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S.P.Mandali's

Ramnarain Ruia Autonomous College

RUIA COLLEGE
Explore • Experience • Excel

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 2022-23)

GRADUATE ATTRIBUTES

GA	Description
A student after completing Master's in Science program will be able to	
GA 1	Demonstrate in depth understanding in the relevant science discipline. Recall, explain, extrapolate and organize conceptual scientific knowledge for execution and application and also to evaluate its relevance.
GA 2	Critically evaluate, analyse and comprehend a scientific problem. Think creatively, experiment and generate a solution independently, check and validate it and modify if necessary.
GA 3	Access, evaluate, understand and compare digital information from various sources and apply it for scientific knowledge acquisition as well as scientific data analysis and presentation.
GA 4	Articulate scientific ideas, put forth a hypothesis, design and execute testing tools and draw relevant inferences. Communicate the research work in appropriate scientific language.
GA 5	Demonstrate initiative, competence and tenacity at the workplace. Successfully plan and execute tasks independently as well as with team members. Effectively communicate and present complex information accurately and appropriately to different groups.
GA 6	Use an objective, unbiased and non-manipulative approach in collection and interpretation of scientific data and avoid plagiarism and violation of Intellectual Property Rights. Appreciate and be sensitive to environmental and sustainability issues and understand its scientific significance and global relevance.
GA 7	Translate academic research into innovation and creatively design scientific solutions to problems. Exemplify project plans, use management skills and lead a team for planning and execution of a task.
GA 8	Understand cross disciplinary relevance of scientific developments and relearn and reskill so as to adapt to technological advancements.

PROGRAM OUTCOMES

PO	Description
A student completing Master's degree in Science Program in the subject of chemistry will be able to :	
PO1	Acquire in-depth knowledge of the advance concepts in the branch of specialization viz, Physical , Inorganic , Organic & Analytical.
PO2	Design and carry out analysis as well as accurately record and analyse the results.
PO3	Explain the findings and share the results with scientists and non scientist with the help of the written and oral communication skills acquire during the course.
PO4	Apply the skills to do specialized research in the core and applied areas of chemical sciences.
PO5	Explore new areas of research in chemistry and allied fields of science and technology.
PO6	Demonstrating the developed skills such as problem solving approach , critical thinking , analytical reasoning ,team work and effective communication for solving the applied research problems related to their field.
PO7	Explain why chemistry plays an integral role in addressing social , economic and environmental problems.
PO8	Become professionally skilled for higher studies in research institutions and to work in industries.

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	Spectral Methods-I	4	15
	II	Hyphenated Techniques		15
	III	Thermal and Radioanalytical Methods		15
	IV	Electroanalytical methods		15
RPSCHEP303	I	Atomic structure	4	15
	II	Atomic spectroscopy		15
	III	Molecular Structure		15
	IV	Molecular spectroscopy		15
RPSCHEPEC-I304	I	Advances in Nanomaterials	4	15
	II	Advanced electrochemistry		15
	III	Statistical Mechanics		15
	IV	Nuclear Chemistry		15
RPSCHEPEC-II304	I	Miscellaneous spectral methods	4	15
	II	Advanced electro-analytical chemistry -I		15
	III	Advanced electro-analytical chemistry -II		15
	IV	Mass Spectrometry and Raman Spectroscopy		15
RPSCHEP3P1		Practical	8	16
RPSCHEP3P2				
RPSCHEP3P3				
RPSCHEP3P4				

Semester IV				
Course Code	**Unit**	**Topic**	**Credits**	**Lectures**
RPSCHEP401	I	Polymer Chemistry-II	4	15
	II	Computational Chemistry		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		15
	III	ESR and Mossbauer Spectroscopy		15
	IV	Catalysis		15
RPSCHEPOC-I404	I	Intellectual Property Right -I	4	15
	II	Intellectual Property Right -II		15
	III	Cheminformatics-I		15
	IV	Cheminformatics-II		15
RPSCHEPOC-II404	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
RPSCHEP3P1	Practical		8	16
RPSCHEP3P2				
RPSCHEP3P3				
RPSCHEP3P4				

Detail Syllabus

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

Course objective:

- The basic objective of the first unit of this paper to acquire a basic knowledge of the properties of polymers and types of polymerization.
- The second unit of this paper aims to know about surfactants and their behaviour in the solution.
- The third unit aims at enabling the student to describe and explain photochemical and photo physical processes using Jablonski diagram and their quantum yield expressions. Students will be able to understand the nature of the photochemical reaction.
- The fourth unit makes student understand the photo physical processes involved in the emission of photons as fluorescence and its applications.

Course Outcome:

After completing this course, the student will be able to:

- Understand molar mass of polymer using different methods.
- Distinguish the various types of polymers.
- Classify the surfactants by their process of formation.
- Know about the various applications of surfactant in different fields.
- Describe the various deactivation processes of molecular excited states.
- Describe the photochemical reactivity of ethenes and carbonyl compounds.
- Give the application of Fluorescence Phenomena.

Unit I	**Polymer Chemistry-I** **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 (homochain,heterochain),the formation(condensation, addition), homo polymers, co polymers(random, alternate, block, graft),the behaviour on application of heat (thermoplastic and (thermosetting),the form and application (plastics, fibre, elastomersandresins). **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.	**(15L)**

	1.3 Types of polymerization: condensation, addition (cationic and anionic) and copolymerization (with kinetics), chain transfer reactions.	
Unit-II	**Modern Applications of Surface Chemistry** **2.1 Surface active agents and micelle:** **Surface-active agents** and their classification, hydrophile-lipophile balance. **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. **Emulsions**: Solubilisation, micro emulsions, characterization of microemulsions, **2.2 Hydrogen storage by Adsorption:** **Hydrogen storage**: fundamentals physisorption, temperature and pressure influence, chemisorption, adsorption energy, 'Electrochemical' adsorption. **Practical adsorption**: storage of hydrogen with carbon materials, activated carbon, graphite graphene, carbon Nano structures, fullerene. Carbon Nano fibres (CNF) and graphite Nano fibres electrochemical storage of hydrogen in carbon materials.	**(15 L)**
Unit-III	**Photo Chemistry-I** **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.	**(15L)**
Unit-IV	**Applications of Fluorescence Phenomena** **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.	**(15L)**

Reference Books:

1. P. Bahadur and N.V. Sastry, Principles of Polymer Science, 2nd Edition, Narosa Publishing House, 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. Vishwanathan and J. Shreedhar, Polymer Science, New Age International Pvt. Ltd., New Delhi, 1990.
5. M.J. Rosen, Surfactants and Interfacial Phenomena, 3rd Edition, John Wiley, 2004.
6. Y. Moroi, Micelles: Theoretical and Applied Aspects, Plenum Press, New York, 1992.
7. Tushar K. Ghosh, Energy Resources and Systems: Volume 2, Springer Link: Bucher, Springer, 2011.
8. R. Strobel, J. Garche, P.T. Mosely, L.J'orrisen, G. Wolfd, "Review Hydrogen Storage by Carbon Materials", Journal of Power Sources, June 2006
9. C.H. De Puy, O.L.Chapman, Molecular reactions and photochemistry, 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 Publications, 2006.

