# ।। सा विद्या या विमुक्तये ।।



# स्वामी रामानंद तीर्थ मराठवाडा विद्यापीठ, नांदेड

"ज्ञानतीर्थ" परिसर, विष्णुपूरी, नांदेड - ४३१६०६ (महाराष्ट्र)

## SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY NANDED

"Dnyanteerth", Vishnupuri, Nanded - 431606 Maharashtra State (INDIA) Established on 17th September 1994 - Recognized by the UGC U/s 2(f) and 12(B), NAAC Re-accredited with 'A' Grade

# ACADEMIC (1-BOARD OF STUDIES) SECTION

Phone: (02462) 229542 : (02462) 229574

Website: www.srtmun.ac.in

E-mail: bos.srtmun@gmail.com

महाविद्यालयांतील विज्ञान तंत्रज्ञान विद्याशाखेतील पदव्युत्तर स्तरावरील द्वितीय वर्षाचे CBCS Pattern नुसारचे अभ्यासक्रम शैक्षणिक वर्ष २०२०–२१ पासून लागू करण्याबाबत.

# प रिपत्रक

या परिपत्रकान्वये सर्व संबंधितांना कळविण्यात येते की, दिनांक २० जून २०२० रोजी संपन्न **झालेल्या ४७व्या मा. विद्या परिषद बैठकीतील विषय क्र.११/४७—२०२०**च्या ठरावानुसार प्रस्तुत विद्यापीठाच्या संलिग्नित महाविद्यालयांतील विज्ञान व तंत्रज्ञान विद्याशाखेतील पदव्यूत्तर स्तरावरील द्वितीय वर्षाचे खालील विषयांचे C.B.C.S. (Choice Based Credit System) Pattern नुसारचे अभ्यासक्रम शैक्षणिक वर्ष २०२०—२१ पासून लागु करण्यात येत आहेत.

1. M.Sc.-II Year-Botany

2. M.Sc.-II Year-Herbal Medicine

3. M.Sc.-II Year-Analytical Chemistry 4. M.Sc.-II Year-Biochemistry

6. M.Sc.-II Year-Physical Chemistry

5. M.Sc.-II Year-Organic Chemistry

7. M.Sc.-II Year-Computer Management 8. M.Sc.-II Year-Computer Science 9. M.Sc.-II Year-Information Technology 10. M.C.A. (Master of Computer Applications)-II Year

11. M.Sc.-II Year-Software Engineering 12. M.Sc.-II Year-System Administration & Networking

14. M.Sc.-II Year-Environmental Science

13. M.Sc.-II Year-Dairy Science

15. M.Sc.-II Year-Applied Mathematics 16. M.Sc.-II Year-Mathematics

17. M.Sc.-II Year-Microbiology

18. M.Sc.-II Year-Physics

19. M.Sc.-II Year-Zoology

20. M.Sc.-II Year-Biotechnology

21. M.Sc.-II Year-Bioinformatics

सदरील परिपत्रक व अभ्यासक्रम प्रस्तृत विद्यापीठाच्या www.srtmun.ac.in या संकेतस्थळावर उपलब्ध आहेत. तरी सदरील बाब ही सर्व संबंधितांच्या निदर्शनास आणुन द्यावी.

'ज्ञानतीर्थ' परिसर,

विष्णुप्री, नांदेड — ४३१ ६०६.

जा.क.: शैक्षणिक—१ / परिपत्रक / पदव्यत्तर—सीबीसीएस अभ्यासक्रम /

२०२०-२१/३३५

स्वाक्षरित/-

उपकलसचिव शैक्षणिक (१–अभ्यासमंडळ) विभाग

**दिनांक :** १६.०७.२०२०.

प्रत माहिती व पढील कार्यवाहीस्तव :

१) मा. कुलसचिव यांचे कार्यालय, प्रस्तृत विद्यापीठ.

