.

SWAMI RAMANAND TEERTH
MARATHWADA UNIVERSITY, NANDED - 431 606

Two Years Post Graduate Degree Program in Chemistry

(Faculty of Science and Technology)

Revised Syllabi as per NEP-2020 for

M.Sc. Second Year

Physical Chemistry

(For Affiliated Colleges)

To be implemented from
Academic year 2024 - 2025

Framed by
BOARD OF STUDIES IN CHEMISTRY

Syllabus for M. Sc. Physical Chemistry, Second Year

Semester – III

As Per NEP- 2020

To be implemented from

Academic Year 2024-2025

SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY, NANDED

M.Sc. PHYSICAL CHEMISTRY (Second Year)

(SEMISTER III & IV) NEP 2020

SEMESTER	COURSE NO.	COURSE	PERIODS / WEEK	TOTAL PERIODS	MARKS
III Semester	SCHECT1501 Compulsory	ADVANCED SPECTROSCOPIC METHODS	04	60	4 Credits / 100 Marks
	SCHECT1502	SOLID STATE CHEMISTRY	04	60	4 Credits / 100 Marks
	SCHECT1503	STATISTICAL THERMODYNAMICS	02	30	2 Credits / 50Marks
	ELECTIVE PAPER (ANYONE A OR B)		04	60	4 Credits /100 marks
	SCHECT1504	A] CHEMICAL DYNAMICS			
	SCHECT1505	B] ADVANCED QUANTUM CHEMISTRY			
	SCHECP 1501	LAB COURSE V	04	60	2 Credits / 50 marks
	SCHECP 1502	LAB COURSE VI	04	60	2 Credits / 50 marks
	SCHERP 1501	RESEARCH PROJECT	04	120	04 credits
				Total	**22 credits**
IV Semester	SCHECT1551	RADIATION CHEMISTRY	04	60	4 Credits / 100 marks
	SCHECT1552	ELECTRO CHEMISTRY	04	60	4 Credits / 100 marks
	ELECTIVE PAPER (ANYONE A OR B)		04	60	4 Credits /50 marks
	SCHECT1553	A] MOLECULAR REACTION DYNAMICS & BIO PHYSICAL CHEMISTRY			
	SCHECT1554	B] LIQUID STATE			
	SCHECP 1551	LAB COURSE VII	04	60	2 Credits

					/50 marks
	SCHERP 1502	RESEARCH PROJECT	06	120	
				Total	**22 credits**
				Grant Total	**44**

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Major Core Theory Course

Course Code – SCHECT1501

Title of the Course: Advanced Spectroscopic Methods

[No. of Credits: 4 Credit] **60 Periods**

Course objectives:

- Students are acquainted with various spectroscopic techniques to elucidate the known and unknown organic molecules.
- Students are familiar with the ultra-violet and visible spectroscopy by determining the absorption maximum of various dienes, enones and aromatic organic compounds.
- Student develops the detail knowledge to get the different peaks of functional groups in organic molecules by infra-red spectroscopy.
- Students understand the importance and applications of proton magnetic resonance spectroscopy for determination of structure of unknown organic compounds.
- Students are recognizable with CMR to authenticate the position of carbon atom in organic molecules.
- Students identified the structure of compounds by fragmentation of various classes of organic molecules.

Module No.	Unit No.	Topic	Hrs. Required to cover the contents
1. 0		**UV-VIS AND IR SPECTROSCOPY:**	17
	1.1	**UV-Vis Spectroscopy:** Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Fieser-Kuhn rules for polyenes. UV spectra of aromatic compounds and heteroaromatic compounds. Calculation of max for the benzene derivatives (R-C6H4-Co-G) by A. I. Scott empirical rules.	
	1.2	**IR spectroscopy:**	

		Recapitulation, Characteristic vibration frequencies of Alkanes, Alkenes, Alkynes, Aromatic compounds, Alcohols, Ethers, Phenols and Amines. Detailed study of vibrational frequencies of carbonyl compounds Ketones, Aldehydes, Esters, Amides, Acids, Anhydride, Lactose, Lactams and Conjugated Carbonyl compounds. Factors affecting group frequencies: overtones, combination bands and Fermi-resonance. FITR and sampling techniques.	
2.0		**Module 2: ^{1}H NMR AND ^{13}C NMR SPECTROSCOPY:**	**18**
	2.1	General introduction and definitions, Chemical shift, Spin-spin interaction, Shielding mechanism of measurement of chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehyde and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto). Factors affecting chemical shift. Deuterium exchange. Spin-spin coupling, factors affecting coupling constant. Complex spin-spin interaction between two and three nuclei. Simplification of complex spectra, nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique. Nuclear Over-Hauser effect (NOE). Resonance of other nuclei; ^{19}Fand ^{31}P.	
	2.2	**^{13}C NMR Spectroscopy:** Resolution and multiplicity of ^{13}C NMR, ^{1}H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR.	
3.0		**MASS SPECTROMETRY**	**10**
	3.1	**Mass Spectrometry:** Theory, instrumentation and modifications; Unit mass and molecular ions; Important terms- singly and doubly charged ions, metastable peak, base peak, isotropic mass peaks, relative	

