

**Rayat Shikshan Sanstha's  
Yashwantrao Chavan Institute of Science, Satara (Autonomous)  
Department of Chemistry**

**M.Sc. II Physical Chemistry: Programme Structure**

Course Code	Title of Course	Credits	Teaching Scheme (h/w)		Evaluation Scheme (Marks)			
			L	P	ISE-I	ISE-II	ESE	Total
<b>M.Sc.-II Semester-III</b>								
MCT-P-301	Advanced Quantum Chemistry	4	4	-	10	10	80	100
MCT-P-302	Electrochemistry	4	4	-	10	10	80	100
MCT-P-303	Molecular Structure –I	4	4	-	10	10	80	100
MCT-P-304	Applied Physical Chemistry	4	4	-	10	10	80	100
MCP-P-305	Chemistry Practical-V	4	-	12	-	-	85+15 (Pro)	100
MCP-P-306	Chemistry Practical-VI	4	-	12	-	-	85+15(Pro)	100
<b>Total</b>		<b>24</b>	<b>16</b>	<b>24</b>	<b>40</b>	<b>40</b>	<b>520</b>	<b>600</b>
<b>M.Sc.-II Semester-IV</b>								
MCT-P-401	Thermodynamics and Molecular Modelling	4	4	-	10	10	80	100
MCT-P-402	Chemical Kinetics	4	4	-	10	10	80	100
MCT-P-403	Molecular Structure-II	4	4	-	10	10	80	100
MCT-P-404	Physicochemical Techniques	4	4	-	10	10	80	100
MCP-P-405	Chemistry Practical-VII	4	-	12	-	-	85+15 (Pro)	100

MCP-P-406	Chemistry Practical-VIII	4	-	12	-	-	85+15(Pro)	100
<b>Total</b>		<b>24</b>	<b>816</b>	<b>24</b>	<b>40</b>	<b>40</b>	<b>520</b>	<b>600</b>

## EVALUATION OF COURSE:

### 1. THIRD SEMESTER

Semester III										
Paper	ESE	Internal Exam		Practical					Total	Grand Total
		ISE-I	ISE-II		Exam	Journal	Project Part-II	Day to day performance		
MCT-P-301	80	10	10	MCP-P-305-V	70	10	15	5	100	
MCT-P-302	80	10	10							
MCT-P-303	80	10	10	MCP-P-306-VI	70	10	15	5	100	
MCT-P-304	80	10	10							
<b>Total</b>	<b>320</b>	<b>40</b>	<b>40</b>		<b>140</b>	<b>20</b>	<b>30</b>	<b>10</b>	<b>200</b>	<b>600</b>

### 2. FOURTH SEMESTER

Semester IV										
Paper	ESE	Internal Exam		Practical					Total	Grand Total
		ISE-I	ISE-II		Exam	Journal	Project Part-II	Day to day performance		
MCT-P-401	80	10	10	MCP-P-405-V	70	10	15	5	100	
MCT-P-402	80	10	10							
MCT-P-403	80	10	10	MCP-P-406-VI	70	10	15	5	100	
MCT-P-404	80	10	10							
<b>Total</b>	<b>320</b>	<b>40</b>	<b>40</b>		<b>140</b>	<b>20</b>	<b>30</b>	<b>10</b>	<b>200</b>	<b>600</b>

## Structure and Title of Papers of M. Sc. II Course

- **M. Sc. II Semester III**

**Paper IX:** Advanced Quantum Chemistry

**Paper X:** Electrochemistry

**Paper XI:** Molecular Structure –I

**Paper XII:** Applied Physical Chemistry

**Paper XII:** Elective I  
Radiation And Photochemistry

- **M. Sc. II Semester IV**

**Paper XIII:** Thermodynamics and Molecular Modelling

**Paper XIV:** Chemical Kinetics

**Paper XV:** Molecular Structure-II

**Paper XVI:** Physicochemical Techniques

**Paper XVI:** Elective II  
Surface Chemistry  
Chemistry of Materials

<b>Course Code</b>	<b>Elective –I</b>	<b>Course Code</b>	<b>Elective –II</b>
MCT-P-304-A	Radiation And Photochemistry	MCT-P-404-A	Surface Chemistry
-	-	MCT-P-404-B	Chemistry of Materials

**Rayat Shikshan Sanstha's**  
**Yashavantrao Chavan Institute of Science, Satara (Autonomous)**  
**Department of Chemistry**  
**Autonomy Draft Syllabus of M. Sc. Part II (Physical Chemistry)-2019-20**

**GENERAL OBJECTIVES OF THE COURSE:**

1. To educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic Laboratories.
2. To provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on qualitative and quantitative technique.
3. To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of interdisciplinary branches of chemistry involving applied organic, inorganic, physical, analytical, industrial, pharmaceutical, polymer, nano science & technology.
4. To conduct lesser written tests and to encourage on non-written tests.
5. To focus on encouraging students to conduct various academic activities like midterm tests, online tests, open book tests, tutorial, surprise test, oral, seminar, assignments and seminar presentation.

**Learning outcomes:**

1. A graduate with a Master's degree in Chemistry has in-depth and detailed functional knowledge of the fundamental theoretical concepts and experimental methods of chemistry.
2. The graduate has expert knowledge of a well-defined area of research within chemistry. The graduate has specific skills in planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques. Skilled in examining specific phenomena theoretically and/or experimentally, the graduate is able to contribute to the generation of new scientific insights or to the innovation of new applications of chemical research.

<b>STRUCTURE OF COURSE: SEMESTER</b>				
<b>Semester</b>	<b>Paper No.</b>	<b>Title</b>	<b>Total Number of lectures/ practical's</b>	<b>Credits</b>
<b>Semester-III</b>	<b>Theory Course</b>			
	MCT-P-301	Advanced Quantum Chemistry	60hrs	4
	MCT-P-302	Electrochemistry	60hrs	4
	MCT-P-303	Molecular Structure –I	60hrs	4
	MCT-P-304	Applied Physical Chemistry	60hrs	4
	<b>Elective paper</b> MCT- P-304 A	Radiation And Photochemistry	60hrs	4
	<b>Practical Course</b>			
	MCP-P-305	Chemistry Practical-V		4
MCP-P-306	Chemistry Practical-VI		4	
<b>Semester-IV</b>	<b>Theory Course</b>			
	MCT-P-401	Thermodynamics and Molecular Modelling	60hrs	4
	MCT-P-402	Chemical Kinetics	60hrs	4
	MCT-P-403	Molecular Structure-II	60hrs	4
	MCT-P-404	Physicochemical Techniques	60hrs	4
	<b>Elective Paper</b> MCT-P-404 A	Surface Chemistry	60hrs	4
	MCT-P-404 B	Chemistry of Materials	60hrs	4
	<b>Practical Course</b>			
	MCP-P-405	Chemistry Practical-VII		4
	MCP-P-406	Chemistry Practical-VIII  OR Internship, Industrial Training		4

- The semester examination will be conducted at the end of each term (both theory and practical examination)
- Theory paper will be of 80 marks each and 20 marks for internal evaluation test conducted in the mid of the term. Two practicals will be of 100 marks each.

