M. Sc Chemistry Programme under
Outcome Based Education (OBE) System
(For students who joined in June 2019 onwards)

SYLLABUS

DEPARTMENT OF CHEMISTRY

(DST-FIST Sponsored Department)

NATIONAL COLLEGE (Autonomous)

(Nationally Accredited at '*A+*' Level by NAAC with CGPA of 3.61 on 4.00 Scale)

(College with Potential for Excellence)

Tiruchirappalli 620 001

Post Graduate and Research Department of Chemistry

Vision Statement

The Chemistry Department is dedicated

- ❖ To develop a Centre of Excellence for teaching as well as research at par with national and international standards.
- ❖ To prepare the students of chemistry in such a way that they are self-reliant, highly informative and a better candidate in the demanding and ever changing world.
- ❖ To prepare the knowledgeable graduates for careers in academia, industry and government.

Mission Statement

- ❖ To develop wholesome and efficient student who will cause transformation in society through a study of chemistry.
- ❖ To extend the best student support services by making them comprehensive and by evolving a curriculum relevant to student community and society at large.
- ❖ To encourage students to face IIT-JAM, CSIR-NET, GATE, SET and other competitive examinations.
- ❖ To invite scientists from National/International laboratories for lectures of global standard.
- ❖ To provide high quality education through effective teaching – learning process for their pursuing high-quality teaching, learning, research, and service.
- ❖ To provide an educational environment where students can realize their full potential in chemistry and attain quality education to face the challenges of the future.

GOALS

1. To improve students basic knowledge of chemistry and to develop skills of scientific inquiry to design and carry out scientific investigations and evaluate scientific evidences to draw conclusions.
2. To make the students to think analytically, critically and creatively to solve problems, judge arguments, and make decisions in scientific and other contexts so that they can start a career in chemical industries.
3. To give training to develop inquiring minds and curiosity about science.

Scope and objective of the M. Sc degree program

- ✓ To understand the main ideas and concepts of chemistry and apply scientific information to solve problems in any situation so that they get a strong foundation in chemistry.
- ✓ Discuss and evaluate scientific information from different sources (internet, newspaper articles, television, scientific texts and publications) and assess its credibility.
- ✓ Enable students to develop scientific inquiry skills to design and carry out scientific investigations by applying the principles of organic, inorganic, physical chemistry, instrumental methods of analysis and analytical chemistry.
- ✓ Draw conclusions supported by scientific explanations and a reasoned interpretation of the analysis of the data.
- ✓ Describe and discuss ways in which science is applied and used to solve local and global problems.
- ✓ Discuss how science and its applications interact with social, economic, political, environmental, cultural and ethical factors.

Programme Outcomes (POs):

1. Graduates are prepared to be creators of new knowledge leading to innovation and entrepreneurship employable in various sectors such as private, government, and research organizations.
2. Graduates are trained to evolve new technologies in their own discipline.
3. Graduates are groomed to engage in lifelong learning process by exploring their knowledge independently.
4. Graduates are framed to design and conduct experiments /demos/create models to analyze and interpret data.
5. Graduates ought to have the ability of effectively communicating the findings of Physical sciences; incorporating with existing knowledge.

Programme Specific Outcomes (PSOs):

1. Human and Social Values and Responsibilities in the context of learning Chemistry
2. Communicative Skills and the Creative scientific mind towards learning chemistry

3. Positive approach towards Environment and Ecology from the Chemistry perspective
4. Critical thinking and the Analytical mind, students develop for the in depth knowledge in advanced-level Chemistry
5. The relevance of extension of Chemistry in the social context for solving social issues
6. Employability Skills shall enable the students to find jobs in corechemistry and other related fields
7. Entrepreneurial Skills shall empower the students to start their own industries / business in core-chemistry fields
8. Analytical or Experimental Skills make the students capable of doing higher-level research works in the emerging fields of chemistry.

Employment opportunity

- ✓ Employability Skills shall enable the students to find jobs in core-chemistry and other related fields
- ✓ Entrepreneurial Skills shall empower the students to start their own industries / business in core-chemistry fields.

