PARISHKAR COLLEGE OF GLOBAL EXCELLENCE (AUTONOMOUS), JAIPUR

SCHEME OF EXAMINATION COURSE STRUCTURE & SYLLABUS AS PER UGC

ज्ञान-विज्ञान विमुक्तये

CHOICE BASED CREDIT SYSTEM (CBCS)

FOR

MASTER OF SCIENCE WITH

CHEMISTRY

Department Members

- Dr Nidhi Sogani
- Dr Nisha Sharma
- Dr Kavita Yadav
- Mrs. Sapna Chaudhary
- Mrs. Hema Jain

SEMESTER WISE DISTRIBUTION OF CREDITS AND COURSES

Proposed Consolidated Scheme for M.Sc. Chemistry

S.No.	Paper	Topic	Credits
SEMESTER I			
1	Chemistry CC 1	INORGANIC CHEMISTRY – I (THEORY OF BONDING, SPECTROSCOPIC METHODS AND NUCLEAR CHEMISTRY)	4
2	Chemistry CC 2	ORGANIC CHEMISTRY – I (ORGANIC REACTION MECHANISM – I)	4
3	Chemistry CC 3	PHYSICAL CHEMISTRY – I (QUANTUM, SURFACE AND ELECTROCHEMISTRY)	4
4	Chemistry CC 4	SPECTROSCOPY – I	4
5	Chemistry CC 5	ANALYTICAL CHEMISTRY	4
6	Chemistry Lab 1	CORE LABORATORY – I	6
7	Chemistry Lab 2	CORE LABORATORY – II	4
9	Chemistry Research 1	SEMINAR	4
		Total Credit	**34**
SEMESTER II			
1	Chemistry CC 6	INORGANIC CHEMISTRY – II (GROUP THEORY, INORGANIC REACTION MECHANISM AND MOLECULAR REARRANGEMENT PROCESSES)	4
2	Chemistry CC 7	ORGANIC CHEMISTRY – II (STEREOCHEMISTRY & ORGANIC REACTION MECHANISM II)	4
3	Chemistry CC 8	PHYSICAL CHEMISTRY – II (THERMODYNAMICS AND CHEMICAL KINETICS)	4
4	Chemistry CC 9	SPECTROSCOPY – II	4
5	Chemistry CC 10	GREEN AND SUSTAINABLE CHEMISTRY	4
6	Chemistry Lab 4	CORE LABORATORY – III	6
7	Chemistry Lab 5	CORE LABORATORY – IV	4
9	Chemistry Research 2	INDUSTRIAL TRAINING	4
		Total Credit	**34**
SEMESTER III			

1	Chemistry CC 11	ORGANIC SYNTHESIS – I	4
2	Chemistry CC 12	ORGANOMETALLIC CHEMISTRY	4
3	Chemistry DSE 1	ELECTIVE – I	4
4	Chemistry DSE 2	ELECTIVE – II	4
5	Chemistry Lab 7	CORE LABORATORY – V	4
6	Chemistry DSE Lab 1	ELECTIVE LABORATORY – I	4
7	Chemistry Research 3	PROJECT PLAN / SYNOPSIS	4
8	Chemistry Research 4	PAPER WRITING	4
		Total Credit	**32**
SEMESTER IV			
1	Chemistry DSE 3	ELECTIVE – III	4
2	Chemistry DSE 4	ELECTIVE – IV	4
3	Chemistry DSE Lab 2	ELECTIVE LABORATORY – II	4
4	Chemistry Research 5	PROJECT WORK + SOCIAL WELLFARE PROJECT	4+4
		OR DISSERTATION	8
		Total Credit	**20**

Chemistry Discipline Specific Elective Paper offered in M.Sc.

Semester	**GROUP A**		**GROUP B**		**GROUP C**	
	Paper	**Papers Name**	**Paper**	**Papers Name**	**Paper**	**Papers Name**
III Semester	CHEMISTRY DSE 1	Environmental Chemistry	CHEMISTRY DSE 1B	Heterocyclic Chemistry	CHEMISTRY DSE 1C	Physical Polymer
	CHEMISTRY DSE 2	Inorganic Polymers	CHEMISTRY DSE 2B	Natural Products	CHEMISTRY DSE 2C	Solid State And Nanomaterials
IV Semester	CHEMISTRY DSE 3A	Bioinorganic Chemistry	CHEMISTRY DSE 3B	Organic Synthesis-II	CHEMISTRY DSE 3C	Advance Electrochemistry
	CHEMISTRY DSE 4A	Supramolecule and Photoinorganic	CHEMISTRY DSE 4B	Medicinal Chemistry	CHEMISTRY DSE 4C	Computational Chemistry

SEMESTER I

CORE COURSE I: CHEMISTRY CC I

INORGANIC CHEMISTRY – I

(THEORY OF BONDING, SPECTROSCOPIC METHODS AND NUCLEAR CHEMISTRY)

CREDIT: 4

Course Objectives:

The course aims to make the students explain about the stereochemistry and the nature of metal-ligand bonding in coordination compounds on the basis of Molecular Orbital Theory. To endow about electronic spectra of transition metal complexes. This course provide the information about the magnetics moment, exchange coupling and spin crossover. To provide knowledge about the working principle of nuclear counters and applications of radioactive isotopes.

Course Learning Outcome:

Concept of VSEPR theory and predict energetics of hybridisation. Comparison between CFT and MOT. Design MOT of different geometry. Discuss ground state and charge transfer spetra in different complexes. Explain the concepts of nuclear counters, functions of their major components and categories of nuclear reactions. Explain the concept of magnetic moments, Optical Rotaory Dispersion (ORD), Circular Dichroism (CD) of Transition Metal Complexes.

SYLLABUS:

UNIT – I : STEREOCHEMISTRY & BONDING IN MAIN GROUP COMPOUND AND METAL LIGAND BONDING **Lecture : 16**

STEREOCHEMISTRY & BONDING IN MAIN GROUP COMPOUND: VSEPR theory, dπ-pπ bond, Bent rule and energetics of hybridization, some simple reaction of covalently bonded molecules.

METAL LIGAND BONDING: Limitation of Crystal field Theory, Molecular Orbital Theory of Octahedral, Tetrahedral and Square Planar Complexes, π Bonding in Molecular Orbital Theory. John Teller distortion.

UNIT – II : ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES **Lecture : 16**

Spectroscopic Ground states, correlation, Orgel diagrams for transition metal complexes (d^1-d^9) states. Calculating Dq, B and β parameter. Charge transfer spectra. Electronic spectra of octahedral and tetrahedral complexes.

UNIT – III : OPTICAL ROTATORY DISPERSION (ORD), CIRCULAR DICHROISM (CD) AND MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES

Lecture : 14

Spectroscopic method of assignment of absolute configuration in optically active metal chelates and stereochemical conformation, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

UNIT – IV : NUCLEAR AND RADIOCHEMISTRY **Lecture : 14**

Laws of radioactive decay: Detection of radiations, Geiger-Nuttal rule GM tubes and their Characteristics, Ionization chamber, Proportional counters, Scintillation counters. Solid state detectors. Calibration of counting equipment's, Determination of absolute integration rates.
Nuclear shell model. Determination of spin parity. Stability of super heavy elements.

