Resolution Number: AC/I(21-22).2(II).RPS5

S.P.Mandali's

Ramnarain Ruia Autonomous College

Syllabus for Semester III & IV

Program: M.Sc. (Physical Chemistry)

Program code: RPSCHEP

(Credit Based Semester and Grading System from the academic year 2021–2022)

SEMESTER III			
Course Code	**Unit**	**Course Title / Unit Title**	**Credits**

RPSCHEP301	**Polymer, Surface & Photochemistry**		**4**
	I	Polymer Chemistry-I	
	II	Modern Applications of Surface Chemistry	
	III	Photo Chemistry-I	
	IV	Applications of Fluorescence Phenomena	
RPSCHEP302	**Advanced Instrumental Techniques**		**4**
	I	Spectral Methods-I	
	II	Hyphenated Techniques	
	III	Thermal and Radioanalytical Methods	
	IV	Electroanalytical methods	
RPSCHEP303	**Atomic and Molecular: Structure and Spectroscopy**		**4**
	I	Atomic structure	
	II	Atomic spectroscopy	
	III	Molecular Structure	
	IV	Molecular spectroscopy	
RPSCHEPEC-I304	**Nano-chemistry, Applied Electrochemistry, Statistical Mechanics & Nuclear Chemistry**		**4**
	I	Advances in Nanomaterials	
	II	Advanced electrochemistry	
	III	Statistical Mechanics	
	IV	Nuclear Chemistry	
RPSCHEPEC-II304	**Modern Methods in Instrumental Analysis**		**4**
	I	Miscellaneous spectral methods	
	II	Advanced electro-analytical chemistry -I	
	III	Advanced electro-analytical chemistry -II	
	IV	Mass Spectrometry and Raman Spectroscopy	
RPSCHEP3P1	**Practical**		**8**
RPSCHEP3P2			
RPSCHEP3P3			
RPSCHEP3P4			

SEMESTER IV

Course Code	Unit	Course Title / Unit Title	Credits
RPSCHEP401	**Chemistry: Polymer, Green, Biophysical and Applied.**		**4**
	I	Polymer Chemistry-II	
	II	Computational Chemistry	
	III	Bio-physical Chemistry and Green Chemistry	
	IV	Photochemistry-II: Kinetics and Applications	
RPSCHEP402	**Material Sciences and Non-equilibrium Thermodynamics**		**4**
	I	Solid State Chemistry	
	II	Instrumental Methods	
	III	Lasers and super conductors	
	IV	Non-equilibrium thermodynamics	
RPSCHEP403	**Symmetry, Spectroscopy and Catalysis**		**4**
	I	Symmetry in Chemistry	
	II	N.M.R. Spectroscopy	
	III	ESR and Mossbauer Spectroscopy	
	IV	Catalysis	
RPSCHEPOC-I404	**Intellectual Property Rights & Cheminformatics**		**4**
	I	Intellectual Property Right -I	
	II	Intellectual Property Right -II	
	III	Cheminformatics-I	
	IV	Cheminformatics-II	
RPSCHEPOC-II404	**Research Methodology**		**4**
	I	Review of Literature	
	II	Data Analysis	
	III	Methods of Scientific Research and Writing Scientific Papers	
	IV	Chemical Safety & Ethical Handling of Chemicals	
RPSCHEP3P1	**Practical**		**8**
RPSCHEP3P2			
RPSCHEP3P3			
RPSCHEP3P4			

SEMESTER III

Course Code: RPSCHEP301

Course Title: POLYMER, SURFACE & PHOTOCHEMISTRY

Credits: 4

Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Determine molar mass of polymers using different methods.
CO 2	Distinguish the various types of polymers.
CO 3	Classify the surfactants by their process of formation.
CO 4	List the various applications of surfactant in different fields.
CO 5	Illustrate the various deactivation processes of molecular excited states.
CO 6	Describe the photochemical reactivity of ethenes and carbonyl compounds.
CO 7	Explain the application of Fluorescence Phenomena.