NATIONAL COLLEGE (AUTONOMOUS), TIRUCHIRAPPALLI-620 001.
NATIONALLY ACCREDITED AT 'A' LEVEL BY NAAC
M.SC CHEMISTRY COURSE STRUCTURE UNDER O.B.E.S
(APPLICABLE TO THE CANDIDATES ADMITTED FROM THE ACADEMIC YEAR (2019-2021)

SEM	PART	COURSE	COURSE TITLE	INS HOURS /WEEK	CRE DIT	EXAM HRS	MARKS			TOTAL
							CIA	EXTERNAL		
								W	O	
I		CORE COURSE-CC1 (P19CH1)	CRYSTAL SYSTEMS ,PHOTOCHEMISTRY AND SUPRAMOLECULAR CHEMISTRY OF INORGANIC COMPOUNDS	6	5	3	25	75	-	100
		CORE COURSE-CC2 (P19CH2)	ORGANIC CHEMISTRY-I	6	5	3	25	75	-	100
		CORE COURSE-CC3 (P19CH3P)	INORGANIC PRACTICALS –I	6	-	-	-	-	-	-
		CORE COURSE-CC4 (P19CH4P	ORGANIC CHEMISTRY PRACTICAL-I	6	-	-	-	-	-	-
		ELECTIVE COURSE-I (P19CH5E)	ADVANCED TECHNIQUES IN CHEMISTRY	6	4	3	25	75	-	100
II			**TOTAL**	**30**	**14**				-	**300**
		CORE COURSE-CC V (P19CH6)	PHYSICAL CHEMISTRY-I	6	5	3	25	75	-	100
		CORE COURSE-CC VI (P19CH7)	REACTION MECHANISM IN CO ORDINATION AND ORGANOMETALLIC CHEMISTRY	6	5	3	25	75	-	100
		CORE COURSE-CC3 (P19CH3P)	INORGANIC PRACTICALS –I	6	5	6	25	75	-	100
		CORE COURSE-CC7 (P19H8P)	INORGNIC CHEMISTRY PRACTICAL-II	6	5	6	25	75	-	100
		CORE COURSE-CC4 (P19CH4P	ORGANIC CHEMISTRY PRACTICAL-I	6	5	6	25	75	-	100
		CORE COURSE-CC8(P19CH9P)	ORGANIC CHEMISTRYIPRACTICAL-II	6	5	6	25	75	-	100
		ELECTIVE COURSE-II (P19CH10E)	GREEN AND ENVIRONMENTAL CHEMISTRY	6	4	3	25	75	-	100
			TOTAL	**30**	**34**				-	**700**
III		CORE COURSE-C9(P19CH11)	ORGANIC CHEMISTRY-II	6	5	3	25	75	-	100
		CORE COURSE-CC10 (P19CH12)	PHYSICAL CHEMISTRY -II	6	5	3	25	75	-	100
		CORE COURSE-CC11 (P19CH13P)	PHYSICAL CHEMISTRY PRACTICAL-I	6	-	-	-	-	-	-
		CORE COURSE-CC14E ELECTIVE COURSE –III (P19CH14E)	SPECTRAL TECHNIQUES IN INORGANIC COMPOUNDS	6	4	3	25	75	-	100
		ELECTIVE COURSE – IV (P19CH15E)	BASIC STRATEGIES OF NANOMATERIALS AND SYNTHETIC ORGANIC CHEMISTRY	6	4	3	25	75	-	100
			TOTAL	**24**	**18**				-	**400**
IV		CORE COURSE –CC12 (P19CH16)	ORGANIC CHEMISTRY-III	6	5	3	25	75	-	100
		CORE COURSE-CC11 (P19CH13P)	PHYSICAL CHEMISTRY PRACTICAL-I	6	5	6	25	75	-	100
		CORE COURSE- 13(P19CH17P)	PHYSICAL CHEMISTRY PRACTICAL –II	6	5	6	25	75	-	100
		ELECTIVE COURSE – V (P19CH18E)	PHYSICAL CHEMISTRY-III	6	4	3	25	75	-	100
		PROJECT P19CHP19	PROJECT-CHEMISTRY	12	5	3	25	75		100
			TOTAL	**36**	**24**					**500**
			GRAND TOTAL	**120**	**90**					**1900**