- २) मा. संचालक, परीक्षा व मुल्यमापन मंडळ यांचे कार्यालय, प्रस्तृत विद्यापीठ.
- ३) प्राचार्य, सर्व संबंधित संलंगिनत महाविद्यालये, प्रस्तुत विद्यापीठ.
- ४) साहाय्यक कुलसचिव, पदव्युत्तर विभाग, प्रस्तुत विद्यापीठ.
- ५) उपकुलसचिव, पात्रता विभाग, प्रस्तृत विद्यापीठ.
- ६) सिस्टम एक्सपर्ट, शैक्षणिक विभाग, प्रस्तुत विद्यापीठ.

# SWAMI RAMANAND TEERTH MARATHWADA UNIVERSITY, NANDED

# M.Sc. PHYSICAL CHEMISTRY Second Year

# (SEMISTER III & IV)

#### **CBCS Pattern**

# w.e.f. Academic Year 2020-21

Semester	Paper	Course No.	Course	Periods / week	Total Periods	Marks
III Semester	XV	PCH-511	Advanced Spectroscopic Methods	4	60	4 Credits
	XVI	PCH-512	Solid State Chemistry	4	60	4 Credits
	XVII	PCH-513	Chemical Dynamics	4	60	4 Credits
	XVIII	PCH-514	Elective Paper (Any one) A] Statistical Thermodynamics B] Advanced Quantum Chemistry C] MOOC NPTEL Courses	4	60	4 Credits
	XIX		Seminar			1 Credit
					Total	17
IV Semester	XX	PCH-521	Radiation Chemistry	4	60	4 Credit
	XXI	PCH-522	Photochemistry	4	60	4 Credit
	XXII	PCH-523	Molecular Reaction Dynamics & Bio Physical Chemistry	4	60	4 Credit
	XXIII	PCH-524	Elective Paper (Any one) A] Electrochemistry B] Liquid State C] MOOC NPTEL Courses	4	60	4 Credit
	XXIV		Seminar			1 Credit
					Total	17
Lab Course Annual	XXV	LPCH-525	Lab course V	6	120	4 Credit
	XXVI	LPCH -526	Lab Course VI	6	120	4 Credit
	XXVII	LPCH -527	Lab Course VII	6	120	4 Credit
	XXVIII	LPCH -528	Lab Course VIII	6	120	4 Credit
					Total	16
					<b>Grant Total</b>	50

Note: 1) Each Laboratory Course of 6 Hrs duration should be completed in 6 Hrs per day.

- 2) Assesment shall consist of continuous assessment (CA) 25 % and end semester assessment (ESE)75%
- 3) Each student has to give one Seminar in each semester.
- 4) Research oriented project to be completed in 12 hrs per week (6hrs per day) having 100 marks. The assessment of project is done by external Examiner at the time practical examination

# M.Sc. Physical Chemistry Second Year semester Pattern

Semester	Paper	Course No	External (ESE)	Internal (CA)	Total
III	XV	PCH-511	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks]	Credits 4 100 marks
	XVI	PCH-512	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks	Credits 4 100 marks
	XVII	PCH-513	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks	Credits 4 100 marks
	XVIII	PCH-514	75 marks	25 marks.[2 tests:15 marks+Assignment:10 marks	Credits 4 100 marks
	XIX	Seminar	25 Marks		Credit 1
IV	XX	PCH-521	75 marks	25 marks.[2tests:15 marks+Assignment:10 marks]	Credits 4 100 marks
	XXI	PCH-522	75 marks	25 marks. [2tests:15marks+Assig nment:10 marks]	Credits 4 100 marks
	XXII	PCH-523	75 marks	25 marks. [2tests:15marks+Assig nment:10 marks]	Credits 4 100 marks
	XXIII	PCH-524	75 marks	25 marks [2tests:15marks+Assig nment:10 marks]	Credits 4 100 marks
	XXIV	Seminar	25 Marks		Credit 1
Lab course Annual pattern	XXV	LPCH-525	75 marks	25 marks [2tests:15marks+Assig nment:10 marks]	Credits 4 100 marks
	XXVI	LPCH -526	75 marks	25 marks [2tests:15marks+Assig nment:10 marks]	Credits 4 100 marks
	XXVII	LPCH -527	75 marks	25 marks [2tests:15marks+Assig nment:10 marks]	Credits 4 100 marks
	XXVIII	LPCH -528	75 marks	25 marks	Credits 4 100 marks

# M. Sc. Second Year, Semester-III

#### Paper-XV, [PCH-511]

#### **Advanced Spectroscopic Methods**

Credits: 04 Periods: 60

# **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.

# **SM-1: UV-Vis Spectroscopy:**

09P

Fieser-Woodward rules for conjugated dienes and carbonyl compounds, Fieser-Kuhn rules for polyenes. UV spectra of aromatic compounds and heteroaromatic compounds. Calculation of Lmax for the benzene derivatives (R-C<sub>6</sub>H<sub>4</sub>-C<sub>0</sub>-G) by A. I. Scott emperical rules.