SEMESTER-III

Paper II

Course Code: RPSCHEP302

Credits: 4

Advanced Instrumental Techniques

Course Objectives:

- Learner in his lower classes has encountered with the basic concept and application of various surface analytical techniques (such as SEM, TEM, and AFM), Atomic emission spectroscopy & Voltammetry. At the M.Sc.-II level, the learner should know the recent developments in these fields, which will enable them to attain industrial readiness.
- The unit one introduces the learner to the surface analytical techniques, electron spectroscopy and NQR. The unit two aims at introducing the learner to the hyphenated techniques, which will bridge the gap between the academic and industry.
- The unit three focuses on thermal methods and radiochemical methods. The unit four deals with electroanalytical methods (voltammetry).
- Voltammetry includes various types. As a whole, the unit four has been detailed as the methods, instrumentation, various types of microelectrodes and their working. Apart from the general coverage, importance is given to the study of organic systems by electrochemical methods.
- Modern techniques used for chemical analysis and mechanistic studies are introduced so that real world analysis problems can be investigated. Focus will be on analytical applications of these techniques and utilizing the correct technique for solving specific analysis problems.

Course Outcome:

After studying this course, the students will be able to-

- Understand the basic working principles and applications of surface analytical techniques (such as SIMS, PIXE) electron spectroscopy and Nuclear Quadrupole Resonance.
- Assess the advantages of development of hyphenated techniques and the different types of interfaces that are used to achieve this hyphenation.
- Know the essential principles underlying the applications of thermal methods and radiochemical methods.
- Develop a working knowledge of various methods used in Voltammetry.
- Explain anodic, cathodic and adsorptive stripping methods in voltammetry.

- Select a suitable method of voltammetry for the analysis of a particular sample.

Unit I	**Spectral Methods-I** **1.1.** Surface Analytical Techniques: Preparation of the surface, difficulties involved in the surface analysis. **1.2.** Principle, instrumentation and applications of the following: i) Secondary Ion mass spectroscopy ii) Particle-Induced X-Ray Emission. **1.3.** Electron Spectroscopy**:** principles, instrumentation and applications of the following ESCA (XPS), AUGER, UPS **1.4.** Nuclear Quadrupole Resonance (NQR), ENDOR, ELDOR.	**(15L)**
Unit-II	**Hyphenated techniques:** **2.1** Introduction, need for hyphenation, possible hyphenations. **2.2** Principle, Interfacing devices, instrumentation and applications of the following- GC-MS, GC-IR, MS-MS, Tandem Mass Spectrometry, LC – MSHPLC-MS, ICP-MS, Head space GC, Spectro-electrochemistry and radio chromatography.	**(15 L)**
Unit-III	**Thermal and Radioanalytical methods** **3.1** Enthalpimetric methods and thermometric titrations. **3.2**Thermal analysis- Principle, Interfacing, instrumentation and Applications of Simultaneous Thermal Analysis- TG-DTA and TG-DSC **3.3** Evolved gas analysis- TG-MS and TG-FTIR **3.4** Activation analysis- NAA, radiometric titrations and radio-release methods Radiometric titrations and Applications **3.5** Auto, X-ray and Gamma Radiography.	**(15L)**
Unit-IV	**Electroanalytical Methods** **4.1** Current Sampled (TAST) Polarography, Normal and Differential Pulse Polarography, Differential double Pulse Polarography **4.2** Potential Sweep methods- Linear Sweep Voltammetry and Cyclic voltammetry. **4.3** Potential Step method- Chronoamperometry **4.5** Stripping Voltammetry- anodic, cathodic, and adsorption **4.6** Chemically and electrolytically modified electrodes and ultra- microelectrodes in voltammetry, **4.7** Applications of electrochemical methods in Organic synthesis.	**(15L)**

Reference Books:

1. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann, 5th Edition (1998).
2. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A. Settle Jr 7th Ed CBS (1986).
3. Introduction to Instrumental Analysis, R. D. Braun, Mc Graw Hill (1987).

4. Analytical Chemistry, G. D. Christian, 4th Ed. John Wiley, New York (1986).
5. Fundamentals of Analytical Chemistry, D .A. Skoog, D. M. West, and F. J. Holler Holt-Saunders 6th Edition (1992).
6. Electroanalytical Chemistry, Ed A. J. Bard and Marcel Dekker, New York, (A series of volumes).
7. Electroanalytical Chemistry, J.J. Lingane, 2nd Ed Interscience, New York (1958).
8. Modern Polarographic Methods in Analytical Chemistry, A. M. Bond, Marcel Dekker, New York, 1980.
9. Introduction to polarography and allied techniques by Kamla Zutski 2006.
10. Surface Analysis –The Principal Techniques, 2nd Edition Edited by John C. Vickerman and Ian S. Gilmore 2009 John Wiley & Sons, Ltd. ISBN: 978-0-470-01763-0.
11. NMR, NQR, EPR, and Mössbauer Spectroscopy in Inorganic Chemistry *R. V. Parish.* Ellis Horwood, Chichester

SEMESTER-III

Paper-III

Course Code: RPSCHEP303

Credits: 4

Atomic and Molecular: Structure and Spectroscopy

Course objectives:

- The basic objective of the first unit of this paper is to learn approximation methods in quantum chemistry used to find solution of Schrodinger equation for complex atomic and molecular structures.
- The second and fourth units of this paper aim to provide a thorough discussion on the basic principles and applications of Atomic and Molecular spectroscopy at the advanced level.
- The third unit explains the theories of chemical bonding like valence bond theory, molecular orbital theory and Hückel theory using the principles of quantum chemistry.