CRYSTAL SYSTEMS, PHOTOCHEMISTRY AND SUPRAMOLECULAR CHEMISTRY OF INORGANIC COMPOUNDS - P19CH1

Semester: I **Core Course: II**

Instruction Hours/Week: 6 **Credits: 5**

Objectives:

1. To study the chemistry and structure of Boron, Sulphur and Nitrogen chain Compounds.
2. To know the structure of ionic compounds and mechanism of solid state reactions.
3. To get the knowledge of crystal systems by X-ray diffraction methods.
4. To understand the concepts of theory and application in inorganic photochemistry and to acquire the knowledge in supramolecular chemistry of inorganic compounds.

UNIT I: Cyclic Inorganic Compounds (18 hours)

Chemistry of boron - carboranes - metallocarboranes - importance of icosahedral frame work of boron atoms in boron chemistry - closo, nido and arachno structure - structural study by Wade's rule. S-N cations and anions. Chains-catenation-heterocatenation - polythiazyl compounds (S_4N_4, S_2N_2 and $(SN)_x$)- homocyclic inorganic systems- reactions of Cp_2TiS_5.

UNIT II: Ionic Bonding and Solid State Reaction (18 hours)

Structure of crystal lattice – The perovskite and spinel structures- radius ratio rule-Lattice energy - Born-Lande equation - Kapustinski's equation – Thermodynamics of complex formation- High-Tc superconductors - solid-state reactions- types and example - tarnish reaction, decomposition reaction, solid-solid reaction - factors influencing reactivity and structure effect - Irradiation - the photographic process.

UNIT III: Crystalline State (18 hours)

Crystal systems and lattice types - Bravais lattices - crystal symmetry - point groups and space groups (No detailed study) - Miller indices - reciprocal lattice concept - close packed structures - BCC, FCC, HCP - voids - coordination numbers - crystal binding - molecular, covalent, metallic and hydrogen bonded crystals. X-ray diffraction by crystals - function of crystals - transmission grating and reflection grating - Bragg's equation (No derivation) - diffraction methods - rotating crystal, oscillation and Weisenberg methods - indexing and determination of lattice types - unit cell dimensions of cubic crystals - structure factor - Fourier synthesis.

UNIT IV: Inorganic Photochemistry **(18 hours)**

Electronic transitions in metal complexes - metal centered and charge transfer transitions - various photophysical and photochemical processes of coordination compounds – uni molecular charge-transfer photochemistry of cobalt (III) complexes - mechanism of CTTM photo reduction. Ligand field photochemistry of Cr (III) complexes - Adamson's rule – conventional flash photolysis and single photon counting- photophysics and photochemistry of Ru-polypyridine complexes - emission and redox properties - photochemistry of organometallic compounds - metal-carbonyl compounds - compounds with metal-metal bonding - Reinecke's salt - chemical actinometer.

UNITV: Supramolecular Chemistry **(18 hours)**

Concepts and languages of supramolecular chemistry - hydrogen bonds - C-H…X interactions - halogen bonds - þi- þi interactions - non-bonded interactions. M.O.F. (Metallo Organic Frameworks) - organometallic systems - combination of different interactions to design molecular rods, triangles ladders, networks etc - design of nanoporous solids – supramolecular metallocatalysis – co- catalysts - catalysis of synthetic reactions - biomolecular and abiotic catalysts - role of supramolecular chemistry in the development of nanoscience and technology - supramolecular devices - supramolecular photochemistry.

Course Outcomes:

With the knowledge of the contents given in the paper, "crystal systems, photochemistry and supramolecular chemistry of inorganic compounds" a student should be able to enter into the field of crystallography and photochemistry.