Reference Books:

- Inorganic Chemistry, Principles of structure and Reactivity, 4" Edition; James E. Huheey: Elleu A. Keiter: Richard L. Keiter.
- Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson.
- Theoretical Inorganic Chemistry; Day and Selbin. FEN.
- Concepts and Models in Inorganic Chemistry, Doughlas Me Daniel.
- Physical Methods in Inorganic Chemistry, R. S. Drago.
- Chemistry of the Elements; N.N. Greenwood and A. Earnshow, Pergamon, 1984.
- Inorganic Electronic Spectroscopy; A.B.P. Lever, Elsevier, 1968,
- Comprehensive Coordination Chemistry eds,, G. Wilkinson RD. Gillas and J.A. Me Clevert,
- megamon, 1987; Vol. 2.
- Nuclear and Radiochemistry; G. Friedlander, J. W. Kennedy, E.S. Macias ind J. M. Miller, 3" Edis Viley: NY, 1981.
- Besentials of Nuclear Chemistry, H. J. Arnikar; 4" Eds., New Age InternationuE N Delhi, India, 2011
- Nuclear and Radiochemistry: Fundamental and Applications, 2 Vols.; "Jets-Volkas Kratz and Ka Heinrich Lieser; 374 Edn., John Wiley & Sons: UK, 2013.

CORE COURSE II: CHEMISTRY CC II

ORGANIC CHEMISTRY – 1

(ORGANIC REACTION MECHANISM – I)

CREDIT: 4

Course Objectives:

The course aims to provide an in-depth knowledge about the organic-chemical reactions with a focus on aromaticity, reactive intermediates and their rearrangements. The course aims to provide students with an in-depth knowledge of different types of reaction mechanisms i.e. substitution, elimination and addition reactions of aliphatic and aromatic organic compounds.

Course Learning Outcome:

Evaluate the stability of various acyclic and cyclic systems using steric, electronic and stereoelectronic effects and correlate them to reactivity. Describe various types of reactive intermediates and factors affecting their stability.Identify the different aromatic, non-aromatic, homoaromatic & antiaromatic compounds and interpret their properties. Illustrate the mechanistic and stereochemical aspects of the nucleophilic substitution reaction of aliphatic and aromatic organic compounds. Explain the mechanistic and stereochemical aspects of the electrophilic substitution reaction of aliphatic and aromatic organic compounds. illustrate the mechanistic concepts to specific name reactions. Apply the basic principles involved in C-C and C-hetero multiple bond formation and be able to illustrate specific name reactions using these principles. Depict the mechanistic aspects of the elimination reaction.

SYLLABUS:

UNIT – I : REACTION MECHANISM, STRUCTURE & REACTIVITY	Lecture : 16
STRUCTURE AND REACTIVITY: Types of mechanisms and reactions, thermodynamic and kinetic control of reactions, Hammond's postulate, Curtin- Hammett principle, Potential enegy diagrams, transition states and intermediates, Methods of determining reaction mechanism, isotope effects. Hard and soft acids and bases Generation, structure, stability and reactivity of carbocation including non-classical carbocation, carbanion, free radical, radical anion, carbene, nitrene, benzyne, nitrenium ion. Effect of structure on reactivity: resonance, field & steric effects. Quantitative treatment of the effect of structure on reactivity. The Hammet equation and linear free energy relationship, substituent and reaction constants & Taft equation. AROMATICITY: Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule and Möbius system, energy level of π molecular orbitals in three to eight membered monocyclic systems having conjugation. Annulenes, fullerenes, antiaromaticity, homoaromaticity, PMO approach, steric inhibition to resonance.	

Bonds weaker than covalent: Addition compounds, phase transfer catalysis and crown ethers, cryptands, inclusion compounds, cyclodextrins, catenanes, rotaxanes and Kekulene.

UNIT – II : NUCLEOPHILIC SUBSTITUTION REACTION **Lecture : 14**

ALIPHATIC NUCLEOPHILIC SUBSTITUTION: S_N^1, S_N^2, mixed S_N^1 and S_N^2, and SET. The neighbouring group mechanism, NGP by π and σ bonds, anchimeric assistance.
Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon, reactivity effect of substrate structure, attacking nucleophile, leaving group, and reaction medium, ambident nucleophile, Regioselectivity.
AROMATIC NUCLEOPHILIC SUBSTITUTION: S_NAr, benzyne and $S_{RN}1$ mechanism, Reactivity - effect of substrate structure, leaving group and attacking nucleophiles on reactivity. Typical reactions– Bucherer reaction, Rosenmund-von Braun reaction, von-Richter, Sommelet-Hauser and Smiles rearrangement.

UNIT – III : ELECTROPHILIC SUBSTITUTION REACTION **Lecture : 14**

ALIPHATIC ELECTROPHILIC SUBSTITUTION: Bimolecular mechanism– S_E2 and S_Ei, the S_E1 mechanism, substitution accompanied by double bond shifts. Effect of substrates, leaving group and solvent polarity on the reactivity.
AROMATIC ELECTROPHILIC SUBSTITUTION: Arenium ion mechanism, orientation and reactivity, energy profile diagrams. o/p ratio, ipso attack, orientation in other ring systems. Quantitative treatment and reactivity in substrates and electrophiles. Substitution reactions involving diazonium ions, Vilsmeir-Haack reaction, Friedel-Craft reaction: Alkylation, arylation (Scholl reaction), acylation (ring closer, Haworth reaction, Hoesch reaction).

UNIT – IV : ADDITION AND ELIMINATION REACTION **Lecture : 16**

ADDITION TO C-C MULTIPLE BONDS: mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radical, regio- and chemo selectivity, orientation and reactivity, addition to cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings, hydroboration, Michael reaction, sharpless asymmetric epoxidation.
ADDITION TO C-HETERO MULTIPLE BONDS: mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles, addition of Grignard reagents, organozinc, organocopper and organolithium reagents to carbonyl and unsaturated carbonyl systems. Witting reaction.
Mechanism of condensation reactions involving enolates - Aldol condensations, Claisen, Dieckmann, Knoevenagel, Stobbe’s condensations, Mannich, Benzoin and Perkin reaction.
ELIMINATION REACTIONS: E2, E1, $E1_{CB}$ and $E2_C$ (syn elimination) mechanisms, orientation of the double bond, effect of substrate structure, attacking base, leaving group and reaction medium on reactivity. Mechanism and orientation in pyrolytic elimination.

Reference Books:

- Advanced Organic Chemistry: Reactions, Mechanisms and Structure; Seventh Edition; J. March; John Wiley and Sons Asia Private Limited, New Delhi, 2015.
- Advanced Organic Chemistry Part A & B; Fifth Edition; F. A. Carey and R. J. Sundberg; Springer, US, 2007.
- Physical Organic Chemistry Vol. I and II; Second Edition; N. Isaacs; Longman Scientific and Technical,1995.
- Named Organic Reactions; Second Edition: T. Lave and A. Plagens; John Wiley and Sons, 2005.
- Organic Chemistry: Vol. I and II; Singh, Mukherjee, Kapoor; Second Edition; New Age International Private Limited, New Delhi, 2018.
- Organic Reaction Mechanism; Fourth Edition; V.K. Ahluwalia and R.K. Parashar; Narosa Publishing House, New Delhi, 2002.

