Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore
Shri Vaishnav Institute of Science
Name of Program: B.Sc. (Major: Chemistry)
(2022-2025)

Semester -VI

COURSE CODE	CATEGORY	COURSE NAME	TEACHING &EVALUATION SCHEME								
			THEORY			PRACTICAL		L	T	P	CREDITS
			END SEM University Exam	Two Term Exam	Teachers Assessmen	END SEM University Exam	Teachers Assessmen				
BSCCH601	CORE	Physical Chemistry II	60	20	20	30	20	4	0	4	6

Legends: **L** - Lecture; **T** - Tutorial/Teacher Guided Student Activity; **P** – Practical; C - Credit.
***Teacher Assessment** shall be based following components: Quiz/Assignment/ Project/Participation in Class, given that no component shall exceed more than 10 marks.

Course Educational Objectives (CEOs):

1. Understand the basic concepts of chemical thermodynamics, the laws of thermodynamics and their applications in chemistry

2. Introduce the empirical and theoretical principles of rates of chemical reactions.

3. Understand the concept of equilibrium as an application of thermodynamic principles.

4. To understand Basic concept of surface chemistry.

5. To acquaint the students with practical knowledge of the concepts of Physical chemistry.

Course Outcomes: -

After completion of this course the students are expected to be able to demonstrate the following knowledge, skills, and attitudes. The student will demonstrate the capability of following.

1. A fundamental understanding of the first and second laws of thermodynamics and their applications to a wide range of systems in chemistry.

2. Understand the concept of reaction rates, order of reaction and rate constant.

3. Calculation of equilibrium constant from thermodynamic parameters and concepts of surface chemistry.

4. Demonstrate a fundamental/systematic understanding of the practical field of Photochemistry.

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SYLLABUS:

UNIT-I: Chemical Thermodynamics:

Intensive and extensive variables; state and path functions; isolated, closed, and open systems. First law: Concept of heat, Q, work, W, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities, calculations of Q, W, ΔU and ΔH for reversible, irreversible, and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. statement of the second law of thermodynamics. Calculation of entropy change for reversible and irreversible processes. Third Law: Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules.

UNIT-II: **Chemical Kinetics**:

Rate of reactions – rate laws and rate constants, order, and molecularity; differential and integrated form of rate equations for simple chemical reactions – zero, first, second order, pseudo first order and equations for half-life; radioactive decay as first order phenomenon. Methods of determining reaction orders and rate laws – integrated rate law method, isolation and initial rate method, half-life method.

UNIT-III: **Thermodynamic Equilibrium:**

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free

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energy of reaction and reaction quotient. Equilibrium constants and their quantitative dependence on temperature, pressure, and concentration (Le Chatelier Principle, Quantitatively). Free energy of mixing and spontaneity. equilibrium between ideal gases and a pure condensed phase.

UNIT-IV: Solutions and Colligative Properties:

Ideal solution-Thermodynamics of Ideal solutions; Raoult's Law- derivation of Raoult's Law; Nonideal or real solutions; activity and activity coefficient; colligative properties: (i) relative lowering of vapor pressure- determination of molecular weight; osmotic pressure- osmosis, measurement of osmotic pressure, Law of osmotic pressure and determination of molecular weight.

UNIT-V: Surface chemistry:

Definition of colloids. Solids in liquids(sols), preparation, purification, properties - kinetic, optical, electrical. Stability of colloids, Hardy-Schulze law, protective colloid. Liquids in liquids (emulsions) preparation, properties, uses. Liquids in solids (gels) preparation, properties and uses.

Adsorption: Physical adsorption, chemisorption. Freundlich, Langmuir adsorption isotherms. Applications of adsorption.