- Question papers will be set in the view of the entire syllabus and preferably covering each unit of the syllabus.

### **Laboratory Safety Equipment's:**

#### **Part: I Personal Precautions:**

1. All persons must wear safety Goggles at all times.
2. Must wear Lab Aprons/Lab Jacket and proper shoes.
3. Except in emergency, over – hurried activities is forbidden.
4. Fume cupboard must be used whenever necessary.
5. Eating, Drinking and Smoking in the laboratories strictly forbidden.

#### **Part: II: Use of Safety and Emergency equipment:**

1. First aid Kits
2. Sand bucket
3. Fire extinguishers (dry chemical and carbon dioxide extinguishers)
4. Chemical Storage cabinet with proper ventilation
5. Material Safety Datasheets.
6. Management of Local exhaust systems and fume hoods.
7. Sign in register if using instruments

**MCT-P-301: ADVANCED QUANTUM CHEMISTRY**

**Learning objectives :**

- i) Distinguish between basics of quantum chemistry
- ii) Understand the variation and perturbation
- iii) Expect the theoretical Ab initio methods
- iv) Understand various semi-empirical methods.

**UNIT–I: Basics of Quantum Chemistry (15)**

Brief review of basic principles of quantum mechanics. Exact solution of Schrödinger wave equation for rigid rotator, linear harmonic oscillator and hydrogen and hydrogen like atoms. Transition dipole moment integral and selection rules for rotational, vibrational and electronic transitions.

**UNIT- II: Variation Principle and Hückel Molecular Orbital Theory (15)**

Variation principle and its application to some simple systems. Hückel molecular orbital theory – Assumptions of HMO theory, the Born-Oppenheimer approximation, -electron approximation, Secular determinant and secular equations, Hückel rule and aromaticity, HMO calculations for organic molecules, free valence index and prediction of chemical reactivity, use of molecular symmetry for simplification of HMO calculations, HMO treatment for molecules containing heteroatoms, extended Hückel methods

**UNIT –III: Ab initio methods (15)**

Self-consistent field (SCF) theory, Hartree-Fock (HF) method, quantum particles and their spins, properties of Slater determinant, HF equation, restricted Hartree-Fock (RHF) and unrestricted Hartree-Fock (UHF) models, Fock matrix, HF calculations, Roothan-Hall equations, Koopman's theorem, electron correlation method. Basis sets: Slater type orbitals (STO), Gaussian type orbitals (GTO), difference between STO and GTO, energy calculations using such orbitals for multielectron systems, classification of basis sets, minimal basis sets, energy calculations for H-atom using STO basis sets at different levels, double- and triple-zeta basis sets, valence-split basis sets, polarized basis sets, truncation and superposition errors in basis sets, methods to overcome above errors. Correlation energy, configuration interactions, many body perturbation theory, Möller-Plesset perturbation, coupled cluster method. Introduction to various software packages for performing ab initio and density functional theory calculations

**UNIT- IV: Semi-empirical methods and Molecular Mechanics, Semi-empirical Methods**

**(15)**

Introduction, need of semi-empirical methods, zero differential overlap (ZDO) approximation, neglect of differential overlap (NDO) method, complete neglect of differential overlap (CNDO), intermediate neglect of differential overlap (INDO), modified intermediate neglect of differential overlap (MINDO), modified neglect of differential overlap (MNDO), neglect of diatomic differential overlap (NDDO). AM1, PM3, PM5, PM6 etc. methods,

Hamiltonian in semi-empirical methods, comparisons in various above mentioned methods, limitations of semi-empirical methods. Introduction to various software packages for performing semi-empirical calculations.

### **Learning Outcomes:**

- i) Student should understand the difference between theoretical quantum chemistry and practical chemistry with respect to energy
- ii) They must know the exact concept of Huckel Molecular Orbital Theory
- iii) They must know the application of quantum chemistry practically in real life
- iv) They should understand difference between ab-initio and semi-empirical methods

### **REFERENCE BOOKS:**

1. A.K. Chandra, Introductory Quantum Chemistry, 4<sup>th</sup> Edition, Tata McGraw- Hill, New 1994.
2. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A molecular Approach, Viva Books, New Delhi, 1998.
3. D. A. McQuarrie, Quantum Chemistry, Viva Books, New Delhi, 2003.
4. P. W. Atkins, Physical Chemistry, 6<sup>th</sup> Edition, Oxford University press, New York, 1998.
5. P. Atkins and R. Friedman, Molecular Quantum Mechanics, 4<sup>th</sup> Edition, Oxford University Press, New York, 2005.
6. Leach, A.R. Molecular Modelling. Principles and Applications, 2<sup>nd</sup> Edition, Prentice-Hall, Harlow, England, 2001.
7. K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.
8. Becker, O.; MacKerell, A.D.; Roux, B.; Watanabe, M. eds. Computational Biochemistry and Biophysics, Marcel Dekker, New York, 2001.
9. F. Jensen, Introduction to Computational Chemistry, 2<sup>nd</sup> Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.
10. D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.

## **Learning objectives**

- i) Understand electrokinetic phenomena of solutions
- ii) Expect the detailed study of ion-solvent interaction
- iii) Expect the exact meaning of electrode reactions in fuel cell
- iv) Understand significance of fuel cells

### **UNIT –I: Electrokinetic phenomena**

**(15)**

Electrical double layer, theories of double layer, electro-capillary phenomena, electro-capillary curve. Electro-osmosis, electrophoresis. Streaming and Sedimentation potentials. Zeta potentials and its determination by electrophoresis, influence of ions on Zeta potential.