CORE COURSE III: CHEMISTRY CC III

PHYSICAL CHEMISTRY – I

(QUANTUM, SURFACE AND ELECTROCHEMISTRY)

CREDIT: 4

Course Objectives:

On successful completion of the course student will be able to Predict aspects of Quantum chemistry. Learn various laws of electrochemistry and their applications & Surface phenomena including three dimensional concept of molecules.

Course Learning Outcome:

Predict the non-relativistic quantum mechanics. Explain time dependent and time independent schrodinger equations for, spin. Explain Angular momentum states, angular momentum addition rules, and identical particles. Familiar with the concepts of surface chemistry. Analyze principles of kinetics & mechanism of surface reactions & understand the relation kinetics and summarize the concepts of adsorption and micelles. Get the fundamentals of electrochemistry and electrochemical cell & dynamics of electrochemistry and electrochemical process.

SYLLABUS:

UNIT – I : QUANTUM CHEMISTRY **Lecture : 17**

Introduction: Historical background - Black body Radiation, de-Broglie concept, Heisenberg's Uncertainty Principle. Postulates of Quantum Mechanics, Operators - Linear, Commutator, Hamiltonian, Hermitian and Angular Momentum Operators, Eigen Value and Eigen Functions, Schrodinger's equation, wave function, physical significance of Ψ^2.

Application of Schrodinger's Equation to (i) particle in one dimensional box, (ii) particle in three dimensional box, (ii) Simple Harmonic Oscillator, (iv) Rigid Rotor and (v) Hydrogen atom; Radial and angular wave functions, quantum numbers and their significance.

UNIT – II : ANGULAR MOMENTUM, APPROXIMATION METHOD & MOLECULAR ORBITAL THEORY **Lecture : 14**

Angular Momentum: Ordinary angular momentum, Eigen functions and Eigen values of angular momentum, Ladder Operator, Addition of Angular Momentum, Spin, antisymmetry and Pauli's exclusion principle.

Approximation Method: The Variation theorem, linear variation principle, perturbation method (First order and nondegenarate). Application of variation method and perturbation method to Helium atom.

Molecular Orbital Theory: Basic ideas, criteria of forming MOs, LCÃO Concept. Huckel's Molecular Orbital (HMD) theory for conjugated organic systems. Application of HMO to ethylene, allylic, cyclopropanyl, butadiene and cyclobutadiene system.

UNIT – III : SURFACE CHEMISTRY **Lecture : 16**

Adsorption: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon)
Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction , critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization -phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

UNIT – IV : ELECTROCHEMISTRY **Lecture : 13**

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination Structure of electrified interfaces, Guoy-Chapman, Stern, Graham Devanatham-Mottwatts, Tobin, Bockris, Devanathan models, Over potentials, exchange, current density derivation of Butler Volmar quation, Tatel plot. Polarography theory, Ilkovic equation; half wave potential and its significance.

Reference Books:

- Physical Chemistry by P.W. Atkins, ELBS.
- Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill
- Quantum Chemistry. Ira N. Levine, Prentice Hall
- Quantum Chemistry; RK Prasad, New Age International.
- Micelles, Theortical and Applied aspects, V. Morai, Plenum Press
- Modern Electrochemistry Vot. I & II; J.O.M. Bockris and A.K.N. Reddy Plenum Press, HNew York.
- Physical Chemistry by Puri, Sharma and Pathania Vishal Publications.

CORE COURSE IV: CHEMISTRY CC IV
SPECTROSCOPY – I

CREDIT: 04

Course Objectives:

The course aims to impart knowledge of origin of basic principles of spectroscopy and its applications to Microwave, Vibrational, Raman, Electronic, Magnetic Resonance and Mossbauer spectroscopy.

Course Learning Outcome:

Recognize spectroscopy in microwave, Rotational spectra of rigid diatomic molecules, selection rules, interaction of spectral lines Study of Vibrating diatomic molecule, energy levels of a diatomic molecule, simple harmonic and anharmonic oscillator, Scattering of light and Raman Spectrum. rotational and vibrational Raman Spectra. Describe working principle and selection rule of electronic spectroscopy. Apply quantum mechanical approach to NMR spectra. Make Students aware of the fine structure of ESR absorption, Hyperfine structure, Techniques of ESR spectroscopy. Understand Principles and Applications of Mossbauer spectroscopy.

SYLLABUS:

UNIT – I : MICROWAVE AND VIBRATIONAL SPECTROSCOPY	**Lecture : 18**
INTRODUCTION: Interaction of electromagnetic radiation with matter, mechanism of absorption and emission of radiation. MICROWAVE SPECTROSCOPY: Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications. VIBRATIONAL SPECTROSCOPY: lnfrared Spectroscopy: vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P,Q,R branches. Breàkdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations. Raman Spectroscopy: Classical and quantum theories of Raman effect. Pure Rotational, Vibrational and Vibrational-Rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS)	
UNIT – II : ELECTRONIC SPECTROSCOPY	**Lecture : 14**
ATOMIC SPECTROSCOPY: Energies of atomic orbitals, vector representation of momenta	

and vector coupling, spectra of hydrogen atom and alkali metal atoms.
MOLECULAR SPECTROSCOPY: Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.
PHOTOELECTRON SPECTROSCOPY: Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy — basic idea.

UNIT – III : MAGNETIC RESONANCE SPECTROSCOPY Lecture : 16

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY: Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, AzB_2 etc.), spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton - ^{13}C, ^{19}F and ^{31}P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.
ELECTRON SPIN RESONANCE SPECTROSCOPY: Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

UNIT – IV : MOSSBAUER SPECTROSCOPY Lecture : 12

Basic Principles, spectral parameters and spectrum display, application of the technique to the study of (i) bonding and structure of Fe^{+2} and Fe^{+3} compounds including those of intermediate (ii) Sn^{+2} and Sn^{+4} compounds, nature of ML bond, coordination number, structure (iii) Detection of oxidation state and equivalent MB atoms

Reference Books:

- Modem Spectroscopy, J.M. Hollas, John Wiley.
- Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
- NMR, NQR, EPR and Mössbauer Spectroscopy in lnorganic Chemistry, R.V. Parish, Ellis Harwood.
- Physical'Methods in Chemistry, R.S. Drago, Saunders College.
- Chemical Applications of Group Theory, F. A. Cotton.
- Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
- Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
- Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
- Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.

- Introduction to Magnetic Resonance, A Carrington and A.D. Maclachalan, Harper & Row.

CORE COURSE V: CHEMISTRY CC V
ANALYTICAL CHEMISTRY

CREDIT: 4

Course Objectives:

To develop an understanding of the range and the uses of analytical methods in chemistry. To get in-depth knowledge of analytical methods such as Sampling, Chromatography, Conductometry and their applications.

Course Learning Outcome:

Explain the fundamentals of analytical chemistry and steps of a characteristic analysis. Express the role of analytical chemistry in science. Compare qualitative and quantitative analyses. Define principle concepts about sampling. Categorizes and defines the sampling methods. Describe the principle and type of Planar and Thin layer chromatography. Describe the set up and process of planar and thin layer chromatography. Determine the values of many physical qualities such as degree of dissociation and dissociation constant of weak electrolyte, ionic products of water and solubility product of salts using conductometry. Describe the application of coulometric titration.