Reference Books:

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1. Peter, A. & Paula, J. de. Physical Chemistry 9th Ed., Oxford University Press (2011).
2. Castellan, G. W. Physical Chemistry 4th Ed., Narosa (2004).
3. Engel, T. & Reid, P. Physical Chemistry 3rd Ed., Prentice-Hall (2012).
4. McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi (2004).
5. Chemical Principles: The Quest for Insight, 6th ed. by P Atkins, L Jones and L Laverman; W H Freeman and Company, New York, 2013.
6. Basic Reaction Kinetics and Mechanism by H E Avery, Mcmillan Publishers Ltd., 1974.

LIST OF PRACTICALS:

1. Determination of enthalpy of neutralization.

2. Determination of Specific heat of metals and liquids

3. Determination of Latent heat of fusion of ice.

4. Determination of solubility product of a sparingly soluble salt and calculation of entropy & enthalpy.

5. Determination of pKa of following compounds by pH titration: Phenol, aniline, ammonia, acetic acid.

6.Kinetics of hydrolysis of methyl acetate - acid and base catalyzed using integrated rate law method.

7. Determination of dissociation constant of CH3COOH by pH meter.

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8.Verification of Debye-Huckel-Onsager equation for true electrolyte.

9.Preparation of lyophobic colloids and verification of Hardy-Schulze rule for coagulation of these colloids by the addition of electrolytes.

10.To study the kinetics of base hydrolysis of ester using conductometry (integrated rate law method).

Practical Reference Books:

1. Experimental Physical Chemistry by G.P. Matthews, Clarendon Press, 1985.
2. Experimental Physical Chemistry by V D Athawale, Parul Mathur, New Age International Publishers, 2001.
3. 1. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
4. 2. Kapoor, K.L. (2019), A Textbook of Physical Chemistry, Vol.7, 1st Edition, McGraw Hill Education.

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BSCCH602A	**DSE**	**Molecules of Life**	60	20	20	30	20	3	0	2	4

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Course Educational Objectives (CEOs):

1. To develop the concept of bioorganic and bioinorganic chemistry.
2. To understand the chemistry and importance of biomolecules in life.
3. To comprehend different bonds, interactions and effects observed in biomolecules at the interface of chemical and biological environment.
4. To acquire knowledge about personalized medicine.
5. To acquaint the students with practical knowledge pertaining to the concepts of bioorganic and bioinorganic chemistry.

Course Outcomes (COs):

1. Students will gain the knowledge of bioorganic chemistry and amino acids specifically, molecular recognition, asymmetric synthesis and application of unnatural amino acids.
2. They will learn the importance of bioorganic chemistry of nucleic acids like single nucleotide polymorphism, HAP-MAP project, Antigene / Antisense therapy.
3. They will be able to understand the role of metal ions in biological systems, structure and functions of electron transfer proteins, enzymes, coenzymes and apoenzymes.
4. Students will be able to understand the chemistry of enzymes in organic synthesis and concept of biomineralization.

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5. They will learn to practically deal with inorganic elements and nanoparticles with reference to medical applications.

Syllabus

Unit – 1

Introduction to Bioorganic Chemistry and Amino acids:

Overview of bioorganic chemistry (from past to present), importance and applications of weak interactions in chemistry and biology, proximity effect in organic chemistry, molecular recognition, chemistry of living cells, analogy between biochemical and organic reactions. Amino acids and their asymmetric synthesis, classification based on chemical constitution, stereochemistry of amino acids, chemistry of peptide bonds, C and N protecting groups in peptide coupling, peptide secondary structures and tools for stabilization. Synthesis and application of unnatural amino acids.

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Unit - 2

Bioorganic Chemistry of Nucleic Acids:

Introduction to nucleic acids, components of nucleic acids – sugars and bases, structure of DNA, conformation of sugar-phosphate back bone, hydrogen bonding by bases, structure and stability of double helix, chemical synthesis of DNA, structure and types of RNA, synthesis and application of unnatural nucleosides, single nucleotide polymorphism (SNP), Hap-Map project, concepts of Antigene / Antisense therapy, goal for personalized medicine.