#### **SM-2: IR spectroscopy:**

09P

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.

# SM-3: <sup>1</sup>H NMR Spectroscopy:

12P

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; <sup>19</sup>F and <sup>31</sup>P.

SM-4: <sup>13</sup>C NMR: 06P

Resolution and multiplicity of <sup>13</sup>C NMR, <sup>1</sup>H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE signal enhancement, off-resonance, proton decoupling, Structural applications of CMR.

#### **SM-5: Mass Spectroscopy:**

09P

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; General fragmentation rules: Fragmentation of various classes of organic molecules, including compounds containing oxygen, sulfur, nitrogen and halogens;  $\alpha$ ,  $\beta$ -, allylic and benzylic cleavage; McLafferty rearrangement.

#### **SM-6: Structural Problems:**

15P

- a) Combined problems on UV, IR, NMR and Mass spectral data for structure determination.
- b) Elucidation of structure of organic molecules using spectra (IR, PMR & CMR).

#### **Outcomes:**

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

#### **Reference Books:**

- 01. Spectroscopic Identification of Organic Compounds, R. M. Silverstern, G. C. Bassler and T. C. Morril.
- 02. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus.
- 03. Application of spectroscopy of organic compounds, J. R. Dyer.
- 04. Spectroscopy of organic compounds, P. S. Kalsi.
- 05. Organic Spectroscopy, William Kamp.
- 06. Organic Chemistry, R. T. Morrison and R. N. Boyd.
- 07. Practical NMR spectroscopy, M. L. Martin, J. J. Delpench and G. J. Martin.
- 08. Spectroscopic methods in organic Chemistry, D. H. William, I. Fleming.
- 09. 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.

# Paper–XVI, [PCH-512] Solid State Chemistry

Marks: 4 Credit Periods: 60

1. Solid State reactions 08P

General Principles, experimental procedures, co-precipitation as precursor to solid state reactions, kinetics of solid state reactions.

# 2. Crystal Defects and Non-Stoichiometry

14P

Perfect and imperfect crystals, intrinsic and extrinsic defects – point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects. Thermodyamics of Schottky and Frenkel defect formation colour centers, non-stocichiometry and defects.

## 3. Electronic Properties and Band Theory

24P

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.

Magnetic properties – classification of materials : quantum theory of paramagnetic cooperative phenomena – magnetic domains hysteresius.

4. Organic solids

Electrically conducting solids, organic charge transfer complex, organic metals, new superconductors.

#### **Books Referred**

- 1. Solid State Chemistry adn 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 Chemisty D.K. Chakarabarty, New Age International

#### **Objectives**

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

- > 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.

# Paper–XVII, [PCH-513] Chemical Dnyamics

Marks: 4 Credit Periods: 60

#### 1. Molecules in Motion

14P

- a. Molecular motion in gases: collision with walls and surface rate of effusion, migration down gradients, transport properties of a perfect gas.
- b. Motion in liquids :Structure of liquids, molecular motion in liquids conductivites of electrolyte solution, mobilities of ions conductivtes and ion-ion interactions.
- c. Diffusion : a Thermodynamic view, the diffusion equation, diffusion probabilities statistical veiw. Problems on every concept.

#### 2. Rate of chemical Reactions

08P

Experimental techniques rates of reactions, integrated rate laws, reactions approaching equilibrium, temperature dependence of reaction rates. According for the rate laws. Elementary reactions, consecutive elementary reactions, unimolecular reactions. Problems.