### **UNIT- II: Ion-solvent Interactions**

**(15 )**

Structure of water, hydration, heats of hydration of electrolytes, individual ions and their comparison, calculation of heats of hydration( Born, Van Arkel& de Boer, Bernal-Fowler methods), entropy of hydration and hydration numbers. Ion transport in solutions, diffusion, chemical potential and work of transport, Ficks laws, expressions for flux and diffusion coefficient. Ionic liquids: Introduction, difference between electrolytes and ionic liquids, diffusion in fused salts, viscosity and diffusion coefficient in molten salts.

### **UNIT-III: Electrode reactions**

**(15)**

Electrified interface, electron transfer under interfacial electric field, symmetry factor, electrode at equilibrium, exchange current density, over potential, Butler-Volmer equation, high field and low field approximations, Tafel equations, kinetics of discharge of hydrogen ions . Diffusion over potentials. Electrode kinetics of semiconductor/ solution interface; n and p type semiconductor, current-potential relation of n and p type semiconductors.

### **UNIT-IV: Fuel cells and corrosion**

**(15)**

Significance of fuel cells: hydrogen - oxygen, hydrocarbon - air, natural gas and carbon monoxide, air fuel cells.

**Corrosion:** concept and importance, mechanism of corrosion and Pourbaix

## **Learning Outcomes:**

- i) Student should understand real application of electrochemistry in fuel cell
- ii) They must know the role of corrosion in fuel cell and electrochemistry
- iii) They must know electrode reactions for the development of green energy
- iv) They should understand the role of ionic liquids in recent research

## **REFERENCE BOOKS:**

1. An Introduction to Electrochemistry by S. Glasstone
2. Modern Electrochemistry Vol. I & II by J. O. M. Bockris and A.K.N. Reddy .
3. Physical Chemistry by S. Glasstone
4. Electrolytic Solutions by R. A. Robinson and R. H. Stokes
5. Physical Chemistry by P. W. Atkins. ELBS.

## MCT-P-303: MOLECULAR STRUCTURE - I

### Learning objectives

- i) Understand symmetry of different inorganic and organic molecules
- ii) Expect the study of aspects of group theory
- iii) Understand the IR, electronic and Raman spectroscopy
- iv) Understand how can analyse electronic spectra of polyatomic molecules

### **UNIT- I: Symmetry properties of molecules and group theory (15)**

Symmetry elements, symmetry operations and point groups, properties of group, symmetry operations as a group, multiplication table. Classes of symmetry operations, basis, representative and matrix representations of operations. Reducible and irreducible representations, orthogonality theorem. Properties of irreducible representations. Constructions of character table for point groups. Explanations for the complete character table for a point group. Representations of vibrational modes in nonlinear molecules. Infrared and Raman activities of normal modes of vibrations.

### **UNIT- II: Introduction of spectroscopy and Rotational Spectra (15)**

Characterization of electromagnetic radiation, The qualification of energy, Regions of Spectrum, transition probability, the width and intensity of spectral transitions. Classification of molecules according to their moment of inertia, Rotational spectra of rigid and non rigid diatomic molecules. The intensities of spectral lines. The effect of isotopic substitution. Polyatomic and symmetric top molecules. The Stark effect.

### **UNIT- III: Infrared spectroscopy and Raman Spectroscopy (15)**

Diatomic molecules: Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero point energy, isotope effect. The anharmonic oscillator, the diatomic vibrating rotator, the interactions of rotations and vibrations.

Polyatomic molecules: Fundamental vibrations and their symmetry, overtone and combination frequencies. The influence of rotations and molecular spin on the spectra of polyatomic molecules. Analysis by Infrared techniques.

Raman Spectroscopy: Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Polarization of light and the Raman effect. Structure determination from Raman and Infra-red spectroscopy.

### **UNIT – IV: Electronic Spectroscopy (15)**

General nature of band spectra. Beer- Lambert Law integrated absorption coefficient and oscillator strength. Term symbols for atoms and molecules. The hydrogen atom and hydrogen like species spectrum.

Sequences and progressions, the vibrational course structure and rotational fine structure of electronic band. The Franck-Condon principle, dissociation energy and dissociation products. Birge-Sponer extrapolation. The Fortrat diagram. Predissociation, classification of electronic states.

The spectrum of molecular hydrogen. Electronic spectra of polyatomic molecules. Chemical analysis by electronic spectroscopy. (d-d), ( ) and ( -n\*) transitions. Photochemical mechanism of vision.

### **Learning Outcomes:**

- i) Student should understand real application spectroscopy in practice
- ii) They must know details of electronic, IR and Raman Spectroscopy
- iii) They must know elements of symmetry for all molecules
- iv) They should understand term symbols for atoms and molecules

### **REFERENCE BOOKS:**

1. Fundamental of molecular spectroscopy by C. N. Banwell Tata McGraw Hill.
2. Physical Chemistry by P. W. Atkins , ELBS, 1986
3. Symmetry, Orbitals and spectra by M. Orchin & H. Jaffe, Willey , interscience.
4. Chemical applications of group theory by F. A. Cotton Willey , interscience
5. Symmetry in chemistry by H. Jaffe and M .Orchin , Jhonwilley.
6. Group theory and its applications to chemistry by K. V. Ramen , Tata McGraw Hill.
7. Molecular Structure and Molecular Spectra by G. Herzberg, Van Nostrand .
8. Molecular Spectroscopy by I. N. Levine , Willey interscience.
9. Molecular Spectroscopy by G. M. Barrow.

## **MCT-P-304 Applied Physical Chemistry**

### **Solid State Chemistry and catalysis**

#### **Learning objectives**

- i) Understand different methods of X-ray structure analysis of crystals
- ii) Expect the study of various solid state reactions
- iii) Understand the kinetics of catalysis
- iv) Distinguish between molecules, nanoparticles and bulk materials

#### **UNIT-I: The solid state**

**(15)**

Introduction, laws of crystallography, lattice types, X-ray diffraction, Bragg's equation, Miller indices, Bragg Method, Debye-Sherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-Ray intensities, structure factor and its relation to intensity and electron density, phase problem, procedure for an X-ray structure determination.

#### **UNIT –II: Solid State Reactions**

**(15)**

General principle, types of reactions: Additive, structure sensitive, Decomposition and phase transition reactions, tarnish reactions, kinetics of solid state reactions, factors affecting the reactivity of solid state reactions.