		intensity, FTMS, etc. Recognition of M+ ion peak.	
	3.2	General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulfur, nitrogen and halogens; α, β-, allylic and benzylic cleavage, McLafferty rearrangement.	
4.0		**Module 4: Structural Problems:**	**15**
	4.1	Combined problems on UV, IR, NMR and Mass spectral data for structure determination.	
	4.2	Elucidation of structure of organic molecules using spectra (IR, PMR&CMR).	
		Total	**60**

Course outcomes

1. Know the use electronic spectroscopy to determine absorption maximum in dienes, enones and aromatic compounds.
2. Know the applications of IR spectroscopy for functional group determination.
3. Learn the structure elucidation of organic compounds by PMR spectroscopy.
4. Gathering basic knowledge to know the position of carbon in carbon compounds.
5. Recognize the molecular mass of the organic molecule by fragmentation pattern.
6. Know the complete structure of compounds using UV, IR, PMR, CMR and Mass spectroscopic methods.

Reference Books

1. Spectroscopic Identification of Organic Compounds, R. M. Silverstern, G. C.Bassler and T. C. Morril.
2. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus.
3. Application of spectroscopy of organic compounds, J. R. Dyer.
4. Spectroscopy of organic compounds, P. S. Kalsi.
5. Organic Spectroscopy, William Kamp.
6. Organic Chemistry, R. T. Morrison and R. N. Boyd.
7. Practical NMR spectroscopy, M. L. Martin, J. J. Delpench and G. J. Martin.
8. Spectroscopic methods in organic Chemistry, D. H. William, I. Fleming.
9. Fundamentals of Molecular spectroscopy, C.N.Banwel.

10. A Handbook of Spectroscopic Data of Chemistry, B. D. Mistry.

11. Elementary Organic Spectroscopy, Y. R. Sharma.

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Major Core Theory Course

Course Code – SCHECT1502

Title of the Course: SOLID STATE CHEMISTRY

[No. of Credits: 4 Credit] **60 Periods**

Course objectives:

- To enable student to acquire knowledge about the various types defects in solids.
- Students can know about the different types of solid-state reactions.
- They understand about classification of solids on basis of band structure and magnetic properties insolid.
- They will know about different types of types of organic solids.

Unit No.	Topic	Hrs.
1	**SOLID STATE REACTIONS**	
	Introduction, General principles, Wagner reaction, Wagner reaction mechanism factors affecting the reactivity of solid state reaction, Experimental procedures of Solid-State, Reactions, Co-precipitation as a precursor to solid state reactions, Solid State reaction method of $Co_{0.5}Zn_{0.5}Cd_{0.2}Fe_{1.8}O_4$ ferrite synthesis kinetics of solid-state reactions	15
2	**CRYSTAL DEFECTS AND NON-STOICHIOMETRY**	
	Perfect and imperfect crystals, intrinsic and extrinsic defects – point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation color centers, non- stoichiometric defects with examples,	15
3	**ELECTRONIC PROPERTIES AND BAND THEORY**	

	Metals, insulators and semiconductors, electronic structure of solids band theory, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, super conductors, Optical properties–optical reflectance, photoconduction–photoelectric effects.	15
4	**ORGANIC SOLIDS**	15
	Introduction, Types of organic solids, examples of organic solids. Electrically conducting solids, organic charge transfer complex, organic metals,new superconductors, applications pf organic solids,	

Course outcomes:

- Student gets knowledge about different types of defects in solids.
- They know about the different types of solid-state reactions and factors affecting reactions.
- Students understand about classification on solids on basis electronic structure.
- They are now able to classify solid on basis of band structure and magnetic properties.