Course Outcome:

After completing this unit, the student will be able to:

- Solve the Schrodinger equation for complex system.
- Understand molecule formation with different theories and comparison.
- Explain the general principles and theory of spectroscopy
- Distinguish the specialties and applications of various types of spectroscopic methods

Unit I	**Atomic structure** Introduction to approximate methods in Quantum Mechanics- **1.1 Variation Method**: Variation Theorem, extension of the variation method, determinants, simultaneous linear equations, linear variation functions. **1.2 Perturbation Theory**: Nondegenerate Perturbation Theory, first order wave function correction, first order and second order energy correction. Perturbation treatment of the Helium atom ground state, Variation treatment of the Helium atom ground state, Perturbation Theory for a degenerate energy level **1.3 Multielectron atoms**: Independent electron approximation, electron spin, spin statistic theorem, symmetric and antisymmetric wave function, the Pauli exclusion principle, slater determinants. **1.4 Hartree's method:** Hartree Folk method, Slater type orbitals, orbital energies	**(15L)**
Unit-II	**Atomic spectroscopy**	**(15 L)**

	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 **2.2** Term symbols, term symbols for multi electron atoms like He, Li, Be, B etc. **2.3** Exchange of interactions and multiplicity of states. **2.4** Anomalous Zeeman Effect and Paschen Back effect. **2.5** Atomic spectra and selection rules, energy level diagram of atomic sodium.	
Unit-III	**Molecular Structure** **3.1 Chemical Bonding:** The Born–Oppenheimer approximation, LCAO method-molecular orbital formation **3.2 Molecular Orbital theory:** MO theory of bonding in hydrogen molecule ion and hydrogen molecule, physical interpretation of bonding and antibonding molecular orbital, calculation of ground state energy, excited state of H_2 singlet and triplet state. **3.3 Valence bond theory:** Heitler-London treatment to hydrogen molecule, resonance, antisymmetric wave function and nature of bonding. Heitler-London Slater Pauling theory. **3.4 Principle of hybridisation:** Directed valence & hybridization in simple polyatomic molecules. (sp, sp^2 and sp^3 hybridisation). **3.5 Hückel theory:** Hückel molecular orbital's Theory for–ethylene, Allyl system, cyclopropenyl, linear butadiene, cyclobutadiene and benzene system.	**(15L)**
Unit-IV	**Molecular Spectroscopy** **4.1 Rotational spectroscopy:** Classification of poly atomic Molecules spherical top, symmetric top and asymmetric top molecules, intensity of spectral lines, non-rigid rotor, spectrum of non-rigid rotor, rotational Spectra of polyatomic molecules, Stark effect, Information derived from the rotational spectra. **4.2 Raman Spectroscopy:** Theory of Raman scattering, quantum theory classical theory of molecular polarizability, pure Rotational Raman spectra, Vibrational Raman spectra, polarization and depolarization of Raman lines, structure determination using IR and Raman spectroscopy (example: XY_2, XY_3 and XY_4), instrumentation. **4.3 Electronic Spectra of molecules:** Introduction, vibrational course structure, progressions and sequences, Frank Condon principle, intensity of vibrational electronic spectra, term symbols for linear molecules, selection rules, dissociation and Predissociation, types of electronic transitions-d-d, vibronic, charge transfer, π-π^*, n-π^*transitions, fate of electronically excited states.	**(15L)**

Reference Books:

1. Atkins P.W, Physical Chemistry, Oxford University Press,6th edition,1998.
2. R. K. Prasad, Quantum Chemistry,3rd Ed., New Age International Publishers,2006.
3. A. McQuarrie, Quantum Chemistry, Viva Books Private Limited, New Delhi, first Indian ed., 2003.

4. M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers, 2001.
5. A.K.Chandra, Introductory QuantumChemistry,4McGrawH edition(1994),Tata McGraw-Hill, New Delhi.
6. I.N. Levine, Quantum Chemistry, 5th 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. Mc Cash, Fundamentals of Molecular Spectroscopy, 4th Ed., Tata-McGraw-Hill, 1994.
9. H.S. Randhawa, Modern Molecular Spectroscopy, McMillan India Ltd., 2003
10. G.Aruldas, Molecular Structure and Spectroscopy, Prentice-HallofIndia, 2001.
11. Donald L. Pavia, Gary M. Lampman and George S. Kriz, Introduction to Spectroscopy, 3rd Ed., Thomson, Brooks/Cole, 2001.

Semester III

Paper IV

Course Code: RPSCHEPEC-I304

Credits: 4

Nano-chemistry, Applied Electrochemistry, Statistical Mechanics & Nuclear Chemistry

Course Objective:

- The basic objective of the first unit of this paper is to recapitulate the various aspects of nanomaterials by student, also their types, application of nanomaterial in research, preparation of nanomaterial is learned through this unit.
- Second unit of this paper significantly underlies application of electrochemistry such as electroplating, batteries and fuel cells wherein student learns elaborately various aspects of these applications.
- Third unit makes student aware of the statistical mechanical relation between bulk properties by classical thermodynamics and microscopic property by statistical thermodynamics.
- Fourth unit makes student aware of the particle accelerators, nuclear models and various applications of nuclear radiations.

Course Outcomes:

After completing this course, the student will be able to:

- Perceive the concept of nanomaterials and preparation of various nanomaterials and apply these concepts in the research of material science
- Understand the concept of applications of electrochemistry in energy creation which is need of new age by fuel cells, batteries etc
- Apply the concept of probability to the thermodynamic properties at micro level
- Derive Maxwell-Boltzmann, Fermi-Dirac statistics.
- Understand how does particle accelerators work viz. Linear, cyclotron.
- Comprehend the concept of nuclear model's Liquid drop, Fermi gas, Shell, Optical etc.
- Know applications of nuclear radiations in pharma, geology, industry.