Text Books:

1. M. C. Day and J. Selbin,"*Theoretical Inorganic Chemistry*", 2nd Edn, **1985**, Affiliated East-West Press Pvt. Ltd, New Delhi.
2. J. E. Huheey, E. A. Keiter and R. L. Keiter, "*Inorganic Chemistry – Principles of Structure and Reactivity*", Harper Collins College Publishers, 4th Edn, **1993**.
3. F. A. Cotton and G. Wilkinson, "*Advanced Inorganic Chemistry*" 5th Edn, Wiley- Interscience Publication, New York, **1988**.
4. L. W. Azaroff, "*Introduction to Solids*", Mc-Graw Hill.
5. N. B. Hannay, "*Solid State Chemistry*", Printice Hall, New Delhi, **1976**.
6. F. C. Philips, "*An Introduction to Crystallography*", Longmans, 3rd Ed., **1963**.

7. K. F. Purcel and J. C. Kotz, "*Inorganic Chemistry*", W. G. Saunder's Company, Philadelphia, **1982**.
8. D. F. Shriver, P.W. Atkins and C.H. Langford, "*Inorganic Chemistry*", ELBS.6th Ed., **1990**.
9. J. Ferraudi, "*Elements of Inorganic Photochemistry*", Wiley, New York, **1988**.
10. W. Adamson and P. D. Fleischauer, "*Concepts of Inorganic Photochemistry*", Wiley, New York, **1975**.
11. J. L. Atwood and J. W. Steed, "*Supramolecular Chemistry: A concise Introduction*", John Wiley & Sons, **2000**.
12. J. M. Lehn, "*Supramolecular Chemistry: Concepts and Perspectives*", Wiley-. VCH, **1995**.

Reference Books:

1. W.E. Jolly, "*Modern Inorganic Chemistry*", McGraw Hill International Ed., New York, **1994**.
2. Gary Wulfsberg, "*Inorganic Chemistry*", University Science Books, **2000**.
3. B.Douglas, D.H.Me Daniel and J.J. Alexander, "*Concepts and Models of Inorganic Chemistry*", John Wiley and Sons, New Delhi, **2001**.

ORGANIC CHEMISTRY I - P19CH2

Semester: I | **Core Course: I**

Instruction Hours/Week: 6 | **Credit: 5**

Objectives:

1. To make the students to know about the nomenclature of organic compound by IUPAC rules
2. To learn the concepts of various methods of determination of reaction mechanism and to comprehend the various factors that operate in organic reactions
3. To appreciate the stereochemical aspects of a reaction and conformational analysis of organic molecules.
4. To learn and understand the path, feasibility and mechanism of a reaction. To understand the techniques involved in the determination of mechanism of reactions and to propose methods to determine the mechanism of reaction.
5. To enable the student to understand and appreciate the importance of carbohydrates, antibiotics and steroids.

UNIT I: Nomenclature of Organic Compounds, Reactive Intermediates and Electronic Effects (18 hours)

Nomenclature of heterocyclics having not more than two hetero atoms such as oxygen, nitrogen and sulphur - Nomenclature of heterocyclic compounds of fused ring system - Nomenclature of alicyclic, bicyclic and tricyclic compounds. **Reactive Intermediates:** Classical and non-classical carbocations, carbanions-free radicals, carbenes, nitrenes, arynes and singlet oxygen-general methods of generation, detection, geometry, stability and reactivity of these intermediates. **Electronic Effects:** Inductive effect - resonance effect – hyper conjugation (Baker-Nathan effect) hydrogen bonding (inter and intramolecular) and steric effects.

UNIT II: Methods of Determining Reaction Mechanisms and Correlation Analysis (18 hours)

Kinetics and non-kinetic methods of determination of reaction mechanisms - Thermodynamic and kinetic aspects of organic reactions ,energy profile diagrams - spectroscopic studies, isotopic effects - intermediate versus transition states - product analysis and its importance - crossover experiments - isotopic labelling studies. **Correlation Analysis:** Linear Free Energy Relations - Hammet equation - significance - sigma and rho applications and limitations - Taft, Swain-Scott-Grunwald-Winstein equations and their applications, classification of solvents.