SYLLABUS:

UNIT – I : INTRODUCTION **Lecture : 14**

Role of analytical chemistry. classification and Limitations of analytical chemistry, Errors and classification, Determinant, constant and indeterminate accuracy, precision, minimization of errors, significant figures and computation rules, mean and standard deviation, distribution of random errors , variance and confidence interval, paired t-test ,least square method ,correlation and regression, linear regression

UNIT – II : SAMPLING IN ANALYSIS **Lecture : 14**

Definition, theory, basis and techniques of sampling, sampling statistics, sampling and physical state, crushing and grinding, hazards in sampling, techniques of sampling of gases, fluids, solids, and particulates, minimization of variables, transmission and storages of sample, high pressure ashing techniques (HPAT), particulate matter, its separation in gas stream, filtering and gravity separation, analysis of particulate matter like asbestos, mica, dust and aerosols etc.
Solvent extraction method in analysis: Principle, classification, theory, instrumentation and application.

UNIT – III : CHROMATOGRAPHY **Lecture : 16**

Types, Ion exchange chromatography, planar chromatography-paper and TLC. Stationary and mobile phases, GC theory, instrumentation and application, liquid-liquid partition chromatography, HPLC, reverse phase chromatography, size exclusion and affinity chromatography

UNIT – IV : CONDUCTOMETRY AND COULOMETRY Lecture : 16

CONDUCTOMETRY: Important laws, definitions, relations, effect of dilution on conductivity, measurement of conductivity, types of conductometric titrations, its applications and limitations.

COULOMETRY

Introductions, principle, experimental details of coulometry at constant current constant potential, titrational applications**.**

Reference Books:

- Analytical Chemistry, Christian G.D., John Wiley & Sons Inc. 2004.ss
- Fundamentals of analytical Chemistry. Skoog. D.A. West D.M. and Hooler F.J., W.B. Saunders.
- Analytical Chemistry-Principles. Kennedy. J.H., W.B. Saunders.
- Analytical Chemistry-Principles and Techniques, LG. Hargis. Prentice Hall.
- Principles of Instrumental Analysis by D.A. Skoog, Holler F.J. and Nieman T.A., 5th Edn, Thomson Brooks/Cole, Bangalor, 2004.
- Principles of Instrumental analysis Skoog D.A. and Loary J.L., Saunders W.B..
- Quantitative Analysis, Day R.A., Jr. and Underwood A.L., Prentice Hall.
- Basic Concepts of Analysis Chemistry, Khopkar S.M., Wiley Eastern.
- Vogels Textbook of Quantitative Chemical Analysis, by Menham J., Denney R.C., Barnes J.D. and Thomas M.J.K., 6th Edn, Low Price Edn, Pearson Education Ltd, New Delhi, 2000.
- Instrumental Analysis, Editors, Christian G.D. and Reilly J.E. O, 2nd Edn, Allyn and Bacon, Inc., Boston,1986.
- Principles and Practice of Analytical Chemistry by. Fifield F.W and Kealey D., 5th Edn, Blackwell Science Ltd, New Delhi, 2004.
- Handbook of Instrumental Techniques for Analytical Chemistry, Editor, Settle F., Low Price Edn, Pearson Education Inc, New Delhi, 2004.
- Instrumental Methods of Chemical Analysis by Ewing G.W., 5th Edn, McGraw Hill Singapore,1985. nalytical Chemistry, Christian G.D., John Wiley & Sons Inc. 2004.

CORE LABORATORY I: CHEMISTRY LAB I

CREDIT: 6

Course Objectives:

The course aims to acquaint the students with various safety measures including handling of chemicals, safe disposal of chemical wastes etc., to make students understand the concept of separation of mixtures containing metal ions, insoluble and interfering radicals. Learn about the synthesis of different metal complexes and to identify them with the help of IR spectra and to make students understand about the different concepts behind the gravimetric and volumetric techniques and its uses in separation of different metal ions from a given mixture. Develop quantitative and qualitative skills to use the basic techniques involved in synthetic organic chemistry. To get knowledge of basic terms regarding surface tension, viscosity and Lambert-Beer law.

Course Learning Outcome:

Apply the knowledge of volumetric and gravimetric techniques in separation and estimation of the amount of different metal ions present in the mixture. Prepare inorganic and organic complexes and interpret their spectra. Apply suitable techniques to separate an inorganic and organic mixture. Perform experiments based on surface tension, viscosity and adsorption phenomena.

SYLLABUS:

INORGANIC CHEMISTRY:

1. Qualitative and Quantitative Analysis
   a) Qualitative analysis of mixture containing of eight cationic / anionic radicals including (i) Interfering anionic radicals (ii) Less common metal ions — TI, Mo, W, Ti, Zr, Th, V, U
   b) Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods
2. Preparation of inorganic compounds and their study by IR, electronic spectra, Mossbauer, ESR and magnetic susceptibility measurements (any four):
   a) cis and trans $[Co(en)2Cl_2]^+$
   b) Tetraamine cupric sulphate $[Cu(NH_3)_4SO_4].H_2O$
   c) $[Ni(NH_3)_6]Cl_2$
   d) $[Cr(H_2O)_6]NO_3.3H_2O$,
   e) cis-$K[Cr(C_2O_4)(H_2O)_2]$
   f) $Na_2S_2O_3.5H_2O$
   g) Prussian Blue

ORGANIC CHEMISTRY:

3. Qualitative Analysis
   Separation, purification and identification of compounds of binary mixture [(one

liquid and one solid) or (two solids) using H_2O, HCl, NaOH, $NaHCO_3$, ether or other reagents. IR spectra to be used for functional group identification and Preparation of derivatives.

4. Organic Synthesis (The Products may be Characterized by Spectral Techniques) (any four)
   a) Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography
   b) Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol
   c) Grignard reaction: Synthesis of triphenylmethanol from benzoic acid
   d) Aldol condensation: Dibenzal acetone from benzaldehyde
   e) Sandmeyer reaction: p-ChlorotoIuene from p-toluidine
   f) Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
   g) Cannizzaro reaction: 4-ChIorobenzaIdehyde as substrate
   h) Friedel Crafts Reaction: §-Benzoyl propionic acid from succinic anhydride and benzene
   i) Aromatic electrophilic sustitutions: Synthesis of p-nitroaniline and p-bromoaniline.

PHYSICAL CHEMISTRY:

Surface tension

5. To study surface tension concentration relationship for solution (Gibbs equation).
6. To determine the critical micelle concentration (CMC) of SDS and CTAB by surface tension techniques.

Adsorption

7. Adsorption of Oxalic acid
8. Acetic acid on charcoal

Viscosity, Solubility and Molecular weight determination

9. Experiments based on definition of viscosity of given liquid using Ostwald's viscometer.
10. Study the variation of viscosity of pure liquid with temperature and determination of temperature coefficient of viscosity of the liquid.
11. Determination of Solubility of various salts like NaCI, KCI, KNO_3 and $NaNO_3$ at different temperature and draw the solubility Curve.
12. Determination of molecular weight of given polymer (Polyvinyl alcohol, polystyrene, methyl acrylate, etc.)
13. Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopy method and to determine the activity coefficient of an electrolyte

Potentiometry/pH-metry

14. Determination of strength of halides in a mixture potentiometrically.
15. Determination of the valency of given ions potentiometrically.
16. Determination of activity and activity coefficient of the given electrolytes.