#### 3. Kinetics of Complex reactions:

19P

- a. Chain reactions: Structure of chain reactions, Explosions, photochemical reactions.
- b. Polymerization Kinetics: Chain Polymerization, stepwise Polymerization
- c. Catalysis and oscillations: Homogenous catalysis, autocatalysis, oscillating reactions, chemical chaos. Problems.

### 4. Molecular Reaction Dynamics:

19P

- a. Reactive encounters: Collision theory, diffusion controlled reactions.
- b. Activated complex theory: The reactions coordinate and transition state, Erying equation, thermodynamic aspects of activated complex theory.
- c. Dynamics of Molecular collisions : reactive collisions, Potential energy surfaces. Problems.

#### **Books Suggested:**

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

## **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.

- > 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 reaction dynamics
- They know about kinetics of the complex reactions which includes chain and polymerization reactions.

# Paper–XVIII, [PCH-514] Statistical Thermodynamics

Marks: 4 Credit Periods: 60

#### 1. Background concepts 08P

Combinatorial problems, 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, Langrange method of undetermined multipliers, distribution and most probable distribution. Problems.

# 2. Statistical Mechanics of a System of Independent Particles

10P

Introduction: distribution laws, partition functions and its significance, limit of applicability of various distribution laws, Relation between partition function and thermodynamics function, illustrative examples and problems.

#### 3. Types of Statistics

08P

Maxwell – Boltzmann statistics, Fermi-Dirac statistics and Bose-Einstein statistics

#### 4. Application of Statistical Mechanics

18P

- **a. Ideal gases:** Partition function of a monatomic gas. Thermodynamics function of a monatomic gas, diatomic and polyatomic gases. Internal rotation of a polyatomic molecule, heat capacity and the residual entropies of polyatomic molecules.
- **b. Solids:** Introduction, Thermal characteristics of crystalline solids. Einstein model, Debye modification, limitations and modifications of Debye theory and comparison between Debye theory and Einstein model.
- **c. Solutions :** Introduction, lattice modals, Ideal solution, non-ideal solutions, polymer solutions.

#### 5. Nuclear spin Statistics:

10P

Introduction, the mean symmetry and the nuclear spin, ortho and Para nuclear states, ortho, and para hydrogen, nuclear spin statistics of deuterium

6. Fluctuations: 06P

Introduction, the mean distribution and mean square deviation, fluctuation in energy in a canonical ensemble, fluctuations in density and radioactive disintegrations, The Brownian movement. Problems.

#### **Book Suggested:**

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

#### **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.

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

# M.Sc. Second Year Semester III Paper–XVIII, [PCH-514] Advanced Quantum Chemistry

Marks: 4 Credit Periods: 60

(Pre-requisite Mathematics at least up to five year B.Sc. Level is necessary. At least one PC among 4 students should be available)

1. Theoretical and Computational Treatment of Atoms and Molecules, Hartee-Fock Theory. 16P
Review of the principles of quantum mechanics, Born-Oppenheimer approximation.
Slater-condon rule. Hartree-Fock equation, Koopmans and Brillouin theories,
Roothan equation, Gaussion basis sets.

#### 2. Configuration Interaction and MC-SCF

16P

Introduction to Cl; full and truncated Cl theorties, size consistency. Introductory treatment of coupled cluster and MC-SCF methods.

#### 3. Semi – empirical theories

16P

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

## 4. Density functional theory

12P

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

#### **Book Referred**

- 1. modern quantum chemistry N.S. ostlund and A. Szabo Mcgrall hill.
- 2. Methods of molecular quamtum mechanics R. McWeeny and B.T. sSutcliffe.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. FrishFoussian Inc

#### **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.

- > Student acquire knowledge about theoretical and Computational Treatment to Atoms and Molecules.
- ➤ They have knowledge of Configuration Interaction and MC-SCF, Semi emerical theories
- > They have understanding about Density functional theory.

# M.Sc. Second Year Semester IV Paper–XX, [PCH-521] Radiation Chemistry

Marks: 4 Credit Periods: 60

# 1. Radioactivity:

Historical background, natural radioactive elements, general characteristics of  $\alpha$ ,  $\beta$ ,  $\gamma$  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  $\alpha$  decay,  $\beta$  decay – energetics of  $\beta$  decay, problems of  $\beta$  decay, Fermi's theory of  $\beta$  decay, nuclear excitation emission, Numerical.

