Errors of Observation and their Treatment 4th Ed., Chapman Hill, London.
   Harris, D. C. (2007) Quantative Chemical Analysis 6th Ed., Freeman Chapters3-5
5. Levie, R. De. (2001) How to use Excel in Analytical Chemistryand in general scientific data analysis Cambridge Universty Press.
6. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press.
7. OSU Safety manual 1.01

Semester –IV

Practicals

Credits: 8

Paper Code	No.	Experiment
RPSCHEP4P1	1.	To determine the formula of the zinc (II) ammonia complex by partition method.
	2.	Determination of the transport no. of silver (I) ions by Hittorf's method.
	3.	To determine the composition of a mixture of hydrochloric acid, potassium chloride and ammonium chloride by titration with sodium hydroxide and silver nitrate conductometrically.
	4.	To determine ΔG, ΔHand ΔS of dissolution of a sparingly soluble salt by conductometry.
	5.	To determine K1 and K2 of a dibasic acid by titration with a base.
	6.	To determine dissociation constant of p-nitro phenol.
RPSCHEP4P2	1.	To construct the phase diagram for a two component system forming a compound
	2.	To determine the energy of activation and other thermodynamic parameters of activation for the reaction between persulphate and potassium iodide.
	3.	To determine the effect of ionic strength of a solution on the reaction between potassium persulphate and potassium iodide.
	4.	To study the order of the reaction between bromate and bromide.
	5.	To determine the van't Hoff's factor by cryoscopic method.
	6.	To determine the liquid junction potential with a concentration cell with and without transference.
RPSCHEP4P3		**Interpretation of spectra/data:**
	1.	Interpretation of vibrational-rotational spectra of rigid and non-rigid diatomic molecules.
	2.	Interpretation of electronic spectra of diatomic molecules.
	3.	Interpretation of electronic spectra of simple polyatomic molecules.
	4.	Interpretation of NMR, ESR spectra
	5.	Interpretation of Interpretation of Mössbauer spectra.
	6.	Analysis of XRD pattern of cubic system
	7.	Interpretation of DTA, TG, and DTG curves
RPSCHEP4P4		**Project Evaluation**

List of reference Books for Practicals:

a. B.Vishwanathan and P.S.Raghavan, Practical Physical Chemistry, Vi va Books Private Limited, 2005.
b.

Note:

1. The candidate is expected to submit a journal certified by the Head of the Department/institution at the time of the practical examination.

2. A candidate will not be allowed to appear for the practical examination unless he / she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.

3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

MODALITY OF ASSESSMENT

Theory Examination Pattern:

A) Internal Assessment - 40% :40 marks.

Sr. No	Evaluation type	Marks
1	Presentation skills (based on communication skill, A.V. presentation and Viva)	15
4	Submission of Hardcopy on presented topic	15
5	Active participation	10

B) External examination - 60 %

Semester End Theory Assessment - 60 marks

i. Duration - These examinations shall be of **2.5 hours** duration.

ii. Paper Pattern: There shall be **4** questions each of **15** marks. On each unit there will be one question. All questions shall be compulsory with internal choice within the questions.

Questions	Options	Marks	Questions on
Q.1)A)	Any 3 out of 5	12	Unit I
Q.1)B)	Any 1 out of 2	3	
Q.2)A)	Any 3 out of 5	12	Unit II
Q.2)B)	Any 1 out of 2	3	
Q.3)A)	Any 3 out of 5	12	Unit III
Q.3)B)	Any 1 out of 2	3	
Q.4)A)	Any 3 out of 5	12	Unit IV
Q.4)B)	Any 1 out of 2	3	

Practical Examination Pattern: External (Semester end practical examination):

1. Major Experiment: 100 marks

Scheme	05		Accuracy	08
Technique	06		Result	05
Observation	30		Viva	05
Calculation	16		Journal	10
Graph	15			

2. Minor Experiment: 50 marks

Scheme	02
Technique	02
Observation	14
Calculation	10
Graph	10
Accuracy	02
Viva	05
Journal	10

PRACTICAL BOOK/JOURNAL

The students are required to present a duly certified journal for appearing at the practical examination, failing which they will not be allowed to appear for the examination.

In case of loss of Journal and/ or Report, a Lost Certificate should be obtained from Head/ Co-ordinator / In-charge of the department; failing which the student will not be allowed to appear for the practical examination.

OVERALL EXAMINATION AND MARKS DISTRIBUTION PATTERN

Semester- III and IV

Course	Semester III			Semester IV			Grand Total
	Internal	External	Total	Internal	External	Total	
Theory	40	60	100	40	60	100	200
Practicals					50	50	100