Course Code	**Unit**	**Course Title / Unit Title**	**Credits/ Lectures**
RPSCHEP301	**POLYMER, SURFACE & PHOTOCHEMISTRY**		**4**
	I	**Polymer Chemistry-I**	**(15L)**

		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, elastomers and resins). **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. **1.3 Types of polymerization**: Condensation, addition (cationic and anionic) and copolymerization (with kinetics), chain transfer reactions.	
	II	**Modern Applications of Surface Chemistry.**	**(15 L)**
		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.	
	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.	
	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.	

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. Shre edhar, 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.

M.Sc. Physical Chemistry
SEMESTER-III
Course Code: RPSCHEP302

Course Title: ADVANCED INSTRUMENTAL TECHNIQUES

Credits: 4

Academic year 2021-22

Course Outcomes:

After studying this course, the learner will be able to-	
CO 1	Make use of the basic working principles of surface analytical techniques (such as SIMS, PIXE) electron spectroscopy and Nuclear Quadrupole Resonance for different applications.
CO 2	Assess hyphenated techniques and the different types of interfaces that are used to achieve this hyphenation.
CO 3	Apply principles of the thermal methods and radiochemical methods for different applications.
CO 4	Develop a working knowledge of various methods used in Voltammetry.
CO 5	Explain anodic, cathodic and adsorptive stripping methods in voltammetry.
CO 6	Select a suitable method of voltammetry for the analysis of a particular sample.

Course Code	**Unit**	**Course Title / Unit Title**	**Credits/ Lectures**
RPSCHEP302	**ADVANCED INSTRUMENTAL TECHNIQUES**		**4**

	I	**Spectral Methods-I**	**(15L)**
		1.1 Surface Analytical Techniques: Preparation of the surface, difficulties involved in the surface analysis. (1L) **1.2** Principle, instrumentation and applications of the following: **a.** ATR-FTIR spectroscopy (2L) **b.** Secondary Ion mass spectroscopy. (SIMS) (2L) **c.** X-Ray Photoelectron Spectroscopy (XPS) (2L) **d.** Low-Energy Ion Scattering Spectroscopy (LEIS) and Rutherford Backscattering (2L) **e.** Scanning Probe Microscopy including AFM, CFM (3L) **1.3** Nuclear Quadrupole Resonance (NQR), ENDOR, ELDOR. (3L)	
	II	**Hyphenated techniques**	**(15 L)**
		2.1 Concept of hyphenation, need for hyphenation, possible hyphenations. (1L) **2.2**. Interfacing devices, instrumentation and applications of GC – MS, (Head space GC , Pyrolysis GC), GC -FTIR, (3L) **2.3** LC-MS: Interface and Ionization techniques for LC-MS, Thermospray, Particle beam, FAB, and Atmospheric Pressure Ionization (API) Techniques. (3L) **2.4** Different Mass Analysers, Magnetic Sector, Quadrupole, Ion Trap, Time of Flight, FTICR (3L) **2.5** LC-MS/MS: Tandem MS, Triple Quad MS, Collision Induced Dissociation Cell, Different scan events, MRM transitions. Hybrid MS/MS. Applications of Tandem MS. (3L) **2.6** Radio chromatography (2L)	
	III	**Thermal and Radioanalytical methods**	**(15L)**
		3.1 Enthalpimetric methods and thermometric titrations. **3.2** Thermal analysis- Principle, Interfacing, instrumentation and Applications of **(a)** Simultaneous Thermal Analysis- TG-DTA and TG-DSC **3.3** Evolved gas analysis- TG-MS and TG-FTIR (8L) **3.4** Activation analysis- NAA, radiometric titrations and radio-release methods, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications. **3.5** Auto, X-ray and Gamma Radiography (7L)	