#### 2. Nuclear Reactions and Reactors:

16P

11P

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- photoncluear reactions, stripping and pickup reactions, evaporation, spallation, fragmentation, direct nuclear reactions, thermonuclear reactions.

Fission energy, natural uranium reactor, four factor formula, classifications of nuclear reactors, reactor power, critical size of thermal reactor, breeder reactor, India's nuclear energy programme, nuclear waste management, energy from nuclear fission.

Numerical

# 3. Elements of Radiation Chemistry:

13P

**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 with matter, 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

#### 4. Effects of Radiation on Matter:

11P

Radiolysis of water and aqueous solutions. Radiolysis of water vapour, liquid water. Radiolysis of oxygenized water. The reduced species-hydrated electrons. Redox reactions due to ray irradiated, radiation induced colour centers in crystals (strong and release 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

#### 5. Application of radioactivity:

09P

Typical reactions involved in the preparations of isotopes: the scillard-chalmers reactions, radiochemical principles in the use of tracers, typical application of radioisotopes as tracers-chemical investigation, physio-chemical research, analytical applications, agricultural applications, industrial applications, use of nuclear radiations, radioisotope as a source of electricity.

#### **Reference Books:**

- Source of atomic energy by s. Glasstone, D. Van Nostrated co. INC
   Essentials of Nuclear Chemistry by H.J. Arnikar 4th Edn, New Age Inter. (p) Ltd.

- Essentials of Nuclear Chemistry by H.J. Armkar 4th Edn, New Age Inter. (p) Etd.
   Introduction to Nuclear Chemistry by B.G. Harvey.
   Nuclear Chemistry by M.G. Arora & M. Singh Anmol publication, New Delhi.
   Elements of Nuclear Chemistry by A.K. Srivastav, P.C. Jain, S. Chand & Co.
   A text book of Nuclear Chemistry by C.V. Shekar Deminat publication & distribution, New Delhi.
   Radiochemistry & Nuclear Chemistry, 3rd edn G. chappin, Butterwerth-Heinemann.

#### **Objectives**

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

- 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

# M. Sc. Second Year, Semester-IV Paper-XXI, [PCH-522] Photochemistry

Marks: 4 Credit Periods: 60

1. Photochemical Reactions 06P

Interaction of electromagnetic radiation with matter, types of excitation, rate of excited molecule, quantum yield, transfer of excitation energy, actionomety.

#### 2. Determination of Reaction Mechanism

06P

Classification, rate constant and life times of reactive energy states determination of rate constants of reactions, effects of light intensity on the rate of photochemical reactions, types of photochemical reactions – photo-dissociation, gas phase photolysis.

#### 3. Photophysical process in electronically excited molecules

14P

Types of photochemistry, pathways with Jabalonski diagram Radiation – Theory, Internal Conversion and intersystem crossing. Fluorescence emission Fluorescence and structure Triplet states and phosphorescence emission Emission property and the electronic configuration Photophysical kinetics of unimolecular process State diagrams Delayed fluorescence The effect of temperature on emission process

# 4. Photophyscial kinetics of Bimolecular Process

13P

Kinetic collisions and optical collision Bimolecular collisions in gases and vapors and the mechanism of Fluorescence quenching Collisions in solution: Kinetics of collisions quenching, stern-Volmer equation Concentration dependence of quenching and exciter formation Quenching by foreign substances.

#### 5. Some aspects of organic and Inorganic photochemistry

13P

Photoreduction and reactions Photoxidation and photooxygenation Cycloaddition reactions Woodward – Hoffman rule of electrocyclic reactions Chemiluminescence Transition mental complexes

#### 6. Some current Topics in photochemistry

08P

Photosynthesis Photo electrochemistry of excites state redox reaction . Solar energy conversion and storage

#### **Book Referred**

- 1. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherji, Wileyeastern
- 2. Essentials of Molecular Photochemistry a. Giolber and J. Baggot, Black well Scientific Publication
- 3. Molecular Photochemisty, N.J. Turro, W.A. Benjamin
- 4. Introductory Photochemistry, A. Cox and T. Camp. Mcgraw-Hill
- 5. Photochemistry R.P. Kundall and A. Gilbert, Thomson Nelson
- 6. Organic Photochemistry, J. Coxon and B. Halton, Camnridge University Press

# **Objectives**

- > To make the student familiar with a broad verities of photochemical systems and their applications.
- > They are expected to learnt about different photo physical process, their kinetics and able to write about the mechanism of photochemical reactions.
- ➤ They also expected to learn about the basic aspects of organic and inorganic photochemistry.