Unit I	**Advantages in nanomaterials** **1.1: Types of nanomaterials** e.g. nanotubes, nanorods, solid spheres, core-shell nanoparticles, mesoporous materials, General preparative methods for various nanomaterials	**(15L)**

	1.2 Important properties on nanomaterials: optical properties of metal and semiconductor nanomaterials, magnetic properties **1.3 Some special nanomaterials:** **Carbon nanotubes-** Types, synthesis using various methods, growth mechanism, electronic structure. **Porous Silicon**- Preparation and mechanism of porous silicon formation, factors affecting porous structure, properties of porous silicon. **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	**Advanced Electrochemistry** **2.1 Kinetics of Electrode reactions (Electrodics):** Essentials of electrode reactions, Butler-Volmmer Model for electrode kinetics, One step, one electron process through potential energy diagram, standard rate constants and transfer coefficients, equilibrium condition and exchange current, current over potential equation, Tafel behaviour. Mass transfer by migration and diffusion, Fick's Law **2.2 Electrochemical device**s: Batteries, Fuel cells, photo electrochemical and dye sensitized solar cells, electrochemical super capacitors, and ion-selective electrodes. **2.3 Corrosion:** Mechanism, Potential – pH diagram, Measurement of corrosion rates, corrosion inhibition-anodic and cathodic protection, passivation.	**(15 L)**
Unit-III	**Statistical Mechanics** **3.1Thermodynamic probability:** combinatorial problems, Stirling approximation**,** Lagrange's 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 heats of solids	**(15L)**
Unit-IV	**Nuclear Chemistry** **4.1 Charged particle accelerator-** linear accelerator, cyclotron, Betatron, Synchro-cyclotron, 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	**(15L)**

	Agricultural applications of radiochemistry, positron emission tomography, Radio immune assay.	

Reference Books:

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 IV

Course Code: RPSCHEPEC-II304

Credits: 4

Modern Methods in Instrumental Analysis

Course Objectives:

- The learner has been introduced to spectroscopy and electroanalytical chemistry in their lower classes.
- This course aims at giving an advanced understanding of these self-same topics, building on concepts previously learnt.
- Unit I of the course describes some miscellaneous topics such as Reflectance IR spectroscopy, photoacoustic spectroscopy, Chemiluminescence methods, and polarimetry.
- The learner at the M.Sc.- II level should be aware of some intriguing methods that have been used for chemical analysis besides the conventional methods that were covered in M.Sc.-I level.
- The second and third unit covers advanced electro-analytical technique, which acquaints the learner with the modern methodology.
- They are introduced to the electrodes currently in use in academic as well as industrial research and explore their superiority over the classical three electrodes set up of Polarography.
- Further, they are introduced to pulsed methods, cyclic voltammetry etc, all of which are used in analysis in routine labs.
- The fourth unit covers modern methods in Mass spectrometry and Raman spectroscopy. The learner will be equipped with the knowledge to interpret mass spectra, and the contemporary techniques in Raman Spectroscopy namely Surface Enhanced and Resonance Raman spectroscopy will be introduced.
- The learner at this stage should be able to correlate how these classical techniques have been adapted and enhanced for their efficient use in routine analysis.

Course Outcome:

After studying this course, the students will be able to-

- Understand the basic working principles and applications of reflectance methods, photoacoustic spectroscopy, Chemiluminescence methods, and polarimetry.

- Understand the advantages of modified electrodes over the classical polarographic methods.
- Develop a working knowledge of various methods used in modern voltammetry.
- Explore some enhanced Raman spectroscopy techniques, namely Surface Enhanced Raman and Resonance Raman Spectroscopy.
- Interpret mass spectra of molecules, recognize metastable ion peaks, and correlate peak presence with possible fragmentation mechanisms to arrive at the structure.

Unit I	**Miscellaneous Spectral Methods** Principle, Instrumentation and Applications of: **1.1.** Reflectance spectroscopy **1.2** Photoacoustic spectroscopy **1.3** Polarimetry: ORD, CD **1.4** Chemiluminescence methods	**(15L)**
Unit-II	**Advanced Electroanalytical Chemistry – I** **2.1** Overview of electrode processes: electrocapillary curve and electro-capillary maximum potential **2.2** Microelectrodes: mercury electrodes, stationary mercury drop electrodes (SMDE), hanging mercury drop electrodes (HMDE), mercury film electrodes (MFE), carbon paste electrodes and chemically modified electrodes. **2.3:** Three electrode systems in modern Polarography, necessity for and development of new voltammetric techniques and their comparison with classical DC Polarography.	**(15 L)**
Unit-III	**Advanced Electroanalytical Chemistry – II** **3.1** Voltammetric methods: Sampled DC Polarography, Linear Sweep voltammetry, cyclic voltammetry, diagnostic criteria of cyclic voltammetry. **3.2** Pulsed techniques in Polarography: Normal pulse Polarography, differential pulse Polarography, double differential pulse Polarography. **3.3** Sinusoidal AC polargraphy, Square wave Polarography **3.4** Applications of electrochemical methods in Organic synthesis.	**(15L)**
Unit-IV	**Mass Spectrometry and Raman Spectroscopy** **4.1 Mass spectroscopy:** recapitulation, correlation of mass spectra with molecular structure- interpretation of mass spectra, analytical information derived from mass spectra- molecular identification, meta stable peaks, Fragmentation Reactions **4.2 Raman spectroscopy:** Principle Theory Instrumentation techniques (SERS and Resonance Raman) and Applications of Raman spectroscopy	**(15L)**

Reference books:

1. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and J.A. Niemann, 5th Edition (1998).
2. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt Jr, J. A. Dean and F. A.

Settle Jr 7th Ed CBS (1986).
3. Introduction to Instrumental Analysis, R. D. Braun, Mc Graw Hill (1987).
4. Analytical Chemistry, G. D. Christian, 4th Ed. John Wiley, New York (1986).
5. Fundamentals of Analytical Chemistry, D .A. Skoog, D. M. West, and F. J. Holler Holt-Saunders 6th Edition (1992).
6. Electroanalytical Chemistry, Ed A. J. Bard and Marcel Dekker, New York, (A series of volumes).
7. Electroanalytical Chemistry, J.J. Lingane, 2nd Ed Interscience, New York (1958).
8. Modern Polarographic Methods in Analytical Chemistry, A. M. Bond, Marcel Dekker, New York, 1980.
9. Introduction to polarography and allied techniques by Kamla Zutski 2006.