	IV	Electroanalytical Methods	(15L)
		4.1 Current Sampled (TAST) Polarography, Normal and Differential Pulse Polarography, Differential double Pulse Polarography (2L) **4.2** Potential Sweep methods- Linear Sweep Voltammetry and Cyclic voltammetry. Potential Step method- Chronoamperomertry (2L) **4.3** Controlled potential technique- Chronopotentiometry (2L) **4.4** Stripping Voltammetry- anodic, cathodic, and adsorption (2L) **4.5**.Chemically and electrolytically modified electrodes and ultra- microelectrodes in voltammetry, Biosensor (2L) **4.6** Corrosion and electrochemistry, Use of Galvano stat and potentiostat (3L) **4.7** Spectro-electrochemistry (2L)	

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.

M.Sc. Physical Chemistry
SEMESTER-III
Course Code: RPSCHEP303
Course Title: ATOMIC AND MOLECULAR: STRUCTURE AND SPECTROSCOPY
Credits: 4
Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Solve the Schrodinger equation for complex system.
CO 2	Compare different theories of Molecule formation
CO 3	Discuss the general principles and theory of spectroscopy
CO 4	Summarize applications of various types of spectroscopic methods.

Course Code	Unit	Course Title / Unit Title	Credits/ Lectures
RPSCHEP303	**ATOMIC AND MOLECULAR: STRUCTURE AND SPECTROSCOPY**		**4**
	I	**Atomic structure**	**(15L)**
		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.	
	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.	
	III	**Molecular Structure**	**(15L)**
		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. **3.3Valence 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 Huckel theory:** Huckel molecular orbital's Theory for–ethylene, Allyl system, cyclopropenyl, linear butadiene, cyclobutadiene and benzene system.	
	IV	**Molecular Spectroscopy**	**(15L)**
		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.	

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, 4thEd., 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).

M.Sc. Physical Chemistry
Semester III
Course Code: RPSCHEPEC-I304
Course Title : Nano-chemistry, Applied Electrochemistry, Statistical Mechanics & Nuclear Chemistry
Credits: 4
Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Perceive the concept of nanomaterials and preparation of various nanomaterials for the research in material science
CO 2	Develop the concept of electrochemistry in energy creation which is need of new age by fuel cells, batteries
CO 3	Apply the concept of probability to the thermodynamic properties at micro level
CO 4	Prove derivation of Maxwell-Boltzmann, Fermi-Dirac statistics.
CO 5	Build knowledge of particle accelerators work viz. Linear, cyclotron.
CO 6	Comprehend the concept of nuclear model's Liquid drop, Fermi gas, Shell, Optical etc.
CO 7	Apply knowledge of nuclear radiations in pharma, geology, industry for various applications

Course Code	Unit	Course Title / Unit Title	Credits/ Lectures
RPSCHEPEC-I 304	**Nano-chemistry, Applied Electrochemistry, Statistical Mechanics & Nuclear Chemistry**		**4**
	I	**Advantages in nanomaterials**	**(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 Important properties on nanomaterials:** Optical properties of metal and semiconductor nanomaterials, magnetic properties **1.3Some 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 **1.5 Application of nanomaterials** in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defence. **1.5 Environmental effects of nanotechnology**	
	II	**Advanced Electrochemistry**	**(15L)**
		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 devices**:	

		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.	
	III	**Statistical Mechanics**	**(15L)**
		3.1 Thermodynamic 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.	
	IV	**Nuclear Chemistry**	**(15L)**
		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-** Geological applications of radioactivity, age of minerals and rocks, age of earth and solar system, medical, industrial and 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, 2nd edition, 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).