Reference Books:

- Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS

- Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall
- Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
- Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
- Vogel's Textbook of Practical Organic Chemistry, A. R. Tatchell, John Wiley
- Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman
- Findley's Practical Physical Chemistry, B.P. Levitt, Longman
- Experimental Physical Chemistry, R.C. Das and B. Behea, Tata McGraw Hill.
- Experiments in Physical Chemistry, J. C. Ghosh, Bharati Bhavan.

CORE LABORATORY II: CHEMISTRY LAB II

CREDIT: 4

Course Objectives:

Conceptual understanding of gravimetric, chromatographic, spectrocopic and conductometric analysis.

Course Learning Outcome:

Technique and application of gravimetric, chromatographic, spectrocopic and conductometric analysis.

SYLLABUS:

1. Gravimetric determination of Nickel (as dmg), Zinc (as Zinc ammonium phosphate), silver (as chloride)
2. To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+} DMG complex in chloroform.
3. Separation of mixtures by chromatography: measure the R_f value in each case.
   Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}.
   Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.
4. Conductometry:
   i. Verification of onsager's equation for strong electrolytes (NaCl, HCl, KNO_3, KCl) and determination of constant A & B.
   ii. Determination of strength of strong and weak acids in a given mixture conductometrically.
   iii. Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.
5. Spectroscopy
   i. Determination of pka of an indicator (e.g., methyl red) in (a) aqueous and (b) micellar media.
   ii. Determination of stoichiometry and stability constant of inorganic (e.g., ferric – salicylic acid) and organic (e.g. amine- iodine) complexes.
   iii. Characterization of the complexes by electronic and IR spectral data.

Reference Books:

- Skoog, D.A. Holler F.J. & Nieman, T.A. *Principles of Instrumental Analysis*, Cengage Learning India Ed.
- Christian, Gary D; Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
- Mikes, O. *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Series on Analytical Chemistry, John Wiley & Sons, 1979.

- Jeffery, G.H., Bassett, J., Mendham, J. & Denney, R.C. *Vogel's Textbook of Quantitative Chemical Analysis*, John Wiley & Sons, 1989.

CHEMISTRY RESEARCH I: SEMINAR

CREDIT: 4

Course Objectives:

The course aims to enhance ability of the students to read, assimilate and discuss scholarly articles and research papers showcasing chemistry as well as the interdisciplinary areas of sciences and to develop strong oral and written communication skills to present their ideas effectively through power-point presentations and appropriate software for the analysis of data. Develop critical thinking and confidence level.

Course Learning Outcome:

Students would be able to create, revise and present ideas in spoken and written forms. Acquired listening, questioning and critical thinking skills. Demonstrate ability to defend and support ideas/claims with appropriate evidence. Students gained experience for how to organize and deliver/disseminate knowledge before audience.

CONTENT:

This activity is important to enhance communication skill of the M.Sc. students, the candidates will have to choose a topic from the syllabi for seminar preparation. They will be expected to submit a write up pertaining to that topic and at the end of semester, a presentation will have to be made in presence of panel of experts from different fields of chemistry.

SEMESTER II

CORE COURSE VI: CHEMISTRY CC VI
INORGANIC CHEMISTRY – II
(GROUP THEORY, INORGANIC REACTION MECHANISM AND MOLECULAR REARRANGEMENT PROCESSES)

CREDIT: 04

Course Objectives:

To impart advanced knowledge on fundamental aspects of classifying molecules based on various symmetry elements, point groups and relate their vibrational spectroscopic feature. To enable the students to learn about reaction mechanism of transition metal complexes. This course provide the information about the electron transfer reactions & Synthesis of coordination compounds.

Course Learning Outcome:

Develop skill for identification symmetry of different elements. Illustrate symmetry operation point groups and their classification. Concept of substitution Reaction. Describe the application of VBT and MOT. Draw mechanism of different complexes and describe their factor affecting and applications. Get to know about stability of co-ordination compounds. Figure out different type of transfer reaction. Describe the Coordination compounds using electron transfer reactions.

SYLLABUS:

UNIT – I : SYMMETRY AND GROUP THEORY IN CHEMISTRY	**Lecture : 18**
Symmetry elements and symmetry operations, definition of group and subgroup, relation between order of a finite group and its subgroup, conjugacy relation and classes, point group, symmetry group, schonfiles symbols, representations of groups by reducible and irreducible representations and relation between them (representation for the C_n, C_{nv}, D_{nh} etc. groups to be worked out explicitly), character of a representation, character tables of C_{2v} and C_{3v} and their use.	
UNIT – II : REACTION MECHANISM OF TRANSITION METAL COMPLEXES – 1	**Lecture : 16**
Basic principles, lability, inertness stability and instability of co-ordination compounds. General principle and mechanism of substitution reaction of tetrahedral, square planar, trigonal bipyramidal, square pyramidal and octahedral complexes; potential energy diagram, transition state and intermediate, isotope effect, Berry's pseudo rotation mechanism.	

UNIT – III : REACTION MECHANISM OF TRANSITION METAL COMPLEX – II **Lecture : 14**

Kinetics of octahedral substitution, acid hydrolysis, factor affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favor of conjugate mechanism, anation reactions, and reactions without metal ligand bond cleavage.

Redox reactions, electron transfer reactions, mechanism of one electron transfer reaction, outer sphere type reactions, inner sphere type reactions.

UNIT – IV : MOLECULAR REARRANGEMENT PROCESSES **Lecture : 14**

Electron transfer reactions (outer and inner sphere), HOMO and LUMO of oxidant and reductant, Chemical activation. Precursor complex formation and rearrangement, nature of bridge ligands, fission of successor complexes, Two-electron transfers, Synthesis of coordination compounds using electron transfer reactions, mixed valence complexes and internal electron transfer.

Reference Books:

- E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.
- R. S. Drago, Physical Methods in Inorganic Chemistry, 1st Edn.(1971), Affiliated EastWest Press, New Delhi.
- Kettle. S. F. A. Physical Inorganic Chemistry: A Coordination Chemistry Approach, Springer, Berlin, Heidelberg (1996).
- Jaffe, H. H. & Orchin, M. Symmetry in Chemistry Dover Publications (2002).
- Cotton, F. A. Chemical Applications of Group Theory Wiley Interscience: N.Y (1990).
- Hatfield, W. E. & Parker, W. E. Symmetry in Chemical Bonding & Structure C. E. Merrill Publishing Co. USA (1974).
- Bishop, D. M. Group Theory and Chemistry, Clarendon Press: Oxford, U.K. (1973).
- F.A. Cotton and G. Wilkinson *Advanced Inorganic Chemistry*, 6th Edn. (1999), John Wiley & Sons, New York.
- J.E. Huheey, E.A. Keiter and R.L. Keiter, *Inorganic Chemistry*, 4th Edn. (1993), Addison Wesley Pub. Co., New York.
- F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Edn (1967), Wiley Eastern Ltd., New Delhi.
- L. Tobe and John Burgess, Inorganic Reaction Mechanisms, Longmans Ist Edn. (1999).