UNIT III: Organic Stereochemistry – I –Optical Isomerism (18 hours)

Optical isomerism - Optical activity and chirality - elements of symmetry - Stereochemistry of overcrowded molecules (hexahelicene, ansa compounds, cyclophanes and trans cycloalkenes - Newmann, Sawhorse and Fischer projections - representation and interconversion - Absolute configuration – R & S notations for special molecules (allenes, spirans, biphenyls) R-S nomenclature of cyclic chiral compounds - molecules with more than one chiral center. Asymmetric synthesis - Optical purity - determination of enantiomeric excess by NMR - definition of terms like prochirality, enantiotopic and diastereotopic atoms, groups and faces - stereoselective and stereospecific reactions.

UNIT IV: Geometrical isomerism and Dynamic Stereochemistry (18 hours)

Geometrical isomerism and ometrical isomerism: E, Z - determination of configuration of geometrical isomers (cyclisation, converting into compounds of known configuration, dipolemoment, converting into less symmetric compounds – spectroscopic methods) configuration of cyclic and bicyclic ring systems - cis-trans nomenclature of three, four and six membered substituted cyclic systems - decalins. **Dynamic Stereochemistry:** Quantitative correlation between conformation and reactivity - Winstein-Eliel equation - Curtin Hammet principle - saponification of an ester - esterification of an alcohol - chromic acid oxidation of cyclohexanols - neighbouring group participation - deamination of 2- amino cyclohexanol.

UNITV: Natural Products (18 hours)

Carbohydrates: Polysaccharides - structure of starch and cellulose, configuration of carbohydrates – photosynthesis. **Antibiotics:** Chemotherapy - definition LD50 - Structural elucidation and synthesis of penicillin, streptomycin - cephalosporin-C. **Steroids:** Classification-structural elucidation of cholestrol (synthesis not required), structural elucidation and synthesis of Vitamin D, estrone, progestrone, ergosterol, androsterone and equilenin - Classification and functions of prostaglandins

Course Outcomes:

1. Students learn bonding in organic molecules and the structural implications on properties
2. Students get learnt the concept of IUPAC nomenclature of bicyclic fusing liquid compounds.

3. Students understand the importance of stereochemical aspects of structure and properties
4. Students get to know the chemical reactions and the mechanisms *via* different intermediates
6. Students learn the techniques of studying the mechanisms of reactions
7. Students get to know the structure and importance of carbohydrates, antibiotics and steroids.

Text Books:

1. R. Panico, W. H. Powell, L. Jean. C. Richer, "*A guide to IUPAC Nomenclature of Organic Compounds*", (**1993**), Jain Inter science.
2. S. C. Pal, "*Nomenclature of Organic Compounds*", (**2008**), Narosa Publishing House.
3. D. Nasipuri, "*Stereochemistry of Organic Compounds-Principles and Applications*", 2nd Ed., New Age International (**2005**).
4. P. S. Kalsi, "*Stereochemistry*", Wiley Eastern Ltd, **1990**.
5. E. L. Eliel and S. H. Wilen, "*Stereochemistry of Organic Compounds*", John Wiley, **2008**.
6. T. H. Lowry and K. S. Richardson, "*Mechanism and Theory in Organic Chemistry*", 2nd Ed., Harper and Row, **1981**.
7. O. P. Agarwal, "*Chemistry of Organic Natural Products*", Volume I & II, Goel Publishers, **2014**.
8. I. L. Finar, "*Organic Chemistry*", Volume-II, 5th Ed., (**2006**).

Reference Books:

1. Structure and Mechanisms, F. Carey, R. Sundberg, "*Advanced Organic Chemistry. Part-A*". 4th Ed., Kluwer Publishers, **2000**.
2. Michael B. Smith, J. March, "*March's Advanced Organic Chemistry*", John Wiley & Sons, 6th Ed., **2007**.
3. J. Clayden, N. Greeves, P. Wothers, "*Organic Chemistry*", Oxford University Press, **2001**.
4. J. Mc. Murry, "*Organic Chemistry*", Brooks/Cole publisher, 5th Ed., **2000**.
5. M. B. Smith, "*Organic Synthesis*', Academic Press, Elsevier, 3rd Ed., **2010**.
6. E.L. Eliel, "*Stereochemistry of Carbon Compounds*", McGraw Hill Book Company, New York, **1975**.