- ➤ Students know about different types of Photochemical Reactions
- > Students are able to write mechanism of different photochemical reactions
- > Students understand about different Photo physical process.
- > They understand about the Photophyscial kinetics of Bimolecular Process
- ➤ They learnt about some basic aspects of organic and Inorganic photochemistry

# M.Sc. Second Year Semester IV Paper–XXII, [PCH-523] Molecular Reaction Dynamics and Biophysical Chemistry

Marks: 4 Credit	Periods: 60
<ol> <li>Molecular Reaction Dynamics</li> <li>Reactive encounters: Collision theory, diffusion controlled reactions.</li> <li>Activated complex theory: The reaction coordinate and transition state, Erying equation, thermodynamic aspects of activated complex theory.</li> <li>Dynamics of Molecular collisions: reactive collisions, Potential energy surfaces. Problems.</li> </ol>	20P
<ul> <li>2. Biophysical Chemistry</li> <li>1. Biological Cell and its Constituents</li> <li>Biological cell structure and functions of proteins, enzymes DNA and RNA in living systems. Helix coil transition.</li> </ul>	03P
2. Bioenergetics Standard free energy change in biochemical reactions, exergonic, endergonic, Hydrolysis of ATP, synthesis of ATP from ADP	04P
3. 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.	06P
<b>4. Biopolymer Interactions</b> 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.	07P
<b>5. Thermodynamics of Biopolymer solutions.</b> Thermodynamics of biopolymer solutions, osmotic pressure, membrane equilibrium muscular contraction and energy generation in mechanoichemical system.	06P
6. Cell Membrane and Transport of lons Structure and functions of cell membrane, ion transport through cell membrane, irreversible thermodynamic treatment of membrane transport. Nerve conduction.	04P
7. Biopolymers and their molecular Weights Evaluation of size, shape, molecular Weight and expect of hydration of Biopolyment by various experimental techniques. Sedimentation equilibrium, hydrodynamic methods, diffusion, sedimentation velocity, viscosity, electrophoresis and rotational motions.	06P
8. Diffraction Methods Light scattering, low angle X-ray scattering, X-ray diffraction and photo correlation spectroscopy, ORD	04P

#### **Book Suggested:**

- 1. Principles opf BioChemistry 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

#### **Objectives**

- To acquire basic knowledge about how physical methods can be applicable to understand biological processes.
- For developing an understanding on how statistical mechanics can be applied to understand about biopolymers and the different biopolymer interactions.

- Students learnt about Biological Cell its Constituents and about Bioenergetics
- > They understand about the Statistical Mechanics in Biopolymers and about the different biopolymer Interactions
- ➤ They understand about the Thermodynamics of Biopolymer solutions.
- > They know about the different Diffraction Methods and photo correlation spectroscopy

# M.Sc. Second Year Semester IV Paper–XXIII, [PCH-524] Electrochemistry

Marks: 4 Credit Periods: 60

1. Introduction 08P

Basic Introduction to eletrolytic conductance, theory of electrolytic dissociation, mechanism of electrolytic conductance and the migration of ions. Problems.

#### 2. Free Energy and Activity

19P

Activity and activity coefficient, equilibrium and free energy changes, Debye-Huckel theory, 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, equilibria in electrolytes, strong intermaediates and weak electorlytes, soulubility, solubility product principle, soulubility for common ions and complexion, determination of instability constant, activity coefficient form soulubility, measurements solubility and Deye-Huckel theory. Problems

3. Reversible Cells

- a. Reversible and irreversible cells, reversible electrodes, application or emf measurements, concentration cells with a single electrolyte., amalgam concentration cells, electrode potential, potentials in nonaqueous soultions, factors affecting electrode potentials, rate or relectrode potentials, electrode potentials and wquilibruim constants, electrode potentials and soulbility proucts.
- b. Oxidation reduction syste: types of oxidations reduction systems, determination of oxidation reduction potentials. Problems.