Reference Books

1. Solid State Chemistry and its Applications, A.R. West Plenum
2. Principles of the Solid State, H.V. Keer, Wiley Eastern
3. Solid State Chemistry N.B. Hannay
4. Solid State Chemistry D.K. Chakrabarty, New Age International

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Major Core Theory Course

Course Code – SCHECT1503

Title of the Course: STATISTICAL THERMODYNAMICS

[No. of Credits: 2 Credit] **30 Periods**

Course objectives:

Objectives

- This course helps students to have basic knowledge of statistical thermodynamic.
- It helps students to have understating about the principle and applications of statistical thermodynamic.
- They will be able to solve numerical based on statistical thermodynamic.

Curriculum Details: SCHECT1503: STATISTICAL THERMODYNAMICS

Unit No.	Topic	Hrs.
1	**BACKGROUND CONCEPTS**	
	Number ways in which particles can be arranged in order or placed in container. The situations of this distribution in Boltzmann, Fermi-Dirac and Bose Einstein statistics, illustrations sterling approximation, Langrage method of undetermined multipliers, distribution, and most probable distribution. Problems.	10
2	**STATISTICAL MECHANICS OF A SYSTEM OF INDEPENDENT PARTICLES**	

	Introduction : Relation between partition function and thermodynamics function, illustrative examplesand problems. Types of statistics: Types of Statistics Maxwell – Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics	10
3	**APPLICATION OF STATISTICAL MECHANICS**	10
	Ideal gases: Partition function of a monatomic gas. Thermodynamics function of a monatomic gas, diatomic and polyatomic gases. Internal rotation of a polyatomic molecule, heatcapacity and the residual entropies of polyatomic molecules. **Solids:** Introduction, Thermal characteristics of crystalline solids. Einstein model, Debye modification, limitations and modifications of Debye theory and comparison between Debyetheory and Einstein model.	

Course outcomes

1. Students will get basic knowledge about the applications of statistical thermodynamic to various systems
2. They will get the basic information of different types of Statistics used in statistical thermodynamics
3. They understated the Statistical Mechanics of a System of Independent Particles.

Book Suggested

1. Statistical Thermodynamics, Donald A. Mc Quarrie, Happer and Row, New York,1973.
2. Statistical Thermodynamics, M.C. Gupta, Wiley Eastern Limited. New Delhi,1990
3. Elements of Statistical Thermodynamics, L.K. Nash, Addison Wesley, Menlo Park, 1992.
4. Text book of Physical Chemistry, Samuel M. Glastone, Littern Educational Publishing In., New York.
5. Physical Chemistry, P.W. Atkins

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Elective Theory Course

Course Code – SCHECT1504

Title of the Course: CHEMICAL DYNAMICS

[No. of Credits: 4 Credit] **60 Periods**

Course objectives

- To enable student to get advanced knowledge about the chemical kinetics of the complex reactions.
- They are expected to know about kinetics chain and polymerization reactions.
- They will learn about the motions of molecules in liquid and gases.
- They will understand the different technique used in study of fast reactions.

Curriculum Details SCHECT1504 : CHEMICAL DYNAMICS

Unit No.	Topic	Hrs.
1	**MOLECULES IN MOTION**	
	Molecular motion in gases: collision with walls and surface rate of effusion, migration down gradients,transport properties of a perfect gas. Motion in liquids: Structure of liquids, molecular motion in liquids conductivitiesof electrolyte solution, mobilities of ions conductivities and ion-ion interactions. Diffusion: a Thermodynamic view, the diffusion equation, diffusion probabilities statistical view.Problems on every concept.	15

2	**RATE OF CHEMICAL REACTIONS** Experimental techniques rates of reactions, integrated rate laws, reactions approaching equilibrium, temperature dependence of reaction rates. According for therate laws. Elementary reactions, consecutive elementary reactions, unimolecular reactions. Problems.	15
3	**KINETICS OF COMPLEX REACTIONS** Chain reactions: Structure of chain reactions, Explosions, photochemical reactions. Polymerization Kinetics: Chain Polymerization, stepwise Polymerization Catalysis and oscillations: Homogenous catalysis, autocatalysis, oscillating reactions, chemicalchaos. Problems.	15
4	**MOLECULAR REACTION DYNAMICS** **Reactive encounters:** Collision theory, diffusion-controlled reactions. **Activated complex theory**: The reactions coordinate and transition state, Eyring equation,thermodynamic aspects of activated complex theory. Dynamics of Molecular collisions: reactive collisions, Potential energy surfaces. Problems.	15

Course outcomes

- Student are now able to calculate the mechanism of various complex reactions
- They know about various experimental techniques to study the kinetics of fast reactions.
- They understood the motions of molecules in liquid and gas as well as about molecular reactiondynamics
- They know about kinetics of the complex reactions which includes chain and polymerizationreactions.