CORE COURSE VII: CHEMISTRY CC VII
ORGANIC CHEMISTRY – II
(STEREOCHEMISTRY & ORGANIC REACTION MECHANISM II)

CREDIT: 4

Course Objectives:

To impart advanced knowledge of stereochemistry of organic compounds, pericyclic and photochemical reactions.

Course Learning Outcome:

Evaluate the stability of various acyclic and cyclic systems using various stereoelectronic effects and correlate their reactivities. Outline the different processes governing the course of photochemical reactions. Distinguish between thermal and photochemical energies and their effect on the course of chemical reactions. Comprehend the orbital interactions and orbital symmetry correlations of various pericyclic reactions. Explain various pericyclic reactions i.e. Electrocyclic reactions, Cycloaddition reactions and Sigmatropic reactions. Predict structures of the products based on the reaction conditions and reagents used in pericyclic reactions. Understand the change of connectivity of an existing organic backbone by using reactions that result in skeletal rearrangements. Interpret Ring expansion and contraction by rearrangement and controlling rearrangements.

SYLLABUS:

UNIT – I : STEREOCHEMISTRY	**Lecture : 14**

Optical activity and Chirality, elements of symmetry, molecules with one, two or more chiral centres. D/L , R/S and Threo/Erythro nomenclature.
Prochirality: Topicity of ligands and faces and their nomenclature. Stereogenicity, pseudoasymmetry, planar chirality, axial chirality, optical purity, chirogenicity, stereogenic and prochiral centres.
Optical activity in the absence of chiral carbons: biphenyls, allenes, alkyldienes, cycloalkyldienes, spiranes, ansa compounds, adamantanes, and cyclophanes, chirality due to helical shape (P & M), chirality in the compounds containing N, S and P.
Configurations, conformations and stability of cyclohexanes (mono, di, and trisubstituted), cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols and decalones, effect of conformation on reactivity, strain in cycloalkanes.
Chiral synthesis, stereoselective and stereospecific synthesis, Prelog's rule, Felkin-anh rule, CD, ORD, octant rule, Cotton effect and their application in determination of absolute and relative configuration and conformation, the axial haloketone rule. Chiral auxiliary and chiral pool.

UNIT – II : PHOTOCHEMISTRY	**Lecture : 14**

Laws of photochemistry. Fate of excited molecules - Jablonskii diagram, energy pooling, exciplexes, excimers, photosensitization, quantum yield, solvent effect, Stern-Volmer equation, delayed fluorescence.

Photochemical reactions of carbonyl compounds –Norrish type I cleavage, Norrish type II cleavage; photo reductions; Paterno-Buchi reactions; Photochemistry of α,β-unsaturated ketones, β,γ-unsaturated ketones, cyclohexadienones (cross conjugated and conjugated).

Photochemistry of alkenes: Intramolecular reactions of the olefinic bond – cis-trans isomerisation (stilbene), cyclization reactions, rearrangement of 1,4 and 1,5-dienes, di-π methane rearrangement.

Photochemistry of aromatic compounds: Photochemical rearrangement, photostationary state, isomerization.

Miscellaneous Photochemical Reactions: Barton reaction, photo Fries rearrangement of ethers and anilides, singlet oxygen reactions (photo oxygenation).

UNIT – III : PERICYCLIC	**Lecture : 16**

General characteristics and classification of pericyclic reaction, molecular orbital symmetry. Woodward-Hoffmann selection rules, Fukui's FMO approach, Woodword-Hoffmann's conservation of orbitals symmetry and correlation daigram and PMO approach.

Electrocyclic Reactions: conrotatory and disrotatory, electrocyclisation and reterocyclisation of 4n, 4n+ 2 π electron and allyl, valence tautomerism.

Cycloaddtion Reactions: antrafacial and suprafacial addition, 4n and 4n+2 π electron systems. Diels Alder reaction- stereo-selectivity (endo, exo), stereo-specificity and region-selectivity, normal and inverse demand Diels Alder reactions, asymmetric Diels Alder reaction, retro Diels Alder reaction, 1, 3-dipolar cycloaddition and cheletropic reactions;

Sigmatropic Rearrangements: Suprafacial and antarafacial shifts of C-H and C-C bonds, retension and inversion of configuration, 3,3- and 5,5-sigmatropic rearrangements; Claisen, Cope and Aza-Cope rearrangements; Fluxional tautomerism (bullvalene); Ene reaction.

UNIT – IV : MOLECULAR REARRANGEMENT	**Lecture : 16**

Mechanistic aspects, nature of the migration, migratory aptitudes, memory effects. A detailed study to the following rearrangements; Wagner-Meerwein, pinacol-pinacolone, Benzil-Benzilic acid rearrangement, rearrangement involving diazomethane (Wolff and Demjanov rearrangement), Stevens, Sommelet and Wittig rearrangements, Favorskii rearrangement in acyclic and cyclic α-halo ketones, Fries Rearrangement, Hoffman, Curtius, Schmidt and Lossen rearrangements and its key reaction intermediates, Neber, Beckmann rearrangement and its stereochemistry, Baeyer–Villiger rearrangement Dakin reaction, Shapiro reaction .

Reference Books:

- Stereochemistry: Conformation and Mechanism; Tenth Edition; P.S. Kalsi; New Age International Publishers Pvt. Ltd, New Delhi, 2019.

- Stereochemistry of Organic Compounds; Third Edition; D. Nasipuri; New Age International Publishers Pvt. Ltd, New Delhi, 2007.
- Stereochemistry and Mechanism through solved Problems; Third Edition; P. S. Kalsi; New Age International Pvt. Ltd., New Delhi, 2004.
- Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).
- Horspool, W. M. Aspects of Organic Photochemistry Academic Press (1976).
- Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc. (1981).
- March, J. Advanced Organic Chemistry John Wiley & Sons (1992).
- Fleming, I., Pericyclic Reactions, Oxford Science Publications (1998).
- Marchand, A. P. & Lehr, R. E. Pericyclic Reactions Academic Press (1977).
- J. Clayden, N.Greeves, S. Warren and P. Wothers, Organic Chemistry, 1st Ed., Oxford University Press, 2001.
- M.B. Smith & J.March, March's Advanced Organic Chemistry, 5th Ed., John Wiley & Sons, New York, 2001.

CORE COURSE VIII: CHEMISTRY CC VIII
PHYSICAL CHEMISTRY – II
(THERMODYNAMICS AND CHEMICAL KINETICS)

CREDIT: 04

Course Objectives:

To understand the basic concepts and principle of classical & Statistical thermodynamics. Determine the rate of reaction and their relation to the way the relation proceeds.

Course Learning Outcome:

Describer the principles concerring solid state structures, understand the different type defects & thermodynamics of defects. Differentiate between metals, insulators and semiconductors.Learn electrically conducting solids. To understand the basic concept's in statistical thermodynamics including the Bolt'zmann distribution law, partition functions, calculations of thermodynamic properties. Understand rate of reactions and the factors that affect the rates of reactions, rate laws different theories of reaction rates and two these account for experimental observations. To understand the general features of fast reactions, collision theory & activated complex theory.

SYLLABUS:

UNIT – I : CLASSICAL THERMODYNAMICS	Lecture : 18
Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropics. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient and its determination. Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.	
UNIT – II : STATISTICAL THERMODYNAMICS	**Lecture : 12**
Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical Onsembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions. Application of partition functions. Heat capacity behavior of solids-chemical equilibria and equilibrium constant in terms of partition functions. Fermi-Dirac statistics, distribution law and	

applications to metal. Bose-Einstein statistics distribution Law and application to helium.