Practical

SEMESTER-III

Credits: 8

RPSCHEP3P1
1. To estimate the amount of hydrochloric acid and acetic acid in a mixture by titration with an alkali using a pH meter. 2. To determine ΔG, ΔH and ΔS of dissolution of a sparingly soluble salt by conductometry. 3. To titrate potassium ferrocyanide with zinc sulphate and hence to determine the formula of the complex. (Potentiometrically) 4. Dissociation constant of an acid- base indicator by spectrophotometry. 5. Thermodynamic data of electrochemical cell by e.m.f. measurements. 6. Simulations determination of $KMnO_4$ and $K_2Cr_2O_7$ by spectrophotometry.
RPSCHEP3P2
1. To determine the formula of the copper (**II**) ammonia complex by partition method. 2. Molecular weight of a polymer by end group estimation. 3. Determination of the energy of activation and other thermodynamic parameters of activation for the acid catalysed hydrolysis of methyl acetate. 4. To study the order of the reaction between bromate and bromide. 5. To estimate the amount of a salt of an organic acid/ sparingly soluble salt like magnesium carbonate by ion exchange chromatography. 6. To measure the radius of glycerol molecule.
RPSCHEP3P3
1. To determine K_1 and K_2 of a dibasic acid by titration with a base. 2. To determine the composition of a mixture of hydrochloric acid, potassium chloride and ammonium chloride by titration with sodium hydroxide and silver nitrate. 3. To determine the E^0 of the quinhydrone electrode. 4. To determine the ionization constant of bromophenol blue. 5. To determine dissociation constant of p-nitro phenol. 6. To determine the proton ligand stability constant of an organic acid and metal ligand stability constant of its complex by pH measurement.
RPSCHEP3P4
1. To determine the isoelectric point of gelatine by viscosity measurement.

2. Hydrolysis constant of aniline hydrochloride by distribution coefficient method.
3. Effect of salt on the distribution of acetic acid between water ethyl acetate.
4. To determine the effect of ionic strength of a solution on the reaction between potassium persulphate and potassium iodide.
5. To investigate reaction between H_2O_2 and KI.
6. To study the effect of the extended conjugation on the λmax of p-nitro phenol by recording spectrum in acidic and alkaline medium

Reference books:

1. Practical Physical Chemistry, A. Findary, T.A. Kitchner (Longmans, Green and Co)
2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.R. Denko, R.M.W. Richett (Pergamon Press)
3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi)

SEMESTER –IV

Paper-I

RPSCHEP401

Credits: 4

Chemistry: Polymer, Green, Biophysical and Applied.

Course objectives:

- The objective of the first unit of this paper to learn techniques of Identification and characterization of polymers.
- The second unit of this paper gives information of advance method in quantum mechanics.
- The third unit gives an idea about biophysical and green chemistry.
- The fourth unit of this paper used to formulate the macroscopic and quantum laws of the absorption of light by molecules and solids.

Course Outcome

After completing this unit, the student will be able to:

- Correlate Macromolecules and their properties, catalyst and its characterization.
- Account for the fundamental background of Density Functional Theory
- Explain the Hohenberg-Kohn theorems and their application.
- Understand photo physical kinetics of unimolecular and bimolecular processes using Stern-Volmer kinetics.
- Understand physical chemistry involved in biological process.
- Account for the different interactions that are important for the formation of structures in biological systems and for how thermodynamic parameters can be measure.
- Know the different techniques of electrophoresis.
- Understand the important uses of the solar cell.

Unit I	**Polymer Chemistry-II** **1.1 Polymers in solid state** – Transitions (glass transition and crystalline melting temperature), crystalline behaviour, 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.	**(15L)**

	1.3 Properties of polymers: Thermal (glass transition temperature, and its determination), mechanical (deformation and fracture) effects in polymers, viscoelasticity surface (surface tension, hardness, friction, abrasion), physical (Impact strength, Tensile strength, solubility) of polymers, weather ability, rheology and mechanical models, mechanical behaviour, Rubber elasticity, **1.4 Polymer degradation and stabilization**: Oxidative, thermal, radiation, Biodegradation	
Unit-II	**Computational Chemistry** **2.1 Semi-empirical Theories:** Recapitulation of Hückel method, extended Hückel method, ZDO approximation, CNDO/INDO methods, Molecular Properties, Computational aspects, **2.2 Density Functional Theory:** Introduction, Hohenberg-Kohn Theorem, N and V representability, Levy Functional, Kohn Sham equations, Functional derivatives and local potentials, Thomas Fermi theory, The Kohn-Sham construction, Fractional occupation numbers, Janak's theorem.	**(15 L)**
Unit-III	**Biophysical Chemistry and Green Chemistry** **3.1 Biophysical Chemistry** **Introduction to Complex Biomolecules:** Proteins, enzymes, DNA, RNA, polysaccharides and lipids. chirality and pH dependence of biomolecules. **Biosensors:** Enzyme based, Electrochemical, immunosensor, fluorescence, optical, Piezoelectric Biosensors. **Electrophoresis (Technique for bio-molecular study):** Principle and factors affecting electro-phoretic mobility, zone electrophoresis–Paper electrophoresis, cellules acetate electrophoresis, Gel electrophoresis. Capillary Electrophoresis, Application of electrophoresis. **3.2 Green Chemistry:** Recapitulation of principles of green chemistry, Waste minimization techniques. Catalysis and Green Chemistry: Phase transfer catalysts, biocatalyst, photo catalysis. Organic solvents, solvent free system, supercritical fluid, ionic liquid, their characteristics, use as catalyst and solvents. Alternative energy sources for initiation and execution of chemical reaction: Microwave and sonochemistry.	**(15L)**
Unit-IV	**Photochemistry-II: Kinetics and Applications** **4.1 Photophysical Kinetics of bimolecular processes.** Mechanism of fluorescence quenching, Collisions in solutions, Kinetics of collisional quenching and Stern-Volmer equation and deviations from Stern Volmer equation, Concentration dependence of quenching and excimer formation, quenching by added substances–charge transfer mechanism and energy transfer mechanism. **4.2 Solar Cells:** photovoltaic and photo galvanic cells; photoelectron chemistry; prospects of solar energy conversion and storage, organic solar cells.	**(15L)**

Reference Books:

1. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition,Narosa Publishing House,2005.
2. C. E. Carraher, Jr., Carraher's Polymer Chemistry, 8thedition, 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. U.N Dash,. A Text Book of Biophysical Chemistry, Macmillan India Ltd
6. Gurtu and Gurtu, Biophysical Chemistry, Pragati Prakashan.
7. Mike Lancaster, Green Chemistry an Introductory Text, Royal Society of Chemistry.
8. K.K.Rohatgi- Mukherjee. Fundamentals of Photochemistry. Reprint 2002. New Age International Publisher, 1978.
9. Approximate Molecular Orbital Theory, J. A. Pople and D. L. Beveridge, McGraw Hill, New York (1971)
10. Molecular Modelling, A. Leach, Longman, Landon (1996)

Semester IV

Paper-II

RPSCHEP402

Credits: 4

Material Sciences and Non-equilibrium Thermodynamics

Course Objective:

- The basic objective of the first unit of this paper is to introduce the aspect of solid-state chemistry in detail by student to understand applications of XRD.
- Second unit of this paper gives clear idea about instrumental methods like XRD and they must learn its different types of XRD.
- Third unit of this paper makes student aware of lasers, its generation's types and applications in different fields.
- Fourth unit of this paper makes student aware of Non-equilibrium thermodynamics and Onsager's theory.

Course Outcomes:

After completing this course, the student will be able to:

- Understand the concept of bonding and structure of crystalline solids.
- Explore different types of lattices, unit cells and defects in crystal in detail
- Understand structure determination by powder diffraction and single crystal X-ray diffraction.
- Understand concept of lasers in chemistry, generations, characteristics and types of lasers.
- Describe applications of lasers in chemistry such as spectroscopy, isotope separation, and kinetics of fast reactions.
- Understands Band theory, superconductors how do they work and magnetic properties.
- Understands second law of thermodynamics at non-equilibrium i.e. entropy production and rate. Also, comprehend principle of microscopic reversibility and transport phenomena across membranes

Unit I	**Solid State Chemistry** **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, Lattices and unit cells. **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. **1.5** Defects and non-stoichiometry: point defects, plane defects, line defects. Solid solutions Diffusion in solids: Mechanisms, Steady state and non-steady state diffusion, factors affecting diffusion.	**(15L)**
Unit-II	**Instrumental Methods** **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.	**(15 L)**
Unit-III	**Lasers and Super conductors** **3.1 Lasers in chemistry** **General principles of LASER action**-Population Inversion, cavity and mode characteristics, Q-switching, Mode locking. **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**.** **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.	**(15L)**
Unit-IV	**Non-equilibrium thermodynamics**: **4.1** Features of non-equilibrium thermodynamics, second law of thermodynamics, uncompensated heat and its relation to thermodynamics function.	**(15L)**

	4.2 Entropy production and its rate. Entropy production in heat transfer process and during mixing of gases. Entropy production and efficiency of galvanic cell. **4.3** Onsager's theory: Reciprocal relation, principle of microscopic reversibility. **4.4** Coupled and uncoupled reactions and their condition. **4.5** Transport phenomena across membranes. Electro kinetic effect and thermo mechanical effects.	

Reference Books:

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.

SEMESTER-IV

Paper-III

Course Code: RPSCHEP403

Credits: 4

Symmetry, Spectroscopy and Catalysis

Course objectives:

- The objective of the first unit of this paper is to learn about the point groups, character table and basic application of symmetry in spectroscopy and chemical bonding. Also, to learn the selection rule for Infrared and Raman-active transitions.
- The objective of second and fourth unit of this paper is to know how nuclear spins are affected by a magnetic field, and be able to explain what happens when radiofrequency radiation is absorbed.
- Student will be enabled to predict the number of proton and carbon NMR signals expected from a compound given its structure and further, predict the splitting pattern in the proton NMR spectrum of a compound given its structure.
- The third unit makes students understand the hyperfine parameters, recoil energy, quadrupole splitting and chemical shift /isomer shift by using Mossbauer spectroscopy.

Course Outcome

After completing this unit, the student will be able to:

- Describe the selection rule for infrared-active transitions.
- Determine whether the molecular vibrations of a triatomic molecule are Raman active.
- Students will be able to analyse the hybridization of given compounds.
- Understand the concepts of equivalent and non-equivalent hydrogens.
- Understand the effect of structure on chemical shift and coupling constants.
- Elucidate the electronic structure of free radicals and paramagnetic transition metal complexes.
- Study the magnetic properties of the materials and its order of orientations.

Unit I	**Symmetry in Chemistry** **1.1** Recapitulation of Points groups and Character tables. **1.2** Applications of Group theory in Infrared and Raman spectroscopy. Molecular Vibrations, determining the Symmetry Types of the Normal Modes; symmetry-based Selection Rules of IR and Raman, application in Infrared and Raman spectroscopy for molecules belongs to point group C_{2v}, C_{3v}, C_{4v}, D_{2h} , D_{3h} , $D_{\infty h}$ and T_d. **1.3** Group theory and quantum mechanics. Wave function as bases for irreducible representation.	**(15L)**

	1.1 Symmetry Adapted Linear Combinations - (SALC) - projection operators and their use to construct SALC. **1.6** Molecular Orbital Theory. Transformation properties of atomic orbitals, MO's for Sigma and pi - molecular orbitals in AB_n molecules, AB_4 (tetrahedral) and AB_6 (octahedral) molecules, Hybrid orbitals.	
Unit-II	**N.M.R. Spectroscopy** **2.1 Nuclear Magnetic Resonance (NMR) Spectroscopy:** Nuclear spin and its interaction with applied field, population of energy state, relaxation time, ^1H NMR Spectroscopy: Chemical Shift; Multiplet Splitting of NMR peaks arises through Spin–Spin Coupling, Multiplet Splitting when more than two spins interact. **2.2 Pulse technique in NMR:** The magnetization vector, spin-spin relaxation, spin-lattice relaxation. **2.3 ^{13}C NMR Spectroscopy:** Fourier Transform NMR; Off-Resonance and Spin-Decoupled, DEPT, Applications, 2-D NMR Spectroscopy (COSY). Nuclear Overhauser Effect Spectroscopy (NOESY). **2.4** Solid-state NMR **2.5** Magnetic Resonance Imaging (MRI); **2.6** NMR Spectroscopy of ^{19}F, ^{15}N and ^{31}P nuclides.	**(15 L)**
Unit-III	**ESR and Mossbauer Spectroscopy** **3.1 Electron spin Resonance Spectroscopy-** **3.1.1** Basic principle, hyperfine splitting (isotropic systems); **3.1.2** g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); **3.1.3** An isotropic effect (the g-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes. **3.2 Mossbauer Spectroscopy:** Basic principles of Mössbauer spectroscopy, instrumentation, spectral parameters a) Mössbauer Parameters- Isomer Shifts, quadrupole splitting, Magnetic hyperfine interaction. b) Application of Mössbauer spectroscopy with respect to i) Oxidation states of metal ion in compounds ii) Structural elucidation iii) Covalent and ionic compounds iv) High spin low spin behaviour	**(15L)**
Unit-IV	**Catalysis** **4.1** Introduction, history and importance of catalysis, concept of activity, selectivity, poisoning, promotion, turnover number and deactivation, **4.2** Types of catalysis: homogeneous catalysis: examples of homogeneous catalysis in gas phase, and in solution phase, acid-base catalysis.	**(15L)**