### **UNIT–III: Electronic Properties and Band Theory**

(15)

Metals, insulators and semi conductors, free electron theory and its applications, electronic structure of solids, band theory, band structure of metals, insulator, and semiconductors, doping in semiconductors, p- n junction, superconductors, Molecular materials, Organic materials, some examples of organic semiconductors, charge carrier injection and transport, Optical properties of organic semiconductors, applications and devices involving optical properties, luminescence photoluminescence, effect of impurity levels on photoluminescence, light emitting diodes, luminous efficiency, photo-conduction and photoelectric effects, laser, principle of laser action, solid state laser and their applications.

### **Unit-IV Catalysis**

(15)

i) Fundamentals of adsorption and catalysis: Physical and Chemical adsorption – adsorption isotherms: evaluation, chemisorption on metals and metal oxides. Catalysis: concept of activity, selectivity, poisoning, promotion and deactivation. Types of catalysis: homogeneous, heterogeneous. Heterogeneous catalysis and catalytic kinetics: concept of Langmuir-Hinshelwood

(4L)

ii) Preparation and Characterization of Catalyst: general methods for 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, FT-IR and thermal methods

(4L)

iii) Nanomaterials and Catalysis: General definition, Nanochemistry basics, distinction between molecules, nanoparticles and bulk materials. Physicochemical considerations of nanomaterials. Size-dependent properties.

(3L)

iv) Catalysis in green chemistry and environmental applications: Purification of exhaust gases from different sources: auto-exhaust catalysts (petrol vehicles, diesel vehicles), VOC removal; ozone decomposition; photocatalysis in effluent treatment.

(2L)

v) Photo-catalysis: Photoprocesses at metals, oxides and semiconductors: concepts and mechanism. Photocatalysis application in organic pollutant degradation present in water and air.

(2L)

### **Learning Outcomes:**

- i) Student should understand the applicative aspect of nanochemistry
- ii) They must know details of characterization methods for catalyst
- iii) They should understand procedure for an X-ray structure determination
- iv) They must know role of heterogeneous catalysis in recent research

### **REFERENCE BOOKS :**

- 1) Molecular Photochemistry , N. J. Turro, W.A. Benjamin
- 2) Fundamentals of Photochemistry , K. K. Rohatagi - Mukherji, Wiley - Eastern

- 3) Elements of Inorganic Photochemistry : G. S. Ferraudi , Wiley
- 4) Concepts of Inorganic Photochemistry , A.W. Adamson & P. J. Fleischauer , Wiley
- 5) A Guide To lasers in chemistry , Gerald R. Van Hecke& Kerry K. Karukstis.
- 6)Photochemistry , R.P. Kundall, A Gilbert, Thomson Nelson
- 7) W. Adamson, Physical Chemistry of Surfaces , Wiley Intersciences, 1990 (5th edition) 1990.
- 8) Bond, G C, Heterogeneous Catalysis: Principles and Application. Oxford University Press 1987
- 9) D.K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, Hardcover - Oct 2008 New Age International Publishers)
- 10) B.C. Gates, Catalytic Chemistry, John Wiley and Sons Inc. (1992).
- 11) G. Cao, Nanostructures and Nanomaterials - Synthesis, Properties and Applications, World-Scientific, 2004.
- 12) P.T. Anastas and J.C. Warner, Green Chemistry, theory and practice,
- 13) Nick Serpone and EzioPelizzetti, Photocatalysis: Fundamentals and Applications, Wiley, New York, NY, 1989.

## MCT-P-304-A Elective Paper: Radiation And Photochemistry

### Learning objectives

- i) Realize the types of radiation, Lasers
- ii) Understand the basics of photochemistry with respect to organic photochemistry
- iii) Expect the study of bond selective chemistry of light atom molecules
- iv) Expect the study of photodegradation of polymers

**UNIT – I: Radiation Chemistry** **(15)**  
Introduction, Radiation Types, their characteristics, Radiation in chemical processes.

**UNIT – II: Lasers and Lasers in Chemistry** **(15)**  
Introduction, characteristics of laser, uses of lasers in chemical process, laser induced chemical reactions, organic photochemistry, lasers as a photochemical tool, laser induced selective bond chemistry , overview , bond selective chemistry of light atom molecules.

**UNIT – III: Basics of photochemistry** **(15)**  
Electrochemistry of excited states , life time measurements , flash photolysis, energy dissipation by radiative and non-radiative processes, properties of excited states, structure , dipole moment, acid-base strength, reactivity , photochemical kinetics, calculations of rates of radiative process , bimolecular quenching, Luminescence for sensors and switches , charge transfer excited state, photoinduced electron transfer reactions.

**UNIT –IV: Miscellaneous Photochemical reaction** **(15)**  
Photo-fries reaction of anilides, photo - fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog, photodegradation of polymers, photochemistry of vision.

## Learning Outcomes:

- i) Student should understand the applicative aspect of radiation chemistry and photochemistry
- ii) They must know details of photo degradation chemistry.
- iii) They must explain the role of radiation and photochemistry in recent advances of science.
- iv) They should understand energy dissipation by radiative and non-radiative processes

## REFERENCE BOOKS:

- 1) Molecular Photochemistry , N. J. Turro, W.A. Benjamin
- 2) Fundamentals of Photochemistry , K. K. Rohatagi - Mukherji, Wiley - Eastern
- 3) Elements of Inorganic Photochemistry : G. S. Ferraudi , Wiley
- 4) Concepts of Inorganic Photochemistry , A.W. Adamson & P. J. Fleischauer , Wiley
- 5) A Guide To lasers in chemistry , Gerald R. Van Hecke& Kerry K. Karukstis.
- 6) Photochemistry , R.P. Kundall, A Gilbert, Thomson Nelson

## M.Sc. Part-II, (Sem-III)

### Physical Chemistry Practical MCP-P-305 Course-V and MCP-P-306 VI

**Course Objective:** Students should

- 1) Study instrumental analysis
- 2) study the determination of thermodynamic parameters for electrochemical reactions.
- 3) Learn to determine order of reactions, equivalence conductance of electrolytes.

#### I) Potentiometry

1. To determine instability constant & stoichiometry of silver ammonia complex potentiometrically.
2. Determination of Thermodynamic Parameters for electrochemical reactions.

(To determine  $G^\circ$ ,  $H^\circ$  and  $S^\circ$  for the formation of 1 mole cadmium in 1 wt. % amalgam at 25<sup>o</sup> C and activity coefficient of solution).