ADVANCED TECHNIQUES IN CHEMISTRY - P19CH5E

Semester: I **Elective Course: I**

Instruction Hours/Week: 6 **Credit: 4**

Objectives:

1. To acquire the knowledge of error analysis and instrumental methods.
2. To study the separation and purification of organic and inorganic compounds.
3. To understand the concepts of thermal methods and fluorescence spectroscopy.
4. To be able to use computers for research in chemistry and also to use C language.
5. To learn the basics of modeling chemical systems.

UNIT I: Error Analysis and Instrumental Methods of Analysis (18 hours)

Various types of Error - accuracy, Precision, significant figures - Standard deviation - Correlation and regression - Fitting of linear equations - Multiple linear regression analysis. Principles and Applications of Extended X-ray absorption fine structure (EXAFS) – Atomic Absorption Spectroscopy (AAS) - Flame Emission Spectroscopy (FES).

UNIT II: Chromatography (18 hours)

Solvent extraction - Principles of ion exchange, paper, thin layer and column Chromatography techniques - Columns, adsorbents, methods, R_f values-McReynold's constants and their uses-HPLC techniques - Adsorbents, Columns, detection methods, estimations - preparative column - GC-MS techniques: methods, principles and uses.

UNIT III: Thermoanalytical Methods and Fluorescence Spectroscopy (18 hours)

Comparison of Thermogravimetric analysis (TGA) and Differential Thermal analysis(DTA) - Differential Scanning Calorimetry (DSC). Principle and instrumentation - Thermometric titrations. Basic aspects of synchronous fluorescence spectroscopy and instrumentation - Instrumentation on fluorescence ratio imaging- Flow cytometry - Fluorimeters (quantization) - applications. XRD- Principles, applications and Instrumentation only.

UNIT IV: Computer Applications in Chemistry (18 hours)

Introduction to computers and computing – World Wide Web-E-journals– search engines for chemistry. Introduction to C language - Structure of C program - Control statements - if statement – Loops- while and for loops - recursion.

Examples of simple chemistry Programmes:

1. Conversion of Celsius temperature to Kelvin temperature
2. Applications of Beer-Lambert Law.
3. Linear least square - Fit log k vs 1/T plot to get Arrhenius parameters.
4. Determination of Anharmonicity constant and dissociation energy calculation.
5. Use of CHEMDRAW and ORIGIN LAB software

UNIT V: Molecular Modelling Basics (18 hours)

Molecular modeling - Coordinate systems - Cartesian and internal coordinate systems - bond lengths, bond angles and torsion angles - distance matrix - stick models space filling models - potential energy surfaces - Molecular mechanics-application and parameterization - advantages and limitations of force fields.

Course Outcomes:

1. Able to minimize errors while reporting the experimental values and justify why continuum radiation sources are usually not practical to use for atomic absorption spectroscopy.
2. Able to do simple chromatographic experiments
3. Able to interpret thermograms and justify why fluorescence measurements are often more sensitive than absorption.
4. Able to develop logics which will help them to create programs, applications in C.
5. Able to describe and comprehend the fundamental concepts of molecular modeling.

Text Books:

1. Willard, Merrit, Dean and Settle, *Instrumental methods of Analysis* CBS Publishers andDistributors, 6th Ed., **1986**. (**UNIT I**)
2. Skoog, D. A. West, D. M. Holler. P. J. "*Fundamentals of Analytical Chemistry"* 7th Ed., Harcourt College Publishers, Singapore. (Page **523-665**). (**UNITS I & IV**)
3. R. Stock and C. B. F. Rice, *Chromatographic Methods*, Chapman and Hall, New York. (**UNIT II**)
4. V. K. Srivastava and K. K. Srivastava, *Introduction to Chromatography*, S. Chand & Co., New Delhi, 2nd Ed., **1981**. (**UNIT II**)
5. Sharma, S. G. Schulman, "*Introduction to Fluorescence Spectroscopy*" Wiley-Interscience, New York, 1999. (**UNIT III**)