Reference Books

1) Physical Chemistry, P.W. Atkins (ELBS)
2) Chemical Kinetics, K.J. Laidler, Tata McGraw Hill Publishing Co. Ltd., News Delhi.
3) Reaction Mechanism and chemical Transformations, J. Rajaram and K. Kuriakose

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Elective Theory Course

Course Code – SCHECT1505

Title of the Course: ADVANCED QUANTUM CHEMISTRY

[No. of Credits: 4 Credit] **60 Periods**

Course objectives:

- After study of this quantum chemistry course students will get knowledge about how to apply theoretical and computational treatment for the study of chemistry.

Curriculum Details SCHECT1505 : ADVANCED QUANTUM CHEMISTRY

Unit No.	Topic	Hrs.
1	**THEORETICAL AND COMPUTATIONAL TREATMENT OF ATOMS AND MOLECULES** Review of the principles of quantum mechanics, Born-Oppenheimer approximation. Slater-Condon rule. Hartree-Fock equation, Koopmans, and Brillouin theories, Roothan equation, Gaussian basis sets, Hartee-Fock Theory	15
2	**CONFIGURATION INTERACTION AND MC-SCF** Introduction to Cl; full and truncated Cl theories, size consistency.	15

	Introductory treatment of coupled cluster and MC-SCF methods.	
3	**SEMI – EMPIRICAL THEORIES** A review of the Huckel, EHT and PPP treatments ZDO approximation detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An Introduction to MOPAC and ANI with hands on experience on personal computers	15
4	**DENSITY FUNCTIONAL THEORY** Derivation of Hohenberg – Kohn theorem, Kohn – Sham formulation, N and V represent abilities, review of the performance of the exiting local (e.g-slater Xa and other methods) and non-local functional treatment of chemical concepts with the density functional theory	15

Course outcomes

1. Student acquire knowledge about theoretical and Computational Treatment to Atoms and Molecules.
2. They have knowledge of Configuration Interaction and MC-SCF, Semi – empirical theories
3. They have understanding about Density functional theory.

Book Referred

1. Modern quantum chemistry N.S. outland and A. Szabo McGraw hill.
2. Methods of molecular quantum mechanics R. McWeeny and B.T. Sutcliffe. Academics press.
3. Density functional theory of Atoms and Molecules R.G Parr and W.yang Oxford
4. Exploring Chemistry with electron structure methods J.B. Foresman and E. Frish Foussian Inc

.

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Major Practical Course

Course Code – SCHECP 1501

Title of the Course: LAB COURSE V

[No. of Credits: 2 Credit] **60 Periods**

Curriculum Details: SCHECP1501: LAB COURSE V

SPECTROSCOPY

1. To determine the indicator constant PK^{IN} of and indicator by using half height method(Bromo cresol purple) (DVJ-200)
2. To determine the stability constant of metal complex between 5-SSA and Fe +3 with the help of job's curve and Bent and French method (for weak complex) (dvJ204)
3. To determine the concentration of Fe (II) and Cu (II) by spectrophotometric titration with EDTA
4. To investigate the effect of ionic strength on pKa of bromo cresol green and thus determine pK_{in} (DVJ-211)
5. To investigate the reaction kineties between K2S2O8 and KI by spectrophotometry (TKC-223)

6. To determine simultaneously the dichromate and permanganate ions in the given solution
7. POLARIMETRY
8. Determine the percentage of two optically active substances in a mixture (TKC-194)
9. To investigate the complex ion formation between Fe (II) and thiocyanate ion
10. To study Kinetics of hydrolysis of sucrose by Hammett-Zuckerman approach (DVJ)
11. Investigate the effect of substitution of chloride ions on rate constant of inversion of cane sugarby using mono, di, and trichloro acetic acid as catalyst

REFRACTOMETRY

12. Determine the refractive indices of series of solution of a salt and determine the concentration of thesalt in the given unknown solution.
13. Determine the molar refraction of ethyl, propyl and butyl acetate and show the constancyof contribution to the molar refraction amide by CH2 group
14. Determine the molar refraction of methyl acetate, ethyl acetate, n-hexane and carbon tetrachlorideand calculate the atomic refraction of C, H and Cl atoms.
15. Study the variation of refractive index with composition of mixtures of carbon tetrachloride and ethyl aetate and determine the molar refraction of the given unknownmixture.