	4.3 heterogeneous catalysis: heterogeneous catalysis with gaseous reactants, liquid reactants, and gaseous reactants, biocatalysis, autocatalysis, negative catalysis, characteristics of catalytic reactions, activation energy and catalysis, theories of catalysis: the intermediate compound formation theory, the adsorption theory **4.4** Mechanism of heterogeneous catalysis, kinetics of heterogeneous catalytic reactions, Langmuir-Hinshelwood model, Catalysis by semiconductors, Boundary Layer theory, Wolkenstein's theory, **4.5** Preparation and Characterisation of Catalysts: General methods of preparation of catalysts: precipitation, sol-gel, hydrothermal, impregnation, hydrolysis, vapour deposition. Activation of catalysts: calcinations, reduction. Catalyst characterization: surface area, pore size distribution, particle size determination, XPS, AES, UV-Vis, FTIR and thermal methods	

Reference Books:

1. Heterogeneous Catalysis, D. K. Chakrabarty and B. Viswanathan, Hardcover - Oct 2008 New Age International Publishers).
2. Catalytic Chemistry, B. C. Gates, John Wiley and Sons Inc. (1992).
3. R.L.Carter, Molecular symmetry and Group theory, Wiley Student Ed., 1996, John Wiley and Sons, (Asia) Pvt.Ltd.
4. C.N.Banwell and E.M.McCash, Fundamentals of Molecular Spectroscopy, 4thEd., Tata-McGraw-Hill, 1994.
5. M. L. Gupta, Atomic and Molecular Spectroscopy, New Age International Publishers, 2001.
6. G. Aruldas, Molecular Structure and Spectroscopy, Prentice-Hall of India, 2001.
7. J.Michael Hollas, Modern Spectroscopy, 4thEd., John Wiley and Sons, 2004.
8. F. A. Cotton, Chemical applications of Group Theory, Wiley Student Ed., 2006, John Wiley and Sons, (Asia) Pvt.Ltd

SEMESTER-IV

Paper-IV

Course Code: RPSCHEPOC-I 404

Credits: 4

INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS

Course Objectives:

- This course aims to introduce the basic tenets of intellectual property rights and patent law.
- The learner, being in the final stage of their Master's course will be familiarized with the procedure of obtaining copyrights, trademarks, etc.
- The legal aspects of trade secrets, various legislation and role of the judiciary in the protection of intellectual property rights will also be explored.
- The course will further cover the use of computers in the application of chemical concepts via Cheminformatics such as in drug design, modelling structures, etc.
- The course aims to introduce the students to technical aids and software models imperative to research- both academic and industrial.

Course Outcome: At the end of this course, the learner is expected to:

- Be well versed with the concept of intellectual property and the terms involved with respect to Indian Patent Law.
- Distinguish between patents and copyrights.
- Understand the economic impact and legislature involved in Intellectual property rights.
- Learn about software tools pertaining to Cheminformatics and Molecular Modelling.
- Conduct structure and sub-structure search online, determine SMILES codes for various molecules.
- To gain knowledge about the application of the research-based tools.

Unit I	**Intellectual Property Rights-I** 1.1 **Introduction to Intellectual Property:** Historical Perspective, Different types of IP, Importance of protecting IP 1.2 **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. 1.3 **Industrial Designs:** Definition, how to obtain, features, International design registration. 1.4 **Copyrights:** Introduction, how to obtain, Differences from Patents. 1.5 **Trade Marks:** Introduction, how to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc. 1.6 **Geographical Indications:** Definition, rules for registration, prevention of illegal exploitation, importance to India.	**(15 L)**

Unit-II	**Intellectual Property Rights-II** **2.1 Trade Secrets:** Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection. **2.2 IP Infringement issue and enforcement:** Role of Judiciary, Role of law enforcement agencies – Police, Customs etc. **2.3 Economic Value of Intellectual Property:** Intangible assets and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer. **2.4 Different International agreements:** - **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 - **Paris Convention** - **WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.	**(15 L)**
Unit-III	**Cheminformatics-I** **3.1 Introduction to Cheminformatics:** History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modelling and structure elucidation. **3.2 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. **3.3 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.	**(15L)**
Unit-IV	**Cheminformatics-II** **4.1** Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modelling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra. **4.2** 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. **4.3** Application of Cheminformatics in Drug Design.	**(15L)**

Reference Books:

1. Vivien Irish, Intellectual Property Rights for Engineers, 2nd Edition, British Library, 2008.
2. David I. Bainbridge, Intellectual Property, 8th Edition, Pearson, 2010.
3. Stephen Elias and Richard Stim, Patent Copyright & Trade Mark, 8th Edition, Nolo and Richard, 2013.
4. Johann Gasteiger and Thomas Engel, Chemoinformatics, Wiley-VCH, 2003.
5. Andrew R. Leach, Valerie J. Gillet, An Introduction to Chemoinformatics, Springer, 2007.
6. Barry A. Bunin, Jurgen Bajorath, Brian Siesel and Guillermo Morales, Chemoinformatics- Theory, Practice and Products, Springer, 2007.