Unit-3

Metal ions in Biological Systems:

Bioinorganic chemistry - General terms, how and why nature selects inorganic elements? Essential and trace metals, Na^+ / K^+ pump, role and chemistry of redox-active and non-redox active metal ions. Structure and functions of electron transfer proteins. Respiratory chain and role of cytochromes, iron and sulphur proteins: Rubredoxin and Ferredoxins. Photosynthesis and photosystem - I, II.

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Unit-4

Transport, Storage of Dioxygen and Enzymes:

Heme proteins, structure and mechanistic functioning of hemoglobin and myoglobin, chemistry behind complete and partial reduction of dioxygen, reactive oxygen species, Introduction of enzymes, enzyme action, transition-state theory, orientation and steric effect. Acid Base catalysis in enzymes, enzyme catalysis by approximation, chemistry of enzymes in organic synthesis and name reaction(s), thermodynamics and kinetics of enzyme catalysis, . Examples of some enzyme mechanisms – chymotrypsin, lysozyme. Coenzymes, prosthetic groups, apoenzymes, vitamin B12, NAD+, NADP+. Mechanisms of reactions catalyzed by the above coenzymes.

Unit-5

Applications of Bioorganic and Bioinorganic Chemistry:

Biomineralization, nature and function of different bio-minerals and understand the mechanism of biomineralization. Nanoparticles and its applications in biosciences, functions of non-redox active elements for protein / DNA. Medical applications of bioorganic chemistry, principles and

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mechanism of homeostasis of a cell, medical applications of metal ions and complexes for the treatment of cancer, diabetes, arthritis.

References:

1. Hermann Dugas, C Penny, Bioorganic Chemistry: A chemical approach to enzyme action,Springer – Verlag
2. AL Lehninger, Principles of Biochemistry, Worth Publishers
3. Collin J Suckling, Enzyme Chemistry: Impact and Applications, Chapman and Hall
4. L Stryer, Biochemistry, W.H. Freeman
5. F Wold, Macromolecules: Structure and Function, Prentice Hall
6. I Bertini, HB Gray, SJ Lippard, JS Valentine, Bioinorganic Chemistry, University ScienceBooks
7. Rekha Dashora, AK Goswami, Supramolecular and Bioinorganic Chemistry, PragatiPrakashan
8. NC Price, L Stevens, Fundamentals of Enzymology, Oxford University Press

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List of Experiments:

1. Stoichiometric Calculations.
2. Preparation and measurement of pH of Standard Buffers and Reagents.
3. Detection of Extra Elements like Nitrogen, Sulphur, and Halogens.
4. Identification of Functional Groups (-COOH, -CHO, -CO, -OH alcoholic and phenolic, $-CONH_2$, $-NH_2$, $-NO_2$).
5. Tests for Carbohydrates, Esters, Anilides.
6. Synthesis of Oil of Wintergreen.
7. Synthesis of Aspirin.
8. Synthesis of Oxalic Acid from Sucrose.
9. Synthesis of Picric Acid.
10. Preparation of Nanoparticle 1.
11. Preparation of Nanoparticle 2.
12. Analysis of nanoparticles by various techniques.

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BSCCH602B	**DSE**	**Unit Operations in Chemical Industries**	60	20	20	30	20	3	0	2	4

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Course Educational Objectives (CEOs):

1. To understand the fundamentals of reaction types.
2. To allude the importance of selection of reagents as per the process opted.
3. To understand the mechanism of name reactions.
4. To acquire knowledge about preparation of commercial products.
5. To acquaint the students with knowledge of the concepts of instruments and processes opted in chemical industries.

Course Outcomes (COs):

1. Students will gain the knowledge of processes like alkylation and halogenation.
2. They will learn the importance of nitration and sulphonation methods.
3. They will be able to develop the concepts pertaining to oxidation and hydrogenation.
4. Students will be able to explain the fundamental concepts used for the synthesis of commercial compounds by esterification, hydrolysis and amination.
5. They will gain practical knowledge of basic processes opted in chemical industries like preparation, isolation, purification and titration needed to become good chemist.