#### II) Spectrophotometry

1. To determine pK value of methyl red indicator at room temperature spectrophotometrically.
2. To determine stoichiometry & stability constant of ferric Sulphosalicylic acid/ salicylic acid complex by Job's Method and mole ratio method spectrophotometrically.
3. To determine equilibrium constant of reaction



#### III) Amperometry

To determine unknown concentration of Iodine using amperometry

#### IV) Chemical Kinetics

To determine the order of reaction between acetone and iodine catalysed by acid.

#### V) Conductometry

To determine equivalent conductance at infinite dilution of strong electrolytes and weak acid by using Kohlrausch Law and dissociation constant for weak acid conductometrically.

#### VI) Cryoscopy

To determine molecular weight and state of benzoic acid in benzene.

#### VII) Moving boundary Method

To determine transport of H<sup>+</sup> ions by using Moving boundary method.

### **VIII) pH - Metry**

To determine dissociation constant of carbonic acid pH metrically.

### **IX) Polarography**

To determine half wave potential of a given ion using half height method, differential method and wave equation method

### **X) Latent heat of Fusion**

Determination of latent heat of fusion of a given solid.

### **XI) Thermochemistry**

Determination of heats of dilution and integral heat of solutions.

**Any other suitable experiments may be added.**

### **Course Outcomes : After completions of experiments students should**

- 1) Understand instrumental analysis.
- 2) Understand operating of various instruments for analysis.
- 3) Understand chemical kinetics, thermochemistry and various physical properties.

### **REFERENCE BOOKS:**

1. Chemical Kinetics by K. J. Laidler.
2. Practical of physical chemistry by A.M. James and F.E.Prichard
3. Vogel's textbook of quantitative analysis by J.Bossett, Denny, Jeffery
4. Lehninger principles of Biochemistry by David L.Nelson, Michael M.cox
5. Instrumental methods of analysis by Willard, Deon, Frank A. Settle
6. Findlay's Practical Chemistry by B.P.Lavitt and J.A.Kitchner
7. Experiens in physical chemistry by David P. Shoemaker
8. An Introduction to Electrochemistry by S. Glasstone
9. Experimental Physical Chemistry by F. Daniels and J. Williams
10. Experimental Physical Chemistry by R.C.Das and B. Behera
11. Practical Physical Chemistry : B. Viswanathan and P.S. Raghavan

**MCT-P-401: Thermodynamics And Molecular Modelling**

**Learning objectives :**

- i) Realize the modern and classical quantum principles
- ii) Understand the statistical and molecular mechanics
- iii) Expect the study of molecular dynamic simulation methods
- iv) Understand the the role of non-equilibrium in thermodynamics

**UNIT-I: Modern Theoretical Principles (15)**

Exact and inexact differential expressions in two variables. Total differentials. Techniques of partial differentiations. Transformation of variables. Maxima and minima. Integrating factors, Paff differential equations, Caratheodary's theory. Legendre transformations. Derivation of thermodynamic identities. The second law of thermodynamics, classical formulations, mathematical consequences of second law. Entropy changes, Clausius inequality. Free energy concept. General condition of equilibrium. Thermodynamic potentials.

**UNIT- II: Statistical and Molecular Mechanics (08)**

Ensembles, ensemble average and time average of the property, ergodic hypothesis, partition functions and thermodynamic properties, classical and quantum statistics, properties of photon gas, thermodynamic properties bosons, use of quantum statistics for evaluation of absolute entropies, condensation of helium, Fermi energy, electron gas in metals.

Heat capacity of solids, Einstein and Debye specific heat equations. Characteristic temperatures. Debye  $T^3$  law

**Molecular Mechanics: (07)**

Introduction, the Morse potential model, harmonic oscillator model, force fields development, various energy terms and non-covalent interactions included in force fields, Lennard-Jones type and truncated Lennard-Jones potentials, Kihara potential, commonly used force fields, parameterization, introduction to software packages used for performing molecular mechanics.

**UNIT –III: Molecular Dynamic Simulation Methods (15)**

Introduction, microscopic and macroscopic properties, time scale of chemical/biological process, force field methods, bonded and non-bonded interactions, advantages and limitations of Force Field Methods, molecular dynamics methods, neighbour searching, Trotter decomposition, cut-offs, temperature and pressure coupling methods, integration algorithms: Verlet algorithm, Leap-frog algorithm, Velocity Verlet, Beeman's algorithm, Constraint algorithms: shake, lincs, etc., Stochastic and Brownian dynamics, topology files, energy minimization: steepest descent method, conjugate gradient method, L-BFGS. Solvent models, Solvation, implicit and explicit solvation, heating dynamics, equilibration dynamics, production dynamics, trajectory analysis, particle mesh Edward dynamics, boundary conditions, Exclusions and 1-4 interactions, gradient based methods, steepest descent method, conjugate gradient method, replica exchange method, conformational analysis, normal mode analysis, free energy calculation: free energy perturbation method, thermodynamic integration

method, thermodynamic cycles for free energy calculations, determination of hydration/solvation free energy, protein folding free energy, protein-ligand binding free energy etc. Software packages for performing Monte-Carlo and Molecular dynamic simulation as well as for visualization and analysis trajectories

#### **UNIT- IV: Non-equilibrium thermodynamics (15)**

Conversion of mass in closed and open systems, conservation of energy in closed and open systems. Law of increasing entropy. Non-adiabatic process and clausius inequality, steady state. Thermodynamic equations of motion. Chemical and electrochemical affinities. Coupling reactions. Rates and affinities. Generalized fluxes, forces and their transformation. Phenomenological equations and coefficients. Concepts of reciprocity relations and Onsager theorem of microscopic reversibility. Entropy production in closed and open systems. Entropy production due to heat flow. Chemical potentials. Diffusion, electromotive force, electro-osmosis, thermoelectric effect and other reactions involving cross relations. Saxens relations

#### **Learning Outcomes:**

- i) Student should understand the the role of non-equilibrium in thermodynamics
- ii) They must know thermodynamic study of coupling reaction.
- iii) They must explain entropy, diffusion, electro-osmosis, diffusion with respect to thermodynamics
- iv) They must know applications and limitations of force field methods

#### **REFERENCE BOOKS:**

1. S. N. Blinder, Advanced physical Chemistry, The Macmilan Company, 1967.
2. L. K. Nash, Elements of statistical thermodynamics, 2<sup>nd</sup> Edition, Addison Wesley, 1974.
3. T.L. Hill, An Introduction to Statistical Thermodynamics, Addison-Wesley, 1960.
4. S. Glasstone, Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists, D. Van Nostrand Company, Inc., 1944.
5. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A molecular Approach, Viva Books, New Delhi, 1998.
6. Allen, M. P., Tildesley, D. J. Computer Simulations of Liquids, Oxford: Oxford Science Publications. 1987.
7. Frenkel, D.; Smit, B. Understanding Molecular Simulation: From Algorithms to Applications, 2<sup>nd</sup> Edition, Academic Press, San Diego, 2002.
8. K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.
9. F. Jensen, Introduction to Computational Chemistry, 2<sup>nd</sup> Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.
10. Schlick, T. Molecular modeling and simulation: an interdisciplinary guide, Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2002.
11. D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.