VISCOSITY

16. Study the variation of viscosity with composition of 1) ethanol – water II) methanol – ethylidenechloride III) the formation of compound (TKC 25)
17. Determine the molecular weight of macromolecules (TKC 251)
18. Determine the iso-electric point of gelation and examine the effect of aging by viscometrical methods(DVJ-29)

FLAME PHOTOMETRY

19. Estimation of Na, K, Li & Ca by flame photometry.

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Major Practical Course

Course Code – SCHECP 1502

Title of the Course: LAB COURSE VI

[No. of Credits: 2 Credit] **60 Periods**

Curriculum Details SCHECP 1502: LAB COURSE VI

POTENTIOMETER

1.Titrate ferrous ammonium sulphate with cerric sulphate and find out formal redox potential of $Re^{2+/}Fe^{3+}$ and Ce^{3+}/Ce^{4+} system

2.Titrate potentiometrically phosphoric acid solution against NaOH and calculate Pk_1, Pk_2 and Pk_3 of the acid

3.Titrate potentiometrically NaCl solution against AgNO3 and find out the concentration of NaCl and hence determine the solubility product of AgCl

4.Determine the activity coefficient of silver ions using a concentration cell without transference

pH METRY

5.To determine the product ligand stability constant of an organic acid and the metal ligand stability constant of its complex by pH measurements

6.Determine the Hammett constant of a given substituted benzoic acid by pH measurements

7.Determine the pH values of various mixtures of sodium acetate and acetic acid in aqueous solution andhence find out the dissociation constant of the acid

8.To determine the hydrolysis constant of aniline hydrochloride by pH measurements

CONDUCTOMETRY

9.To determine the thermodynamic dissociation constant of weak acid conductometrically.

10.Investigate the kinetics of basic hydrolysis of ethyl acetate conductometrically.

11.Conductometric titration of a mixture of strong acid weak acid and a salt

12.To determine the degree of hydrolysis and hydrolysis constant of sodium acetate Conductometrically

MAGNETO CHEMISTRY

13.To determine the magnetic susceptibility and number of unpaired electrons in a given compound.

14. Verification of Weidemann's law using nickel chloride solutions

SURFACE TENSION

15. Study the effect of surfactant (n- propyl alcohol) at various concentrations on the surface tension ofwater and hence determine the limiting cross-sectional area of alcohol molecule by stalagmometer

16. Determine the parachor of a solid by stalagmometer

THERMODYNAMICS

17. Determine the partial molar volume of ethanol and water in a given composition by density measurements.

18. To determine heat of neutralization of strong acid and heat of ionization of weak acid calorimetrically.

19. To determine the integral hear of solution of KNO_3

20. To determine the heat of dissociation of benzoic acid in water

21.To determine heat of precipitation of $BaSO_4$

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - III)

Research Project Course

Course Code – SCHERP 1501

Title of the Course: RESEARCH PROJECT

[No. of Credits: 4 Credit] **120 Periods**

Course objectives:

1. To train the students with different experimental and analytical skills considering opportunities in academic and industrial research.
2. To gain the knowledge of referring research journals, writing research articles and submit the dissertation report.

Curriculum Details: SCHECP1501: Research Project

1. 0		**RESEARCH PROJECT**	
		Small research project designed by the teacher based on the interest of the student and capabilities should be worked out.	
		Total	**120**

Note:

1. External and Internal Examiners will examine this project jointly at the time of Practical examination.
2. The students will have to give at least one seminar in each semester in their subject of specialization is compulsory.
3. Project work must be carried out only in specialized branch.
4. All synthesized organic compounds should be submitted at the time of University Examination.
5. The project work carried out during the year should be presented in power point presentation in presence of University Examiners.

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - IV)

Major Core Theory Course

Course Code – SCHECT1551

Title of the Course: RADIATION CHEMISTRY

[No. of Credits: 4 Credit] **60 Periods**

Course objectives:

- Students should be able to improve their knowledge about basic information of radiation andnuclear chemistry.
- They should know about the different types of nuclear reactions, nuclear reactors, and applications

of radioactivity in various fields.