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Syllabus

Unit – 1

Alkylation and Halogenation:

Alkylation: Introduction, types of alkylation, alkylating agents, mechanism of alkylation reactions, manufacturing process of phenyl ethyl alcohol. Halogenation: Introduction, reagents for halogenations, halogenations of aromatics – side chain and nuclear halogenations, commercial manufacture of chlorobenzene, chloral.

Unit - 2

Nitration and Sulphonation:

Nitration: Introduction, nitrating agents, mechanism and nitration of paraffin hydrocarbons - benzene to nitrobenzene, m-dinitrobenzene, chlorobenzene to o & p-nitrochlorobenzenes. Sulphonation: Introduction, sulphonating agents, chemical and physical factors in sulphonation, mechanism of sulphonation, commercial sulphonation of benzene, naphthalene.

Unit-3

Oxidation and Hydrogenation:

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Oxidation: Introduction, types of oxidation reactions, oxidizing agents, mechanism of oxidation, liquid phase oxidation and vapour phase oxidation, commercial manufacture of benzoic acid, acetic acid. Hydrogenation: Introduction, catalysts for hydrogenation reactions, hydrogenation of vegetable oil, manufacture of methanol from carbon monoxide and hydrogen, catalytic reforming.

Unit-4

Esterification and Hydrolysis:

Esterification: Introduction, esterification by organic acids, by addition of unsaturated compounds, esterification of carboxy acid derivatives, commercial manufacture of ethyl acetate. Hydrolysis: Introduction, hydrolyzing agents, mechanism of hydrolysis.

Unit-5

Amination:

Introduction, methods of reduction by metal and acid, catalytic sulfide, electrolytic, metal and alkali sulfites, metal hydrides, sodium metal. Commercial manufacturing process of m-nitroaniline, p-aminophenol. Aminolysis: Introduction, aminating agents, factors affecting.

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References:

1. P. H. Groggins: Unit Processes in Organic Synthesis (MGH)
2. F. A. Henglein: Chemical Technology (Pergamon)
3. M. G. Rao and M. Sittings: Outlines of Chemical Technology (EWP)
4. Clausen, Mattson: Principles of Industrial Chemistry
5. H A. Lowenheim and M. K. Moran: Industrial Chemicals
6. Kirk and Othmer: Encyclopedia of Chemical technology
7. Kent, Riegel's Industrial Chemistry (N-R)
8. S. D. Shukla and G. N. Pandey: A Textbook of Chemical Technology, Vol-II
9. J. K Stille: Industrial Organic Chemistry (P.I I.)

List of Experiments:

1. Stoichiometric calculations.
2. Preparation of reagents, standard acids, alkalis and buffers.
3. Preparation of complex 1.
4. Preparation of complex 2.
5. Preparation of complex 3.
6. Isolation of casein from milk.
7. Isolation of lycopene from tomato paste.
8. To purify a given sample of phthalic acid by sublimation.
9. Estimation of hardness of water by EDTA method.
10. Determination of alkalinity in given water sample.
11. Determination of acidity in given water sample.

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BSCCH603A	DSE	Quantum Chemistry & Photochemistry	60	20	20	30	20	3	0	2	4

Legends: **L** - Lecture; **T** - Tutorial/Teacher Guided Student Activity; **P** – Practical; C - Credit.
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Course Educational Objectives (CEOs):

1.To give basic knowledge of concept of quantum Chemistry and Photochemistry.
2.To develop an understanding of Quantum Chemistry and Photochemistry.
3.To introduce concept of energy quantization to understand the failure of classical mechanics and analysis of microscopic particles/systems
4. To explore the photochemistry of organic compounds and their applications in synthesis.