#### 4. Dyanmic Electrochemistry:

14P

Process at electrodes., electrical double layer, rate of charge transfer, polarisation, electrochemical process, electrolysis, characteristics of working eclls,. Power production and corrosion, types of electrochemical corrosions, fuel cells, powere generation in fule cells, power storage, secondary cells, thermodynamics and kinetics of corrsion and their prevention methods, applications of electrolysis in electrorefining, electroplating and electrotyping. Problems.

## **Books Suggested:**

- 1. Text book of Physical Chemistry, Samuel. M.Glastone, LitternEducational publishing in., New York
- 2. Physical Chemeistry, P.W. Atkins (ELBS)
- 3. Introduction to electrochemistry, Samuel M. Glastone, LitternEducational. Publishing inc., New Yourl.
- 4. Theoritical electrochemistry, L. J. Antropov., Mir Publioshers, Moscow
- 5. Modern electrochemistry vol I & II Bokris J.O.M. and Reddy A.K.M (pLENUM)

#### **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 in electrochemistry
- ➤ They will be aware about electrochemical theory of corrosion and method of prevention of corrosion..

- 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 to solve numerical on it.
- > Students get knowledge about electrochemical theory of corrosion and method of prevention of corrosion..

# M. Sc. Second Year, Semester-IV Paper-XXIII, [PCH-524] Liquid State

Marks: 4 Credit Periods: 60

# 1. General properties of liquids

15P

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.

14P

Theory of liquids, partition function method or model approach; single cell models, communal energy and entropy LTD model, significant structure model.

#### 3. Distribution Function and Related Equations

18P

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 and computational Techniques.

13P

Spectroscopic techniques for liquid dynamic structure studies, Neutron and X-ray scattering spectroscopy 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.

#### **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.

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

# M. Sc. Second Year Laboratory Course-V, Paper- XXV, LPCH-525

Marks: 4 Credit Periods: 120

# **Spectroscopy**

- 1) To determine the indicator constant  $P_{K}^{\mathbb{N}}$  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 soectrophotmetric titration with EDTA
- 4) To investigate the effect of ionic strength on pKa of bromo cresol green and thus determine pkin (DVJ-211)
- 5) To invistigate the reaction kineties between K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and KI by spectrophotometry (TKC-223)
- 6) To determine simultaneously the dichromate and permanganate ions in the given soulution

#### **POLARIMETRY**

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

# REFRACTOMETRY

- 11) Determine the refractive indices of series of solution of a salt and determine the concentration of the salt in the given unknown solution.
- 12) Determine the molar refraction of ethyl, prooyl and butly acetate and show the constancy of contribution to the molar refraction amde by CH2 group
- 13) Determine the molar refraction of methyl acetate, ethyl acetate, n-hexane and carbon tetrachloride and calculate the atomic refraction of C, H and Cl atoms.
- 14) Study the variation of refractive index with composition of mixtures of carbon tetrachloride and ethyl aetate and determine the molar refraction of the given unknown mixture. VISCOSITY
- 15) Study the variation of viscosity with composition of 1) ethanol water II) methanol ethylidene chloride III) the formation of compound (TKC 25)
- 16) Determine the molecular weight of macromolecules (TKC 251)
- 17) Determine the iso-electric point of gelation and examine the effect of aging by viscometric methods (DVJ-29)