M.Sc. Physical Chemistry
Semester III
Course Code: RPSCHEPEC-II304
Course Title: MODERN METHODS IN INSTRUMENTAL ANALYSIS
Credits: 4
Academic year 2021-22

Course Outcomes:

After studying this course, the learner will be able to-	
CO 1	Make use of principles of reflectance methods, photoacoustic spectroscopy, Chemiluminescence methods, and polarimetry for various applications.
CO 2	Discuss advantages of modified electrodes over the classical polarographic methods.
CO 3	Develop a working knowledge of various methods used in modern voltammetry.
CO 4	Outline enhanced Raman spectroscopy techniques, namely Surface Enhanced Raman and Resonance Raman Spectroscopy.
CO 5	Interpret mass spectra of molecules, recognize metastable ion peaks, and correlate peak presence with possible fragmentation mechanisms to arrive at the structure.

Course Code	Unit	Course Title / Unit Title	Credits/ Lectures
RPSCHEPEC-II304	**MODERN METHODS IN INSTRUMENTAL ANALYSIS**		**4**
	I	**Miscellaneous Spectral Methods**	**(15L)**
		Principle, Instrumentation and Applications of: **1.1.** Reflectance spectroscopy **1.2** Photoacoustic spectroscopy **1.3**Polarimetry: ORD, CD **1.4** Chemiluminescence methods	
	II	**Advanced Electroanalytical Chemistry – I**	**(15 L)**
		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.	
	III	**Advanced Electroanalytical Chemistry – II**	**(15L)**
		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 polarography, Square wave Polarography **3.4** Applications of electrochemical methods in Organic synthesis.	

	IV	**Mass Spectrometry and Raman Spectroscopy**	**(15L)**
		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.	

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).

M.Sc. Physical Chemistry
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, ΔHand 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)

MODALITY OF ASSESSMENT

Theory Examination Pattern:

A) Internal Assessment - 40% (40 Marks)

Presentation: 20 Marks

Continuous Internal Assessment (CIA): 20 Marks

For each paper, learners are evaluated from their presentation based on the topic selected from syllabus. The assessment of presentation is as follows:

Sr. No	Evaluation type	Marks
1	Presentation content	10
2	Presentation skills	05
3	Viva	05
4	Continuous Internal Assessment (CIA) e.g. Test, Group discussion, assignment, open-book tests etc.	20
	Total	40

B) External examination - 60 %

Semester End Theory Assessment - 60 marks

1. Duration - These examinations shall be of **2.5 hours** duration.
2. Paper Pattern:
   - **2.1** There shall be **04** questions each of **15** marks. On each unit, there will be one question.
   - **2.2** 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:

Semester End Practical Examination: 50 marks

Experimental work	**40**
Viva	**05**
Journal	**05**

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, a Lost Certificate should be obtained from Head/ Coordinator / 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

Course	**301**			**302**			**Grand Total**
	Internal	**External**	**Total**	**Internal**	**External**	**Total**	
Theory	**40**	**60**	**100**	**40**	**60**	**100**	**200**
Practical			**50**			**50**	**100**
Course	**303**			**304**			**Grand Total**
	Internal	**External**	**Total**	**Internal**	**External**	**Total**	
Theory	**40**	**60**	**100**	**40**	**60**	**100**	**200**
Practical			**50**			**50**	**100**

Total: 600 marks

M.Sc. Physical Chemistry
SEMESTER –IV
Course Code: RPSCHEP401
Course Title : CHEMISTRY: POLYMER, GREEN, BIOPHYSICAL AND APPLIED.
Credits: 4
Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Elaborate Macromolecule, their properties and its characterization.
CO 2	Account for the fundamental background of Density Functional Theory
CO 3	Prove Hohenberg-Kohn theorems and their application.
CO 4	Apply photo physical kinetics of unimolecular and bimolecular processes using Stern-Volmer kinetics.
CO 5	Appraise physical chemistry involved in biological process.
CO 6	Measure thermodynamic parameters for different interactions that are important for the formation of structures in biological systems.
CO 7	Compare the different techniques of electrophoresis
CO 8	Discuss important uses of the solar cell.