UNIT – III : CHEMICAL KINETICS - I **Lecture : 18**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects : Steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain reactions (hydrogen-bromine reaction, pyrolysis of acetaldchyde, decomposition of ethane), photochemical reactions (hydrogen-bromine and hydrogen-chlorine).

UNIT – IV : CHEMICAL KINETICS - II **Lecture : 12**

General features of fast reactions, study of fast reactions by flow method, relaxation method; flash photolysis and the nuclear magnetic resonance method. Collision theory of reaction rates, Arrhenius equation and the effect of temperature on reaction rate.
Activated complex theory, Modified collision theory (steric effect) names of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus (RRKM) theories of unimolecular reactions).

Reference Books:

- P. W Atkins, Physical Chemistry, ELBS.
- ER K Laidler, Chemical Kinetics; McGraw Hill.
- J. Raraman and J. Kuriacose, Kinetics and Mechanism of Chemical Transforma ion, Plenum.
- Samuel Glasstone, Thermodynamics for Chemist, East West Press,
- R. P.Rastogi and R. R. Mishra, Introduction to Chemical Thermodynamics, Vikash Publication House.
- Purt, Sharma and Pathaniya, Principles of Physical Chemistry, Vishal Publications.

CORE COURSE IX: CHEMISTRY CC IX
SPECTROSCOPY – II

CREDIT: 4

Course Objectives:

To impart knowledge of spectroscopic techniques (UV, IR, NMR and Mass) and understand structural elucidation of unknown organic compound using combined spectral data.

Course Learning Outcome:

To understands the basic principle of UV and IR. To interpret relevant terms of uv-spectroscopy. To describe molecular vibration with the interaction of matter and electromagnetic wave. To interpret the basic principle of NMR spectroscopy. Be able to predict the splitting pattern in the proton NMR of a compound given its structure. To describe how ionization of molecules can take place. Explain how a mass spectrum should be used to identify unknown component. To determine the number of distinct C atoms in a molecule. Assign a chemical shift to each carbon in a given molecule.

SYLLABUS:

UNIT – I : UV AND IR SPECTROSCOPY	Lecture : 18
ULTRAVIOLET AND VISIBLE SPECTROSCOPY : Various electronic transitions (185-800 nm), Beer—Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls. INFRARED SPECTROSCOPY: Instrumentation and sample handling, Characteristic vibrational 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, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT IR. IR of gaseous, solids and polymeric materials. Definition, deduction of absolute configuration, octant rule for ketones.	
UNIT – II : NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY	**Lecture : 14**
General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of	

deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve- variation of coupling constant with dihedral angle. Simplification of complex spectra- nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei-F, P.

UNIT – III: MASS SPECTROMETRY	**Lecture : 14**
Introduction, ion production - El, Cl, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.	
UNIT – IV: CARBON-13 NMR SPECTROSCOPY	**Lecture : 14**
General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques. Application of Spectroscopy: Problem based on UV, IR, NMR spectroscopy, and mass Spectrometry for structural elucidation of organic compounds.	

Reference Books:

- Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
- Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
- Progress in Inorganic Chemistry vol., 8, ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley
- Transition Metal Chemistry eck R.L. Carlin vol. 3, Dekker
- Inorganic Electronic Spectroscopy,. A.P.B. Lever, Elsevier.
- NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
- Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J. f\/ttrtin, Heyden.
- Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley
- Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
- Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
- Spectroscopic Methods in Organic Chemistry, D. H. Williams, l. Fleming, Tata McGr.

CORE COURSE X: CHEMISTRY CC X
GREEN AND SUSTAINABLE CHEMISTRY

CREDIT: 4

Course Objectives:

Learn principle green chemistry for designing chemical synthesis in future trends. Students will acquire knowledge to use various diffraction methods in structural analysis and to understand the different aspects of nano materials.

Course- Learning Outcome:

This part of course provides introduction to green chemistry aspects and the approaches to be adopted for greener synthesis. Students will understnad the significance of green chemistgry in industries specially to provide cleaner energy.

SYLLABUS:

UNIT – I : INTRODUCTION, PRINCIPLE AND CONCEPT OF GREEN CHEMISTRY **Lecture : 14**
Introduction, principle and concepts of Green Chemistry Need for green chemistry; Inception and evolution of green chemistry; Twelve principles of green chemistry with their explanations and examples; Designing a green synthesis using these principles; Green chemistry in day to day life.
UNIT – II : NON-TRADITIONAL GREENER ALTERNATIVE APPROACHES **Lecture : 14**
Different approaches to green synthesis: (a) Uses of green reagents in organic synthesis · Dimethyl carbonate, polymer supported reagents - per acids and chromic acid (b) Green catalysts, role of catalysis in sustainable development, homogeneous and heterogeneous catalysts; Introduction, advantages and applications of (i) Nanocatalysts, (ii) Phase transfer catalysts, (iii) Biocatalysts, (iv) Organocatalysts, in organic synthesis.
UNIT – III : APPLICATIONS OF NON-CONVENTIONAL ENERGY SOURCES **Lecture : 16**
Introduction of microwave induced synthesis: Microwave activation, equipment, time and energy benefits, limitations; Organic transformations under microwaves Fries rearrangement, Diels-Alder reaction, decarboxylation, saponification of ester, alkylation of reactive methylene compounds; Heterocyclic synthesis - B-Lactams, pyrrole, quinoline. Introduction of ultrasound assisted green synthesis: Instrumentation, physical aspects, applications in organic transformations. Electrochemical synthesis: Introduction, synthesis of sebacic acid and

adiponitrile.

UNIT – IV : ENVIRONMENTALLY BENIGN SOLUTIONS TO ORGANIC SOLVENTS **Lecture : 16**

Ionic liquids as green solvents: Introduction, properties and types of ionic liquids. Synthetic applications - Diels-Alder reaction, epoxidation and Heck reaction. Aqueous phase reactions: Enhancement of selectivity, efficiency. Synthetic applications - 1,3-Dipolar Cycloadditions, Carbon-Carbon bond-forming processes and bromination reactions. Fluorous solvents in green chemistry: Scope, definition and their synthetic applicability. Role of supercritical carbon dioxide in green chemistry, Ethyl lactate as a renewable green solvent: Properties and applications.

Reference Books:

- P.T. Anastas and J.C. Warner. Green Chemistry: Theory and Practice, Oxford University Press.
- M. Lancaster, Green Chemistry: Introductory Text. Royal Society of Chemistry (London).
- M.A. Ryan and M.Tinnesand, Introduction to Green Chemistry, American Chemical Society (Washington).
- F.M. Kerton. Alternative Solvents for Green Chemistry, Royal Society of Chemistry (London).
- V.K. Ahluwalia, M. Kidwni, New Trends in Green Chemistry, Springer.

CORE LABORATORY III: CHEMISTRY LAB III

CREDIT: 04

Course Objectives:

The course aims to make the students aware of the different spectrophotometric and electroanalytical techniques. Acquire the knowledge of basic terminology regarding chemical kinetics, viscosity and surface tension.