12. Online Manuals for simulation and visualization packages such as GROMACS, VMD, NAMD, AMBER, TINKER, etc.
13. I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Wiley, New York, 1968.
14. R.P. Rastogi, Introduction to Non-equilibrium Physical Chemistry: Towards Complexity and Non-linear Science, Elsevier, Oxford, 2008.

## MCT-P-402 Chemical Kinetics

### Learning objectives

- i) Realise difference between fast reactions and their rates
- ii) Understand the value of heterogeneous catalysis for feasibility of reaction
- iii) Expect the kinetics of organic reactions
- iv) Understand Hammett plots and Hammett equation

### UNIT-I: Fast Reactions

(15)

Kinetics of Fast reactions: Relaxation techniques, pressure jump and temperature jump methods, NMR relaxation, flash photolysis and molecular beam methods. **Hydrogen ion dependence of reaction rates:** Protonation and hydrolysis equilibria, determination of active reactant species from kinetic data, interpretation of hydrogen ion effect with example.

### UNIT – II: Theories of Reaction Rate

(15)

Equilibrium and rate of reaction, Partition function and activated complex, Collision theory of gas reaction, collision frequency. The rate constant, molecular diameters, collision theory vs. experiment Transition state theory (Thermodynamic and partition function approach) Activated complex theory of reaction rates, reaction coordinate and transition state, formation and decay of activated complex, Eyring equation, thermodynamic aspects, Theory of unimolecular reactions.

### UNIT–III: Heterogeneous Catalysis

(15)

Chemical reactions on surfaces, unimolecular surface reactions, bimolecular surface reactions, Electronic theories of chemisorption's and heterogeneous catalysis. Photocatalysis, Reaction mechanism of photocatalysis Effect of photocatalysis reaction. Heterogeneously catalysed oxidation and reduction reactions: oxidation of hydrogen with oxygen (Determination of Pt, Pd, Ir and Rh) Reduction of silver bromide (Determination of S and Se), Trace metal ion catalysis and their mechanisms. Micellar catalysis, Berezini, Menger-Portonoy, cooperative and pseudo-phase ion exchange models and examples.

### UNIT- IV : Organic Reaction Mechanisms

(15)

Linear free energy relationships: Hammett plots, Hammett equation, substituent and reaction constants and their physical significance, calculation of k and K values, Yukawa- Tsuno equation. Taft equation, steric parameters Solvent effects, Grunwald-Winstein equation.

## Learning Outcomes:

- i) Student should understand organic transformations through kinetics
- ii) They must know details of rates of fast reaction.
- iii) They must know the role of catalyst and its mechanism during catalysis.
- iv) They should understand physical significance of substituent and reaction constants

## REFERENCE BOOKS:

1. Chemical Kinetics by K. J. Laidler.
2. Kinetics and Mechanism by A. A. Frost and R. G. Pearson .
3. Fast Reactions by Haque .
4. Theory of chemical reaction rates by K. J. Laidler, McGraw Hill, New York , 1969.
5. Fast Reactions by J. N. Bradley , Clarendon Press Oxford , 1974
6. Physical Chemistry by W. J. Moore.
7. Physical Chemistry by P.W. Atkins
8. Micellar effect on the kinetics and mechanism of chromium(VI) oxidation of organic substrates  
By Asim K. Das, Coordination Chemistry Reviews, Vol 248, p 81-89 ( 2004 ).
9. Some aspects of electron transfer reactions involving organic molecules by B. Sethuram, Allied Publishers, 2003.
10. Surfactants and polymers in aqueous solution by Bo Jonsson, Bjorn Lindman, Krister Holmberg and Bengt Kronberg, John-Wiley & Sons, 1998.
11. Inorganic reaction mechanisms, Part II Edited by John O. Edwards, Interscience, 1972.

## MCT-P-403-Molecular structure-II

### Learning objectives

- i) Understand the electric and magnetic properties of molecules
- ii) Understand Nuclear Magnetic Resonance, Electron Spin Resonance Spectroscopy
- iii) Expect the application of Mossbauer Spectroscopy
- iv) Expect the application of magnetism to coordination complexes and complex ions of transition metals.

### UNIT – I: The Electric Properties of Molecules (15)

Electric dipole moment of molecule, polarization of a dielectric, polarizability of molecules, Clausius-Mossotti equation. Debye equation. limitation of the Debye theory , determination of dipole moment from dielectric measurements in pure liquids and in solutions. Dipole moment and ionic character, Bond moment, Group moment, vector addition of moments, bond angles, The energies due to dipole-dipole, dipole induced dipole and induced dipole-induced dipole interaction. Lennard-Jones potential .

### UNIT – II: The Magnetic properties of Molecules (15)

Diamagnetism and Para magnetism. Volume and mass susceptibilities. Lengevins classical theory of diamagnetism and paramagnetism Atomic and ionic susceptibility. Pascal constants, Curie - Weiss law. Van Vleck general equation of magnetic susceptibility.

Determination of magnetic susceptibility. Ferro and ferri magnetism, application to coordination complexes and complex ions of transition metals.

### **UNIT – III: Nuclear Magnetic Resonance Spectroscopy (15)**

The nature of spinning particles, interaction between spin and a magnetic field. Population of energy levels, The Larmor precession. relaxation times. the meaning of resonance and the resonance condition. NMR experiment, significance of shielding constants and chemical shift. The origin and effect spin - spin coupling , factors affecting chemical shift, chemical analysis by NMR. Exchange phenomena,  $^{13}\text{C}$  NMR spectroscopy, double resonance and nuclear-overhauser effect.