Curriculum Details: SCHECT1551: RADIATION CHEMISTRY

Unit No.	Topic	Hrs.
1	**RADIOACTIVITY**	

	Historical background, natural radioactive elements, general characteristics of α, β, γ rays, detection and measurement of radioactivity, the theory of radioactive disintegration, decay kinetics, units of radioactivity parent daughter growth relationship secular and transient equilibrium, theory of α decay, β decay – energeticsof β decay, problems of β decay, Fermi's theory of β decay, nuclear excitation emission, Numerical.	15
2	**NUCLEAR REACTIONS AND REACTORS**	
	Definition and Bethes notation, nuclear reaction energetics, nuclear reaction and threshold energy, characteristics of nuclear reactions, types of nuclear reactions, conservation in nuclear reactions, specific nuclear reactions-photonuclear reactions,stripping and pickup reactions, evaporation, spallation, fragmentation, direct nuclearreactions, thermonuclear reactions. Fission energy, natural uranium reactor, four factor formula, classifications of nuclearreactors, reactor power, critical size of thermal reactor, breeder reactor, India's nuclear energy programme, nuclear waste management, energy from nuclear fission. Numerical	15
3	**ELEMENTS OF RADIATION CHEMISTRY**	
	Introduction: Primary effects due to charged particle/radiation, Linear energy transfer (LET), interactions of electron with matter, interaction of neutrons with matter, interaction of heavy charged particles with matter, interaction of rays withmatter, units for measuring radiation absorption, absorption in water. Radiation dosimeter-units of radiation energy, Chemical dosimeter- the Fricke dosimeter, ceric sulphate dosimeter, other chemical dosimeters conversions of measured dose values. Numerical	15
4	**EFFECTS OF RADIATION ON MATTER**	
	Radiolysis of water and aqueous solutions. Radiolysis of water vapor, liquid	

	water. Radiolysis of oxygenized water. The reduced species-hydrated electrons. Redox reactions due to ray irradiated, radiation induced color centers in crystals (strong andrelease of energy), effect of pH on radiolytic product of water solution, Radiolysis of aqueous solution: Radiolysis of ferric solution, ferrous sulphate, cupric sulphate solution, Radiolysis of aqueous solution of organic compounds Numerical	15

Course outcomes

- They know about different types of nuclear reactions and reactors
- They understand about the effect of radiation on matter
- Students understand about the about applications of radioactivity in various fields.
    - They are be able to solve numerical of different concepts of radioactivity

Reference Books

1. Source of atomic energy by S. Glasstone, D. Van Nostrated co. INC
2. Essentials of Nuclear Chemistry by H.J. Arnikar 4th Edn, New Age Inter. (p) Ltd.
3. Introduction to Nuclear Chemistry by B.G. Harvey.
4. Nuclear Chemistry by M.G. Arora & M. Singh Anmol publication, New Delhi.
5. Elements of Nuclear Chemistry by A.K. Srivastav, P.C. Jain, S. Chand & Co.
6. A text book of Nuclear Chemistry by C.V. Shekar Deminat publication & distribution, Delhi

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - IV)

Major Core Theory Course

Course Code – SCHECT1552

Title of the Course: ELECTROCHEMISTRY

[No. of Credits: 4 Credit] **60 Periods**

Course objectives

- Students will be able to know about reversible and irreversible cell.
- Students will understand different processes which takes place over metal surface
- They will be able explain different Debye Huckel theory and its application inelectrochemistry
- They will be aware about electrochemical theory of corrosion and method of prevention ofcorrosion.

Curriculum Details: SCHECT1551: ELECTROCHEMISTRY

Unit No.	Topic	Hrs.
1	**FREE ENERGY AND ACTIVITY**	
	Activity and activity coefficient, equilibrium, and free energy changes, Debye-Huckeltheory, Debye-Huckel limiting law, Debye-Huckel equation of appreciable concentration, Huckel and Bronsted equation, quantitative verification of appreciable concentrations, Huckel and Bronsted equation, quantitative verification of Debye- Huckel equation, tests, of Debye Huckel limiting equation, activities in concentration solutions., extension of Debye-Huckel theory, ion association	15
2	**EQUILIBRIA IN ELECTROLYTES**	
	equilibria in electrolytes, strong intermediates and weak electrolytes, solubility, solubility product principle, solubility for common ions and complexion, determination of instability constant, activity coefficient form solubility, measurements solubility andDeye-Huckel theory. Problems	15
3	**REVERSIBLE CELLS**	
	Reversible and irreversible cells, reversible electrodes, application or emf measurements, concentration cells with a single electrolyte., amalgam concentration cells, electrode potential, potentials in nonaqueous solutions, factors affecting electrode potentials, rate or electrode potentials, electrode potentials and equilibrium constants, electrode potentials and solubility products.	15
4	**DYNAMIC ELECTROCHEMISTRY**	
	Process at electrodes., electrical double layer, rate of charge transfer, polarization, electrochemical process, electrolysis, characteristics of working cells, Power production and corrosion, types of electrochemical corrosions,	15

	fuel cells, power generation in fuel cells, power storage, secondary cells, thermodynamics and kinetics of corrosion and their prevention methods, applications of electrolysis in electrorefining, electroplating and electrotyping. Problems	

Course outcomes

- They acquire knowledge about the reversible and irreversible cell and their examples,
- They now know about different processes which takes place over metal surface
- Student know about Debye Huckel theory and its application in electrochemistry and able tosolve numerical on it.
- Students get knowledge about electrochemical theory of corrosion and method of prevention of corrosion.