SEMESTER-IV

Course Code: RPSCHEPOC-II 404

Credits: 4

RESEARCH METHODOLOGY

Course Objectives:

- This course aims to introduce the basic principles of scientific research.
- The student who will soon obtain a Master's degree in Science will be introduced to the systematic methodology of conducting fundamental research, right from literature surveys to developing a problem.
- They will be taught methods in statistical analysis of data pertaining to research, writing of research papers in the various formats available.
- Finally, they will be guided about laboratory safety protocols which are absolutely essential for the new research student.

Course Outcome: At the end of this course, the learner is expected to:

- Understand basics of research methodology
- Get the technical know-how of research from developing a problem.
- Be able to write a research paper, study formats of existing research papers and review papers
- Be aware about importance of lab-safety and the safety protocols in R&D laboratories.

Unit I	**Review of Literature** **1.1 Print:** Primary, Secondary and Tertiary sources. **1.2 Journals:** **1.3** 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. **1.4 Digital:** **1.5** 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, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus. **1.6 Information Technology and Library Resources:** **1.7** The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	**(15L)**
Unit-II	**Data Analysis** **2.1 The Investigative Approach:**	**(15 L)**

	Making and recording Measurements, SI units and their use, Scientific methods and design of experiments. **2.2 Analysis and Presentation of Data:** Descriptive statistics, choosing and using statistical tests, Chemometrics, 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, r and its abuse, basic aspects of multiple linear regression analysis	
Unit-III	**Methods of Scientific Research and Writing Scientific Papers** **3.1** Reporting practical and project work, writing literature surveys and reviews, organizing a poster display, giving an oral presentation. **3.2** 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.	**(15L)**
Unit-IV	**Chemical Safety & Ethical Handling of Chemicals** **4.1** 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 **4.2** 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.	**(15L)**

Reference Books:

1. C. R. Kothari, Research Methodology- Methods and techniques, New Age International (P) Limited Publisher, 2004.
2. Yogesh Kumar Singh, Fundamental of Research Methodology and Statistics, New Age International (P) Limited Publisher, 2006.
3. Carol Ellison, Concise Guide to Writing Research Ppaers, McGraw-Hill, 2016.
4. Introductory Statistics, Prem S. Mann, C. Jay Lacke, 7th Edition, John Wiley and Sons, 2010.
5. Statistics From A to Z - Confusing Concepts Clarified, Andrew A. Jawlik, John Wiley and Sons, 2016.

Semester –IV

Practical

Credits: 8

RPSCHEP4P1
1. To determine hydrolysis constant and degree of hydrolysis of ammonium chloride and hence to estimate the dissociation constant of the base. 2. To determine the liquid junction potential with a concentration cell with and without transference. 3. To determine the molar conductance of a weak electrolyte at infinite dilution hence to determine its dissociation constant. 4. Determination of energy of n to Π* transition in acetone and study of effect of solvent on energy of this transition by recording absorbance spectra in n-hexane and water. 5. Determination of isosbestic point of a given dye molecule by spectrophotometric method. 6. To determine the proton ligand stability constant of an organic acid and metal ligand stability constant of its complex by pH measurement.
RPSCHEP4P2
1. To determine the formula of the zinc (II) ammonia complex by partition method. 2. Determination of the chain linkage in poly (vinyl alcohol) from viscosity measurements. 3. To study the kinetics of the decomposition of hydrogen peroxide in presence of ferric chloride solution and hence to study the effect of the catalyst on the decomposition reaction. 4. To determine the rate constant and the order of the reaction between persulphate and iodide ions. 5. To determine the energy of activation and other thermodynamic parameters of activation for the reaction between persulphate and potassium iodide. 6. To determine the equilibrium constant for the reaction. $CaSO_4$ (s) + $2Ag^{+1}$ (aq) = Ag_2SO_4(s) + Ca^{-2} (aq)
RPSCHEP4P3
A. 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. Analysis of XRD pattern of cubic system 6. Interpretation of DTA, TG, and DTG curves **B. Use of plane-wave DFT based code: Quantum Espresso** **Part 1:** Using DFT for structure optimization or relaxation of structures and self-consistent field calculations for simple molecules or crystals.

Part 2: Interpretation of data from relaxation process, plotting of total and partial atom projected Density of States (DOS), obtaining band gap and deducing magnetic properties.
RPSCHEP4P4
Project Evaluation

Reference books:

1. Practical Physical Chemistry, A. Findary, T.A. Kitchner (Longmans, Green and Co)
2. Experiments in Physical Chemistry, J.M. Wilson, K.J. Newcombe, A.R. Denko, R.M.W. Richett (Pergamon Press)
3. Senior Practical Physical Chemistry, B.D. Khosla and V.S. Garg (R. Chand and Co., Delhi)

MODALITY OF ASSESSMENT

Theory Examination Pattern

A. Internal Assessment: 40%

<table>
<tr><td>Presentation</td><td>20 M</td><td>For each paper, students are evaluated from their presentation based on the topic selected from syllabus. The assessment of presentation is as follows:
<table>
<tr><td>Sr.no.</td><td>Evaluation Type</td><td>Marks</td></tr>
<tr><td>1</td><td>Presentation content</td><td>10</td></tr>
<tr><td>2</td><td>Presentation skills</td><td>05</td></tr>
<tr><td>3</td><td>Viva</td><td>05</td></tr>
<tr><td colspan="2">Total</td><td>20</td></tr>
</table></td></tr>
<tr><td>Continuous Internal Assessment (CIA)</td><td>20 M</td><td>e.g. Test, Group discussion, assignment, open-book tests etc.</td></tr>
</table>

B. External Examination: 60%

Semester end theory assessment worth 60 marks

i. Duration: These exams will be conducted for the duration of 2.5 hours.

ii. Paper pattern

1. There shall be 04 questions each of 15 marks. On each unit there will be one question.

2. All questions shall be compulsory with internal choice within the question.

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

Semester end practical examination: 50 marks per paper

Experimental work	40 M
Journal	05 M
Viva	05 M

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, 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

Theory Examination

Course		301	302	303	304
Marks	**Internal**	40	40	40	40
	External	60	60	60	60

Practical Examination

Course	P301	P302	P303	P304
Marks	50	50	50	50

Total : 600 marks

Semester: IV

Theory Examination

Course		401	402	403	404
Marks	**Internal**	40	40	40	40
	External	60	60	60	60

Practical Examination

Course	P401	P402	P403	P404
Marks	50	50	50	50

Total : 600 marks