### **UNIT – IV: A) Electron Spin Resonance Spectroscopy (8)**

Electron spin and Magnetic moment, Resonance condition in ESR and significance of 'g' value. ESR spectra of organic free radicals, McConnell relation , Electron Exchange reactions , applications of ESR,

### **B) Mossbauer Spectroscopy (7)**

Basic principle of Mossbauer spectroscopy, hyperfine structure, quadrupole splitting, instrumentation and applications of Mossbauer spectroscopy, Problems related to Mossbauer spectra.

### **Learning Outcomes:**

- i) Student should understand Electric dipole moment, dielectric, polarizability of molecules
- ii) They must know application of ESR spectroscopy.
- iii) They must explain application of Nuclear Magnetic Resonance Spectroscopy
- iv) They should understand applications of Mossbauer spectroscopy

### **REFERENCE BOOKS:**

1. Fundamentals of molecular spectroscopy by C. N. Banwell.
2. Physical chemistry by P. W. Atkins. ELBS. 1986
3. Introduction to molecular spectroscopy by G. M. Barrow.
4. Molecular spectroscopy by I. N. Levine , Wiley interscience.
5. Nuclear magnetic Resonance by J. D. Roberts, McGrawHill .
6. Introduction to Magnetic resonance by A. Carrington and A. D. McLachlan. Harper and Row.
7. Electron Spin Resonance , Elementary theory and practical applications by J. E. Wetz and J. R. Boulton , McGraw Hill .
8. Introduction to Magneto chemistry by Earnst Shaw. Academic Press
9. Electrical and optical properties of molecular behaviour by M. Davies, pergman press.
10. Polar molecules by P. Debye, Dover publications.

## **Learning objectives**

- i) Learning advanced instrumentation techniques
- ii) Understand different physicochemical techniques
- iii) Expect the introduction and applications of instrumentation
- iv) Understand STEM, SEM

### **Unit I . X-ray methods (15L)**

Generation and properties of X-rays, generation of X-rays, -spectra, X-ray absorption, Concept of absorption edge, application, X-ray absorptive apparatus, radiography and radiotherapy, applications, X rays fluorescence, fundamental principles, instrumentation, wavelength dispersive and energy dispersive, quantitative analysis, X-ray emission, fundamental principles, X ray diffraction, powder diffractometer, applications in material science, electron microprobe, further advanced techniques, Introduction to STEM, SEM

### **Unit II. XPS (X-ray photoelectron spectroscopy) and Mass spectrometry (15L)**

Theory satellite peaks, chemical shift, apparatus, chemical analysis, using ESCA, AES-fundamental principles UP Luminescence, chemiluminescence, gas phase, liquid phase chemiluminescence, apparatus, bioluminescence, electrochemiluminescence

**Mass spectrometry:** Theory, instrumentation-basic components, ionization sources, analyzers, resolution, chemical analysis, advanced techniques-GC/MS, MS/MS introduction

### **Unit III. Neutron Activation Analysis (15L)**

Principle, target, matrix, cross-section, fluxes, saturation activity, excitation function, Different steps involved in NAA, radiochemical and instrumental NAA, prompt radiation and pulse neutron activation analysis, applications

### **Unit IV. A) Inductively coupled plasma atomic emission spectroscopy (5L)**

Principle, instrumentation, analysis and applications

#### **B) Thermal methods of analysis: (6L)**

TGA, DTA, DSC and thermometric titrations – principle, instrumentation, factors affecting TGA curve, applications

#### **C) Radiometric titrations : (4L)**

Principle , types and instrumentation

## **Learning Outcomes:**

- i) Student should understand instrumentation techniques
- ii) They must know details of instrumentation and applications
- iii) They must know the role of different physicochemical techniques
- iv) They should understand TGA, DTA, DSC, thermometric titrations

## **Reference Books :**

1. Introduction to Instrumental Analysis- R. D. Braun, Pharmamed Press, Indian Reprint (2006)
2. Principles of Instrumental Analysis, 5th edition- D.A. Skoog, F.J. Holler, T.A. Nieman, Philadelphia Saunders College Publishing (1988)

3. Principles of activation analysis - P. Kruger , John Wiley (1971)

4. Nuclear analytical chemistry- J. Tolgyessy and S. Verga Vol. 2 , University park press (1972)

## MCT-P-404-A Elective Paper: Surface Chemistry

### Learning objectives :

- i) Understand Surface Chemistry of interfaces
- ii) Realize experimental aspects based on use of Langmuir-Adam surface pressure balance
- iii) Expect the study of B.E.T. equation, methods of determination of surface area
- iv) Realize the meaning of Colloids and emulsion

### UNIT-I: Surface Chemistry of interfaces (15)

Types of interfaces, Liquid-vapour interface, Surface tension and interfacial tension, surface tension across curved surfaces, capillary action, methods of determination of surface tension, , vapor pressure of droplet ( Kelvin equation ) ,Surface activity and adsorption phenomenon, Trube's Rule, Gibb's Adsorption equation, liquid-liquid interfaces, work of cohesion and adhesion, surface spreading , spreading of one liquid on the surface of other liquid, spreading coefficient and derivation for its relation with surface tension, monomolecular films, preparation of monolayer films, Langmuir-Boldget method, physical states of films, ideal equation of states, experimental aspects based on use of Langmuir-Adam surface pressure balance,

### Unit-II: Solid-gas interfaces (15)

Adsorption of gases on solids, factors affecting adsorption, Experimental methods of determining gas adsorption, volumetric method, Gravimetric method, types of adsorption isotherms, The B.E.T. equation, methods of determination of surface area, Herkins's Jura method, BET method, Point B Mehhod, Heat of adsorption, Calorimetric method of determination of heat of adsorption, Chemisorption, Kinetics of chemisorptions, Heterogenous catalysis (Contact catalysis), mechanism of catalysis, factors influencing catalytic activity.

### UNIT- III: Colloids and emulsion (15)

The Colloidal state: Introduction, types, preparation and stability of colloids, properties of colloids, Electrokinetic phenomena: Electrophoresis, electro-osmosis, Emulsion: Types of emulsion, theories of emulsion and emulsion stability, identification of emulsion types, inversion emulsion, microemulsion : theory and application , micellisation, structure of micelle, reverse micelle , solubisation of water insoluble organic substances

### UNIT –IV: Solid-Liquid and Solid - Solid interfaces (15)

Solid-liquid interfaces, Introduction, wetting phenomenon, contact angle and wetting, heat of wetting, methods of determination of contact angle, contact angle hysteresis, wetting agents, selective wetting, applications in detergency, and pesticide affectivity, Solid-Solid interfaces, introduction, Surface energy of solids, adhesion and adsorption, sintering and sintering

mechanism, Tammann temperature, importance of impurities, surface structure and surface composition. Friction and lubrication, mechanism of lubrication, solid state lubricants.