#### FLAME PHOTOMETRY

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

# M. Sc. Second Year Laboratory Course-VI, Paper– XXVI, LPCH-526

Marks: 4 Credit Periods: 120

#### **Potentiometer**

- 1) Titrate ferrous ammonium sulphate with cerric sulophate and find out formal redox potential of  $Re^{2+/}Fe^{3+}$  and  $Ce^{3+/}Ce^{4+}$  system
- 2) Titrate potentionmetriaclly phosphoric acid solution against NaOH and calculate Pk1, Pk2 and Pk3 of the acid
- 3) Titrate potentiometrically NaCl soulution against AgNO3 and find out the concentration of NaCl and hence determine the solubility product of AgCl
- 4) To determine the standad free energy change ^G0 and equilibrium constant for the reaction. Cu +2Ag+ ----- Cu++ Ag (TKC-167)
- 5) Determine the activity coefficient of sivlver ions using a concentration cell without transference (TKC-154)

#### PH METRY

- 6) To determine the product lignd stability constant of an organic acid and the metal ligand stability constant of its complex by pH measurements (TKC-176)
- 7) Determine the Hammett constant of a given substituted benzoic acid by pH measurements (TKC-170)
- 8) Determine the pH values of various mixtures of sodium acetate and acetic acid in aqueous solution and hence find out the dissociation constant of the acid (TKC-173)
- 9) To determine the hydrolysis constant of aniline hydrochloride by pH measurements (TKC-174)

# Conductometry

- 10) To determine the thermodynamic dissociation constant of weak acid conductometrically.
- 11) Investigate the kinetics of basic hydrolysis of ethyl acetate conductometrically.
- 12) Conductometric titration of a mixture of strong acid weak acid and a salt (DVJ)
- 13) To determine the degree of hydrolysis and hydrolysis constant of sodium acetate Conductometrically

#### **MAGNETO – CHEMISTRY**

- 14) To determine the magnetic susceptibility and number of unpaired electrons in a given compound.
- 15) Verification of Weidemann's law using nickel chloride solutions

#### SURFACE TENSION

- 16) Studythe effect of surfactant (n-propyl alcohol) at various concentrations on the surface tension of water and hence determine the limiting cross sectional area of alcohol molecule bystalagmomenter
- 17) Determine the parachor of a solid by stalagmometer

#### **THERMODYNAMICS**

- 18) Determine the partial molar volume of ethanol and water in a given composition by density measurements.
- 19) To determine heat of neutralization of strong acid and heat of ionization of weak acid calorimetrically.
- 20) To determine the integral hear of solution of KNO<sub>3</sub>
- 21) To determine the heat of dissociation of benzoic acid in water
- 22) To determine heat of precipitation of BaSO<sub>4</sub>

# M. Sc. Second Year Laboratory Course-VII, Paper– XXVII, LPCH-527

Marks: 4 Credit Periods: 120

#### **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<sub>2</sub>O<sub>2</sub> 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 distribution method.

#### **ADSORPTION**

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

#### **SECTION (A): APPLICATION OF COMPUTER IN CHEMISTRY**

- 10) Calculate the mole fraction of liquid mixture from given data by using Excel-Software
- 11) Determine the excess molar volume of binary liquid / ternary liquid mixture by using Excel / MATLAB softwere from given data.
- **12**) Calculate mean deviation, relative mean deviation and standard deviiation byusing Excel / MATLAB softwere from given data.
- 13) Calculate the excess viscosity of binary / ternary liquied mixtures by using Excel/Matlab
- **14**) Plot the graph of Emf Vs volume of titrant added E/V Vs volume of titrant added from the experimentally observed data by using Excel softwere and justify thenature of graph.
- **15**) Determine proton ligand formation number (nA) dissociation constant (pK) andmetal—ligand stability constant (pL) by using Excel programme.
- 16) Draw the molecular structure of given molecules using chem. Draw Windows.
- 17) Draw the graph of ionization potantial Vs. Atomic number or II, III, IV, V, VI row elements and justify the nature.
- **18**) Draw the graph between atomic number Vs I.P. and electro-negativity of first group elements by using Excel softwere from given data and justify the nature of the graph.

M. Sc. Second Year M. Sc. Second Year Laboratory Course-VIII, Paper– XXVIII, LPCH-528

Marks: 4 Credit Periods: 120

#### **PROJECT**

The students will develop utilities such as analytical spectra, simulation programmes 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.

#### **SEMINAR**

The students will have to give at least one seminar in each semester in their subject of specialization. For this submission of synopsis of seminar delivered by every student is compulsory which is to be produced before exa