References books

1. Text book of Physical Chemistry, Samuel. Gallstone, Litter Educationalpublishing in., New York
2. Physical Chemistry, P.W.Atkins (ELBS)
3. Introduction to electrochemistry, Samuel M. Gallstone, Litter Educational.Publishing inc., New YoRK
4. Theoretical electrochemistry, L. J. Antropov., Mir Publishers, Moscow
5. Modern electrochemistry vol I & II Bokris J.O.M. and Reddy A.K.M (PLENUM)

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - IV)

Elective Theory Course

Course Code – SCHECT1553

Title of the Course: MOLECULAR REACTION DYNAMICS AND BIOPHYSICAL CHEMISTRY

[No. of Credits: 4 Credit] **60 Periods**

Course objectives:

- To acquire basic knowledge about how physical methods can be applicable to understand biologicalprocesses.

- For developing an understanding on how statistical mechanics can be applied to understand aboutbiopolymers and the different biopolymer interactions.

Curriculum Details: SCHECT1551: MOLECULAR REACTION DYNAMICS AND BIOPHYSICAL CHEMISTRY

Unit No.	Topic	Hrs.
1	**MOLECULAR REACTION DYNAMICS**	
	a. Reactive encounters: Collision theory, diffusion-controlled reactions. **b. Activated complex theory:** The reaction coordinate and transition state, Eyring equation, thermodynamic aspects of activated complex theory. **c. Dynamics of Molecular collisions:** reactive collisions, Potential energy surfaces. Problems.	15
2	**BIOPHYSICAL CHEMISTRY**	
	A. Biological Cell and its Constituents Biological cell structure and functions of proteins, enzymes DNA and RNA in living systems. Helix coil transition **B. Bioenergetics:** Standard free energy change in biochemical reactions, exergonic, endergonic, Hydrolysis of ATP, synthesis of ATP from ADP **C. Statistical Mechanics in Biopolymers:** Chain configuration of macromolecules, statistical distribution end to end dimensions, calculation of average dimension of various chain structures, polypeptide and protein structures, introduction to protein folding problem.	15
3	**BIOPOLYMER INTERACTIONS**	
	Forces involved in biopolymer interactions. Electrostatic charges and molecular expansion, hydrophobic forces, dispersion force interactions. Multiple equilibria and various types of binding processes in biological systems. Hydrogen ion titration curves.	15

4	**THERMODYNAMICS OF BIOPOLYMER SOLUTIONS**	
	Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium muscular contraction and energy generation in mechanochemical system. **Biopolymers and their molecular Weights** Evaluation of size, shape, molecular Weight and expect of hydration of Biopolymer, by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis, and rotational motions.	15

Course outcomes:

- Students learnt about Biological Cell its Constituents and about Bioenergetics
- They understand about the Statistical Mechanics in Biopolymers and about the different biopolymerInteractions
- They understand about the Thermodynamics of Biopolymer solutions.

They know about the different Diffraction Methods and photo correlation spectroscopy

Reference Books

1. Principles of Bio Chemistry A.L.Lehniger, Worth Publisher
2. Biochemistry, L. Stryer, W.H. Freeman
3. Biochemistry, J. Devidrawn, Neil Patterson
4. Biochemistry, Voet, Jphn Wiley
5. Qutines of Biochemisty E.E. Conn and P.K. Stumpf, Jojn Wiley
6. Bioinorganic Chemistry, A Chemical Approch to Enzyme Action, H. Dugas and C. Penny, Springer-Vertag.
7. Macromolecules structure and function F. Would, Prentice Hall

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - IV)

Elective Theory Course

Course Code – SCHECT1554

Title of the Course: LIQUID STATE

[No. of Credits: 4 Credit]	60 Periods

Course objectives:

- After learning this unit students should know about general properties, theories of liquid,
- Distribution Function and Related Equations.
- They will learn about Spectroscopic techniques for liquid dynamic structure studies
- They will get knowledge about Computation Techniques- Monte Carlo and molecular dynamics methods