Course Outcomes: -

After completion of this course the students are expected to be able to demonstrate the following knowledge, skills, and attitudes. The student will demonstrate the capability of following.

1. Theoretical understanding of concepts of quantum mechanics
2. Became aware of Quantum Chemistry and Photochemistry.
3. Became aware of Quantum Chemistry and laws of Photochemistry.
4. Demonstrate a fundamental/systematic understanding of the practical field of Photochemistry.

SYLLABUS:

Unit I: Quantum Chemistry

Postulates of quantum mechanics, quantum mechanical operators, Schrödingerequation and its application to free particle and “particle-in-a- box” (rigorous treatment).

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Semester -VI

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Unit II: Quantum Chemistry

Quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions, probability distribution functions, nodal properties, Extension to two- and three-dimensional boxes, separation of variables, degeneracy.

Unit III: Quantum Chemistry

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy. Rigid rotator model of rotation of diatomic molecule.

Unit IV: Photochemistry

Laws of photochemistry: Grotthus-Draper law, Stark-Einstein law of photochemical equivalence and Lambert-Beer's law; quantum yield and its measurement for a photochemical process.

Unit V: Photochemistry

Actinometry. Photo stationary state. Photosensitized reactions. Kinetics of HI decomposition, H_2 -Br_2 reaction, dimerization of anthracene.

REFERENCE BOOKS:

1. F. L. Pilar: Elementary Quantum Chemistry, Dover Publications, Inc. NY, 1990.2nd Ed.
2. P. W. Atkins and R. S. Friedman: Molecular Quantum Mechanics, 3rd Ed., Oxford Univ. Press, 1997

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3. Ira N. Levine: Quantum Chemistry, Prentice Hall
4. A. K. Chandra: Introduction to Quantum Chemistry, Tata McGraw Hill
5. Fleming: Pericyclic Reactions, Oxford University Press, Oxford, 1999.
7. S.M. Mukherjee, S.P. Singh: Pericyclic Reactions, MacMillan India, New Delhi.
8. Sankararaman, S: Pericyclic Reactions -Applications and Theory, Wiley –VCH,2005.

. 9. Modern Molecular Photochemistry of Organic Molecules, N. J. Turro, V. Ramamurthy and J. C. Scaiano, University Science Books

10. Advanced organic chemistry, F. A. Carey and R. J. Sundberg, Springer, 5th Edition

11. Organic Photochemistry, Coxon J. and Halton B., Cambridge University Press.

List of Experiments:

1. Verify Lambert-Beer's law and determine the concentration of CuSO4/KMnO4/K2Cr2O7 in a solution of unknown concentration.
2. Study the kinetics of iodination of propanone in acidic medium.
3. Determine the amount of iron present in a sample using 1, 10-phenathroline.
4. Determine the dissociation constant of an indicator (phenolphthalein).
5. 1.Study the 200-500 nm absorbance spectra of KMnO4 and K2Cr2O7 (in 0.1 M H2SO4) and determine the λmax values. Calculate the energies of the two transitions in different units (kJ molecule-1, kJ mol-1, cm-1, eV).

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6. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.
7. Determine the concentrations of KMnO4 and K2Cr2O7 in a mixture.
8. Study the decomposition of oxalic acid in solution photosensitized by uranyl sulphate.
9. Investigate the complex ion formation between Fe(III) and salicylic acid by Job's method.
10. Titrate copper (III) solution with EDTA spectroscopically.

REFERENCE BOOKS

Practical:

1.Khosla, B. D.; Garg, V. C. & Gulati, A., Senior Practical Physical Chemistry, R. Chand & Co.: NewDelhi (2011).

2.Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).

3.Halpern, A. M. & McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co. NewYork (2003).

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Course Objective:
To develop the understanding of fundamentals of Spectroscopy.
To develop the understanding of structure determination.
To give basic knowledge of Spectroscopic Methods.