Course Learning Outcome:

Understand the student the principle behind flamephotometery and spectrophotometry. Predict the kinetics of different reactions. Perform experiment based on surface tension and viscosity measurements.

SYLLABUS:

INORGANIC CHEMISTRY

1. Flame Photometric Determinations:
   - i. Sodium and potassium when present together
   - ii. Lithium/calcium/barium/stronlium
   - iii. Cadmium and magnesium in tap water.
2. Spectrophotometric Determinations:
   - i. Nickel/molybdenum/tungston/vanadium/uraniumby extractiv spectrophotometric method.
   - ii. Iron-phenanthroline complex: Job‘s Method of continuous variations.
   - iii. Zirconium-Alizarin Red-S complex: Mole-ratio method.
   - iv. Copper-Ethylene diamine complex: Slope-ratio method.

ORGANIC CHEMISTRY

3. Stereochemical study of organic compounds via models:
   - i. R and Z configuration of optical isomers
   - ii. E, Z configuration of geometrical isomers
   - iii. Conformational analysis of cyclohexanes and substituted cyclohexanes.
4. Multi-step Synthesis of Organic Compounds

   The exercises should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.
   - i. Photochemical reaction: Benzophenone→Benzpinacol→Benzpinacolone
   - ii. Beckmann rearrangement: Benzanilide from benzene (Benzene→Benzophenone→Benzophenone oxime → Benzanilide)
   - iii. Benzilic acid rearrangement: Benzilic acid from benzoin (Benzoin→Benzil→Benzilic acid)
   - iv. Synthesis of heterocyclic compounds:
     Skraup synthesis: Preparation of quinolone from aniline
     Fisher -Indole synthesis: Preparation of 2-phenylindoIe from phenylhydrazine.

v. Synthesis using microwaves: Alkylation of diethyl malonate with benzyl chloride.

PHYSICAL CHEMISTRY

5. Chemical Kinetics
   i. Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).
   ii. Determination of the effect of (a) Change of temperature (b) Changer of concentration of reactant and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reaction.
   iii. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
   iv. Determination of the rate constant for the oxidation of iodide ions by peroxide studying the kinetics as an iodine clock reaction.
   v. Determination of partial molar volume of solute (e.g. KCI) and solvent in a binary mixture.
   vi. Determination of the temperature dependence of the solubility of a compound in the sullying having similar intermolecular interactions (benzoic acid in water and in DMSO Mixture) and calculate the partial molar heat of solution.
6. Thermodynamics
   i. Determination of partial molar volume of solute (e.g., KCI) and solvent in a binary mixture.
   ii. Determination of the temperature dependence of the solubility of a compound in two Solvents having similar intermolecular interactions (benzoic acid in water and in DMSO-water mixture) and calculate the partial molar heat of solution.

Reference Books:

- Inorganic Experiments, J. Derek Woollins, VCH.
- Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike and M. M. Singh, Wiley.
- Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand
- Experimental Physical Chemistry, D. P. Shoemaker, C. W. Garland and J. W. Niber, McGraw Hill lnterscience.
- Findlay's Practical Physical Chemistry, revised B.P. Levitt, Longman.
- Experiments in Physical Chemistry, J. C. Ghosh, Bharati Bhavan.

CHEMISTRY LABORATORY IV: CHEMISTRY LAB IV

CREDIT: 4

Course Objectives:

The course aims to provide an in-depth knowledge about the **Green chemical approaches of synthesis.** Provide knowledge of various methods for the synthesis of nanoparticles,

Course Learning Outcome:

Choose safer starting material, Use renewable resources, avoid waste to increase atom economy, use of enzyme as catalyst, use green solvent, use alternative source of energy

SYLLABUS:

1. Synthesis of hydrogel by co-precipitation method.
2. Synthesis of silver and gold metal nanoparticles.
3. USING RENEWABLE RESOURCES: Preparation and characterization of biodiesel from vegetable oil/ waste cooking oil
4. AVOIDING WASTE: Principle of atom economy. Use of molecular model kit to stimulate the reaction to investigate how the atom economy can illustrate Green Chemistry.
   Preparation of propene by two methods can be studied
   (I) Triethylamine ion + OH^- → propene + trimethylpropene + water, H_2SO_4/H_2O
   (II) 1-propanol →propene + water
   The other types of reactions, like addition, elimination, substitution and rearrangement should also be studied for the calculation of atom economy.
5. USE OF ENZYMES AS CATALYSTS: Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide
6. ALTERNATIVE GREEN SOLVENTS: Extraction of D-limonene from orange peel using liquid CO_2 prepared from dry ice.
   Mechanochemical solvent free synthesis of azomethines
7. ALTERNATIVE SOURCES OF ENERGY: Solvent free, microwave assisted one pot synthesis of phthalocyanine complex of copper (II).
   Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
8. Spectroscopy: Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

Reference Books:

- Anastas, P.T and Warner, J.C. *Green Chemistry: Theory and Practice*, Oxford University Press, 1998
- Kirchoff, M. and Ryan, M.A. *Greener approaches to undergraduate chemistry experiment*. American Chemical Society, Washington DC, 2002
- Ryan, M.A. *Introduction to Green Chemistry*, Tinnesand; (Ed), American Chemical Society, Washington DC, 2002

- Sharma, R.K.; Sidhwani, I.T. and Chaudhari, M.K. *Green Chemistry Experiments: A monograph*, I.K. International Publishing House Pvt Ltd. New Delhi, Bangalore ISBN 978-93-81141-55-7, 2013
- Cann, M.C. and Connelly, M. E. *Real world cases in Green Chemistry*, American Chemical Society, 2008
- Cann, M. C. and Thomas, P. *Real world cases in Green Chemistry*, American Chemical Society, 2008
- Lancaster, Mike *Green Chemistry: An introductory text*: *2nd Ed.* RSC Publishing, ISBN 978-1-84755-873-2
- Pavia, D.L., Kriz, G.S., Lampman, G.M. and Engels, R.G. *Introduction to Organic Laboratory Techniques – a Microscale Approach* 4th Ed., Brooks-Cole Laboratory Series for Organic Chemistry, 2006.

CHEMISTRY RESEARCH II: INDUSTRIAL TRAINING

CREDIT: 4

Course Objectives:

The objective of this training is to provide basic skills and knowledge required to work safely in environments which involve the transport, storage, use and disposal of chemicals. Provide the skills to identify the hazards, as explain the controls needed to stay safe working around the chemicals.

Course Learning Outcome:

Demonstrate the applications of chemistry concepts and principles learned in classroom. Illustrate processes and products manufactured in the chemical industries. Develop awareness of the engineering and technological aspects in the chemical industries. Improve interpersonal skill by communicating directly with industrial personnel. Aware of the roles and ethics of chemists in related industries. Aware of the impacts of industrial processes on health, safety, environment and society.

CONTENT:

This activity is important for M.Sc. students to relate their theoretical knowledge to practical aspects of the studied courses, in terms of industrial unit operations, process and design concepts, and impact of its activities on health, safety, environment and society. The students should be exposed to industrial visits after the examination of second semester during their summer break. To enhance their research interest the candidates will have to choose their chemical industry/ laboratory. They will be expected to submit a write up pertaining to that visit and a presentation will have to be made in presence of panel of experts from different fields of chemistry.