Curriculum Details: SCHECT1553: LIQUID STATE

Unit No.	LIQUID STATE	Hrs.
1	**GENERAL PROPERTIES OF LIQUIDS**	15
	a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations, internal pressure, and its significance in liquids. Equations of state, critical constants. Different types of intermolecular forces in liquids, different potential function for liquids, additivity of pair potential approximation. b) A classical partition function for liquids, correspondence principle, configuration integral, configuration properties.	
2	**THEORY OF LIQUIDS**	15
	Theory of liquids, partition function method or model approach; single cell models, communal energy and models, communal energy and entropy LTD model, significant structure model	
3	**DISTRIBUTION FUNCTION AND RELATED EQUATIONS**	15
	Radial distribution function method, equation of state ion terms of RDF, Molecular distribution functions, pair distribution function, relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, clusters expansion.	
4	**METHODS FOR STRUCTURE DETERMINATION**	15

	AND COMPUTATIONAL TECHNIQUES	
	Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy Computation Techniques- Monte Carlo and molecular dynamics methods.,	
		60

Course outcomes:

- They know about the general properties, theories of liquid,
- They now know about spectroscopic techniques for liquid dynamics structure studies
- Student know about computation Techniques- Monte Carlo and molecular dynamics methods.

Books Referred :-

1. An introduction to Liquid state P.A. Egelstaff, Academic Press
2. The Dynamic Liquid State, A.F.M. Bartion, Longman.
3. The Liquid State, J.A. Pryde
4. Significant Liquid Structures, H.Eyring and M.S. John.

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - IV)

Major Practical Course

Course Code – SCHECP 1551

Title of the Course: LAB COURSE VII

[No. of Credits: 4 Credit] **60 Periods**

Course objectives:

- To train the students in estimation of organic molecules.
- Gain the practical knowledge to estimate the drug molecules by instrumentation methods.

Curriculum Details: SCHECP1551: LAB COURSE VII

CHEMICAL DYNAMICS

1) Investigate the influence of ionic strength on the rate constant of the reaction between $K_2S_2O_8$ and KI(TKC-335)

2) Determine the order of a reaction by I) substitution method (II) fractional change method and (III)differential method

3) Investigate the reaction between bromic acid and hydrochloric acid (TKC 346)

4) Investigate the reaction between H_2O_2 and KI kinetically

5) Investigate the kinetics of iodination of acetone.

PHASE EQUILIBRIA

6) Determine the critical solution temperature of phenol and water in presence of 1)1`% NaCl 2)0.5% naphthalene 3) succinic acid

7) Construct the phase diagram of a three- component system containing ethanol benzene and water.

8) Determine the equilibrium constant of the tri- iodide formation in aqueous solution by distributionmethod.

ADSORPTION

9) Investigate the adsorption of acetic/ oxalic acid by activated charcoal and test the validity of Freundlich and Langmuir's isotherm

APPLICATION OF COMPUTER IN CHEMISTRY

1. Determine the excess molar volume of binary liquid / ternary liquid mixture by using Excel /MATLAB software from given data.

2. Calculate mean deviation, relative mean deviation, and standard deviation by using Excel / MATLABsoftware from given data.
3. Plot the graph of Emf Vs volume of titrant added E/V Vs volume of titrant added
4. from the experimentally observed data by using Excel software and justify the nature of graph.
5. Determine proton ligand formation number (nA) dissociation constant (pK) and metal– ligandstability constant (pL) by using Excel programme.
6. Draw the molecular structure of given molecules using chem. Draw Windows.
7. Draw the graph of ionization potential Vs. Atomic number or II, III, IV, V, VI row elements andjustify the nature.
8. Draw the graph between atomic number Vs I.P. and electro-negativity of first group elements byusing Excel software from given data and justify the nature of the graph.
9. Calculate the mole fraction of liquid mixture from given data by using Excel–Software

National Education Policy 2020

M.Sc. Chemistry, II Year (Semester - IV)

Course Code – SCHERP 1502

Title of the Course: RESEARCH PROJECT

[No. of Credits: 6 Credit] **180 Periods**

Course objectives:

- To train the students with different experimental and analytical skills considering opportunities in academic and industrial research.
- To gain the knowledge of referring research journals, writing research articles and submit the dissertation report.

Curriculum Details: SCHECP1501: RESEARCH PROJECT

1. 0		**RESEARCH PROJECT**	
		The students will develop utilities such as analytical spectra, simulation programmers that will supplement laboratory exercises in their subject of specialization. For this, variety of small research project designed by the teacher based on the interest of the student and capabilities should be worked out.	
		Total	**180 Hrs**

Note:

1. External and Internal Examiners will examine this project jointly at the time of Practical examination.
2. The students will have to give at least one seminar in each semester in their subject of specialization is compulsory.
3. Project work must be carried out only in specialized branch.
4. The project work carried out during the year should be presented in power point presentation in presence of University Examiners.