Course Outcomes: -
After completion of this course the students are expected to be able to demonstrate following knowledge, skills, and attitudes. The student will demonstrate capability of:

Fundamentals of Organic Chemistry and Spectroscopy.
Interpret various types of spectra and know about their application in structure elucidation.
Apply fundamental/systematic different Spectroscopic Methods.

Unit I
Rotational and Vibrational spectra: Basic principles, selection rule, fundamental vibrations, Raman Effect. Identification of some representative organic and inorganic compounds.

Electronic spectra: Frank-Condon principle, Fluorescence, Phosphorescence, electronic spectra of diatomic molecules, chromophores, auxochromes, absorption and intensity shifts, solvent effects, Woodward Fieser rules.

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Unit II

Nuclear Magnetic Resonance Spectroscopy: Basic principles, origin of chemical shifts, factors affecting the chemical shifts and their interpretation, spin-spin coupling, relaxation processes, coupling constants. Nuclear Overhouser Effect (NOE) 2D-NMR, 1H, 13C, and 19F NMR spectra of selected compounds. Shift reagents.

Unit III

EPR spectroscopy: Basic principles, origin of g-shifts, spin orbit coupling, line shape, zero field splitting, Kramer degeneracy, ESR analysis of organic radicals, transition metal complexes of vanadium, copper.

Mass spectrometry: Basic principles and instrumentation, mass spectral fragmentation of organic compounds, factors affecting fragmentation, applications of mass spectrometry.

Unit IV

Mössbauer Spectroscopy: Nuclear resonance absorption, recoil energy, Doppler effect, Mössbauer effect, Isomer shift, quadruple interactions, effect of magnetic field, determination of oxidation states of iron (including bioinorganic systems, ferredoxins) tin and cobalt compounds.

Unit V

X-ray Diffraction: X-ray diffraction by single crystal – Space groups –Systematic absences in X-ray data and identification of lattice types, glide planes and screw axes. X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Structure solution by Heavy atom method and direct method. Determination of absolute configuration of molecules.

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Ramchandran Diagram of Protein.

Neutron Diffraction by solids and liquids– magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell. Neutron diffraction vs X- ray diffraction.

Books:

1. C.N. Banwell, Fundamentals of molecular Spectroscopy, TMH, New Delhi.
2. B.P. Straughan and S.Walker Spectroscopy Vol.3, Chapman Hall London.
3. P.M. Silverstein, F. X. Wester, Spectroscopic Identification of Organic Compounds, Wiley.
4. Y.R. Sharma, Elementary Organic Spectroscopy – Principles and Chemical applications, S.Chand.
5. Kakkar, R. (2015), Atomic & Molecular Spectroscopy, Cambridge University Press.
6. Drago, R. S. Physical Methods for Chemistry, (Saunders Company).
7. Nakamoto, K. Infrared and Raman Spectra: Inorganic and Coordination Compounds, (John Wiley).

List of Practical's:

1. To determine the specific rotation of a sugar using Polarimeter.
2. To study the Optical rotatory dispersion of some Chiral Substances.
3. To study the thermal study of proteins.

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4. To determine Critical Micelle Concentration (CMC) of a surfactant.
5. Familiarization with the UV- Visible Absorption Spectroscopy.
6. Verification of Beer- Lambert Law.
7. Solvent effects on UV Visible Absorption Spectra.
8. Study of Kinetics of a reaction by using spectroscopic methods.
9. Instrumentation and working principle of IR Spectroscopy using salt plates.
10. Instrumentation and working principle of Solution IR Spectroscopy.
11. Instrumentation and working principle of Mass Spectroscopy.
12. Determination of molar mass of simple compounds using mass spectroscopy.
13. NMR Spectroscopy and evaluation of simple 1H NMR spectra of selected organic compounds.
14. Identification of unknown compounds using spectroscopic techniques.
15. Estimation of Protein by Lowry Method.
16. Quantitative estimation of Carbohydrates by Anthrone method.

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