Course Code	Unit	Course Title / Unit Title	Credits/ Lectures
RPSCHEP401	**CHEMISTRY: POLYMER, GREEN, BIOPHYSICAL AN APPLIED.**		**4**
	I	**Polymer Chemistry-II**	**(15L)**
		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. **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	
	II	**Computational Chemistry**	**(15 L)**
		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.	
	III	**Biophysical Chemistry and Green Chemistry**	**(15L)**
		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.	
	IV	**Photochemistry-II: Kinetics and Applications**	**(15L)**
		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.	

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).

M.Sc. Physical Chemistry
Semester IV
Course Code: RPSCHEP402
Course Title : Material Sciences and Non-equilibrium Thermodynamics
Credits: 4
Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Relate concept of bonding for structure of crystalline solids.
CO 2	Explain different types of lattices, unit cells and defects in crystal in detail.
CO 3	Assess structure determination by powder diffraction and single crystal X-ray diffraction.
CO 4	Develop concept of lasers in chemistry, its generation, characteristics and types of lasers.
CO 5	Describe applications of lasers in chemistry such as spectroscopy, isotope separation, and kinetics of fast reactions.
CO 6	Make use of Band theory for working of superconductors and magnetic properties.
CO 7	Explain second law of thermodynamics at non-equilibrium i.e. entropy production and rate. Also, comprehend principle of microscopic reversibility and transport phenomena across membranes.

Course Code	Unit	Course Title / Unit Title	Credits/ Lectures
RPSCHEP402	**Material Sciences and Non-equilibrium Thermodynamics**		**4**
	I	**Solid State Chemistry**	**(15L)**
		1.1. Bonding and Structure: Classification of solids based on nature of force.(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. **1.4.** 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.	
	II	**Instrumental Methods**	**(15 L)**
		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.	
	III	**Lasers and Super conductors**	**(15L)**
		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.	
	IV	**Non-equilibrium thermodynamics**:	**(15L)**
		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 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 thermomechanical 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, Principlesand Applications, McMillanIndia Ltd.,(2002).

8. S. Glasstone, Theoretical Chemistry, Affiliated East–West Press Pvt. Ltd., New Delhi, (1973).

M.Sc Physical Chemistry
SEMESTER-IV
Course Code: RPSCHEP403
Course Title : Symmetry, Spectroscopy and Catalysis
Credits: 4
Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Describe the selection rule for infrared-active transitions.
CO 2	Determine whether the molecular vibrations of a triatomic molecule are Raman active.
CO 3	Analyse the hybridization of given compounds.
CO 4	Explain concepts of equivalent and non-equivalent hydrogens.
CO 5	Assess effect of structure on chemical shift and coupling constants.
CO 6	Elucidate the electronic structure of free radicals and paramagnetic transition metal complexes.
CO 7	Comprehend magnetic properties of the materials and its order of orientations.

Course Code	Unit	Course Title / Unit Title	Credits/ Lectures
RPSCHEP403	**Symmetry , Spectroscopy & Catalysis**		**4**
	I	**Symmetry in Chemistry**	**(15L)**
		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. **1.1** Symmetry Adapted Linear Combinations - (SALC) - projection operators and their use to construct SALC. **1.5** 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.	
	II	**N.M.R. Spectroscopy**	**(15 L)**
		2.1 Nuclear Magnetic Resonance (NMR) Spectroscopy: Nuclear spin and its interaction with applied field, population of energy state, relaxation time, ^{1}H NMR Spectroscopy: Chemical Shift; Multiplet Splitting of NMR peaks arises through Spin–Spin Coupling, Multiplet Splitting when more than two spins interact. **2.3 Pulse technique in NMR:** The magnetization vector, spin-spin relaxation, spin-lattice relaxation. **2.4 ^{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.	

	III	**ESR and Mossbauer Spectroscopy**	**(15L)**
		3.1 Electron spin Resonance Spectroscopy- **3.1.1** Basic principle, hyperfine splitting (isotropic systems); **3.1.2**.g-value and the factors affecting there of; 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	
	IV	**Catalysis**	**(15L)**
		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. **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 Learner 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 Learner Ed., 2006, John Wiley and Sons,(Asia) Pvt.Ltd.