### **Learning Outcomes:**

- i) Student should understand types of interfaces, Liquid-vapor interface, Surface tension and interfacial tension
- ii) They must know Heat of adsorption, Calorimetric method of determination of heat of adsorption, Chemisorption.
- iii) They must explain structure of micelle, reverse micelle, solubilisation of water insoluble organic substances
- iv) They should understand applications of solid-liquid interfaces in detergency, and pesticide affectivity

### **REFERENCE BOOKS:**

1. Physical chemistry of surfaces: A. W. Adamson.
2. Theory of adsorption and catalysis by Alfred Clark ,
3. Chemisorption by B. M. W. Trapnell and H.O. Hayward.
4. Introduction to colloids and surface chemistry by D. J. Shaw.
5. Theories of chemical reaction rates by A. J. K. Laidler
6. Surface chemistry by J. J. Bikermann
7. The Surface Chemistry of Solids, by S. J. Gregg, Second Edition, Chapman & Hall Ltd. London.
8. Advanced Physical Chemistry, by Gurdeep Raj ,Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP)
9. Principles of Physical Chemistry, Puri B.R., Sharma L.R. & Pathania M.S., Vishal Publishing Co., Jalandar-144008
10. Physical Chemistry by Pahari S. New Central Book Agency (P) Ltd. Kolkata-700009.

## **MCT-P-404-B Elective Paper-II: Chemistry Of Materials**

### **Learning objectives**

- i) Understand the synthesis of Ceramics, Composite and Nanomaterials
- ii) Understand fibre - reinforced composites, macroscopic composites
- iii) Expect the study of polymer types and their applications
- iv) Realize the methodology of thin film synthesis.

### **UNIT –I: Glasses, Ceramics, Composite and Nanomaterials (15)**

Glassy state, glass formers and glass modifiers, applications, Ceramic structures, mechanical properties, clay products. Reformatories, characterizations, properties and applications.

Microscopic composites; dispersion - strengthened and particle - reinforced, fibre - reinforced composites, macroscopic composites. Nanocrystline phase, preparation procedures, special properties, and applications.

**UNIT-II: High Tc Materials** (15)

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, and normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption - pairing and multigap structure in high Tc materials, applications of high Tc materials.

**UNIT-III: Polymeric Materials** (15)

Molecular shape, structure and configuration, crystallinity, stress-strain behavior, thermal behavior, polymer types and their applications, conducting and ferro-electric polymers.

**UNIT-IV: Thin films and Langmuir-Blodgett Films** (15)

Preparation techniques; evaporation / sputtering, chemical processes, MOCVD, sol-gel etc. Langmuir-Blodgett (LB) film, growth techniques, photolithography, properties and application of thin and LB films.

**Learning Outcomes:**

- i) Student should understand the applications of thin films and Langmuir-Blodgett Films
- ii) They must know crystallinity, stress-strain behavior, thermal behavior.
- iii) They must explain application glasses, ceramics and nanomaterials.
- iv) They should understand properties and application of thin and LB films.

**REFERENCE BOOKS:**

1. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders College
2. Material Science and Engineering, An introduction, W. D. Callister, Wiley.
3. Principles of Solid State, H. V. Keer, Wiley Easton.
4. Materials Science, J. C. Anderson, K. D. Leaver, J. M. Alexander and R. D. Rawlings, ELBS
5. Thermotropic Liquid Crystals, Ed, G. W. Gray, John Wiley.
6. Text book of liquid crystals, Kelkar and Halz, Chemie Verlag

**M.Sc. Part-II (Sem-IV)**  
**Physical Chemistry Practical Course-VII and VIII**  
**MCP-P-405 and MCP-P-406**

**Course Objectives : Students should**

- 1) Learn the characterisation of complexes.
- 2) Study the synthesis of nanoparticles
- 3) Study the Preparation and characterization of thin film.

**1. Spectroscopy:**

- 1) Characterization of the complexes by electronic and IR spectral data.
- 2) Determination of indicator constant and isobestic point of an indicator.
- 3) Determination of stability constant of ferric thiocyanate complex.

2. To synthesize metal nanoparticles and to study their size-dependent optical properties
3. 'Green' synthesis of metals and their oxide nanoparticles: applications for environmental remediation
4. Preparation and characterization of thin film
5. To synthesize thin film and study their optoelectronic properties
6. Analytical study of medicinal plants via HPLC
7. To synthesize carbon nanoparticle.
8. To synthesize carbon nanoparticle and study adsorption behavior of dye.
9. Kinetic study by i) spectrophotometric method ii) conductometric method.
10. Industry oriented Practicals

**Course Outcomes : After completions of experiments students should**

- 1) Understand characterisation of complex molecules by spectroscopically.
- 2) Understand operating of HPLC instrument for analysis.
- 3) Prepare and characterise thin film.

**REFERENCE BOOKS:**

1. Fundamental of molecular spectroscopy by C. N. Banwell Tata McGraw Hill.
2. Practical of physical chemistry by A.M. James and F.E.Prichard
3. Vogel's textbook of quantitative analysis by J.Bossett, Denny, Jeffery
4. Instrumental methods of analysis by Willard, Deon, Frank A. Settle
5. Findlay's Practical Chemistry by B.P.Lavitt and J.A.Kitchner
6. Experiments in physical chemistry by David P. Shoemaker
7. Experimental Physical Chemistry by F. Daniels and J. Williams
8. Experimental Physical Chemistry by R.C.Das and B. Behera
9. Practical Physical Chemistry : B. Viswanathan and P.S. Raghavan

**Research project: Lab Project in Parent Institute**

External and internal examiners will examine the project (50 Marks) jointly at the time of practical examination

(Any other experiment may be added when required)

**Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.**

OR

**Internship, Industrial Training:**

Students should complete their internship programme or industrial training or research project work in well reputed organisations like IIT, NIT, IISER, NCL, ICT, Universities, Chemical Industries and Pharmaceutical Industries etc. The minimum period of their internship is 30 days. Students should submit their project report in details with certificate is compulsory.