M.Sc. Physical Chemistry
SEMESTER-IV
Course Code: RPSCHEPOC-I 404
Course Title : INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS
Credits: 4
Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Relate concept of intellectual property and the terms involved with respect to Indian Patent Law.
CO 2	Distinguish between patents and copyrights.
CO 3	Compare the economic impact and legislature involved in Intellectual property rights.
CO 4	Build knowledge about software tools pertaining to Cheminformatics and Molecular Modelling.
CO 5	Determine structure and sub-structure search online, determine SMILES codes for various molecules.
CO 6	Summarize knowledge about the application of the research-based tools.

Course Code	Unit	Course Title / Unit Title	Credits/ Lectures
RPSCHEPOC-I 404	**INTELLECTUAL PROPERTY RIGHTS & CHEMINFORMATICS**		**4**
	I	**Intellectual Property Rights-I**	**(15 L)**
		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.	
	II	**Intellectual Property Rights-II**	**(15 L)**
		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.	
	III	**Cheminformatics-I**	**(15L)**
		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.	
	IV	**Cheminformatics-II**	**(15L)**
		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.	

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).

M.Sc Physical Chemistry
SEMESTER-IV
Course Code: RPSCHEPOC-II 404
Course Title : RESEARCH METHODOLOGY
Credits: 4
Academic year 2021-22

Course Outcomes:

After completing this course, the learner will be able to:	
CO 1	Perceive basics of research methodology
CO 2	Conduct research by developing a problem
CO 3	Develop research paper writing, study formats of existing research papers and review papers
CO 4	Appraise importance of lab-safety and the safety protocols in R&D laboratories.

Course Code	Unit	Course Title / Unit title	Credits/ Lectures
RPSCHEPOC-II 404	**RESEARCH METHODOLOGY**		**4**
	I	**Review of Literature**	**(15L)**
		1.1 Print: Primary, Secondary and Tertiary sources. **1.2 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. **1.3 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, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus. **1.4 Information Technology and Library Resources:** The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	
	II	**Data Analysis**	**(15 L)**
		2.1 The Investigative Approach: 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.	

	III	**Methods of Scientific Research and Writing Scientific Papers**	**(15L)**
		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.	
	IV	**Chemical Safety & Ethical Handling of Chemicals**	**(15L)**
		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.	

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).

M.Sc Physical Chemistry
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:

B) Internal Assessment - 40% (40 Marks)

Presentation: 20 Marks

Continuous Internal Assessment (CIA): 20 Marks

For each paper, learners are evaluated from their presentation based on the topic selected from syllabus. The assessment of presentation is as follows:

Sr. No	Evaluation type	Marks
1	Presentation content	10
2	Presentation skills	05
3	Viva	05
4	Continuous Internal Assessment (CIA) e.g. Test, Group discussion, assignment, open-book tests etc.	20
	Total	40

B) External examination - 60 %

Semester End Theory Assessment - 60 marks

1. Duration - These examinations shall be of **2.5 hours** duration.
2. Paper Pattern:

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

2.2 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:

Semester End Practical Examination: 50 marks

Experimental work	**40**
Viva	**05**
Journal	**05**

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, a Lost Certificate should be obtained from Head/ Coordinator / 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: IV

Course	**401**			**402**			**Grand Total**
	Internal	**External**	**Total**	**Internal**	**External**	**Total**	
Theory	**40**	**60**	**100**	**40**	**60**	**100**	**200**
Practical			**50**			**50**	**100**
Course	**403**			**404**			**Grand Total**
	Internal	**External**	**Total**	**Internal**	**External**	**Total**	
Theory	**40**	**60**	**100**	**40**	**60**	**100**	**200**
Practical			**50**			**50**	**100**

Total: 600 marks