6. E. Balaguruswamy, "*Programming in ANSI C*", Tata McGraw Hill, 2nd Ed., New Delhi, **1999**. (**UNIT IV**)
7. R. Leach, "*Molecular Modelling Principles and Applications*", 2nd Ed., Prentice Hall, **2001**. (**UNIT V**)
8. W. B. Smith, "*Introduction to Theoretical Organic Chemistry and Molecular Modelling*" John Wiley, New York, **1996**. (**UNIT V**)
9. Tim Clark, "A Handbook of Computational Chemistry", John Wiley, New York, **1985**. (**UNIT V**)

Reference Books

1. H,W. Willard, L.I. Merrit, J.J.A. Dean and F.A. Settle, "*Instrumental methods of analysis*", CBS publishers, 6th Ed., **1986**
2. Skoog D A, Holler F J and Crouch S R, "*Principles of Instrumental Analysis*", 6th Ed., Thompson Brooks/Cole, Belmont CA, **2007**.
3. Skoog D A, West D M, Holler F J and Crouch S R, "*Fundamentals of Analytical Chemistry*", 9th Ed., Brooks/Cole, Belmont CA, **2014**.

INORGANIC CHEMISTRY PRACTICAL –I P19CH3P

Semester: I **Core Course: II**

Instruction Hours/Week: 6 **Credit: 5**

Objectives:

1. To learn and identify the inorganic cation in a mixture.
2. To know the colourimetric techniques for estimation of ions.
   - Semi-micro qualitative analysis of a mixture containing two common and two rare cations.
   - Estimation of Copper, Ferric, Nickel, Chromium and Manganese using photoelectric colorimeter.

Course Outcomes:

1. Students will be able to identify and estimate the amount of inorganic ions present in a sample.
2. Students learn the instrumentation technique of Photocolorimeter.

References:

1. Vogel, "*Quantitative Inorganic Analysis*", ELBS, 3rd Ed., **1971**.
2. V. V. Ramanujam, "*Inorganic Semimicro Qualitative Analysis*", The National Publishing Company, Madras, **1974**.

ORGANIC CHEMISTRY PRACTICAL – I – P19CH4P

Semester: I & II **Core Course: IV**

Instruction Hours/Week: 6 **Credits: 5**

Objectives:

1. To learn the separation techniques of binary organic mixtures and characterize them.
2. To study some single stage preparation of organic compound.

Qualitative Analysis of an Organic Mixture Containing Two Components

Pilot separation, analysis and derivatization.

Preparation of Organic Compounds (Single Stage)

(a) Methyl-m-nitrobenzene from methyl benzoate (nitration)

(b) Glucose penta acetate from glucose (acetylation)

(c) Resacetophenonone from resorcinol (acetylation)

(d) Phenyl-azo-2-naphthol from aniline (diazotization)

(e) 2-Naphthylmethylether from 2- Naphthol (methylation)

(f) Dibenzalacetone from benzaldehyde

Course Outcomes:

1. Students learn the separation of binary organic mixtures
2. Students understand the green chemistry concepts
3. Students learn the skills of doing micro level analysis
4. Students get to know the methods of qualitative analysis of organic compounds
5. Students understand the single stage preparation of organic compounds
6. Students learn about the derivative of the organic functional groups

Text Books:

1. Dey and Sitaraman, "*Laboratory Manual of Organic Chemistry*", Allied Publishers, **1992**.
2. N. S. Gnanaprakasam, G. Ramamurthy, "*Organic Chemistry Lab Manual*", S. Viswanathan Printers and Publishers Pvt. Ltd., **2015**.

References:

1. Furniss, S. B.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. "*Vogel's Text Book of Practical Organic Chemistry*", 5th Ed., Longman Scientific & technical, England, **1989**.

PHYSICAL CHEMISTRY I - P19CH6

Semester: II **Core Course: V**

Instructions Hours per Week: 6 **Credits: 5**

Objectives:

1. To learn to apply quantum mechanics to simple chemical systems.
2. To learn in detail rotational, vibrational and electronic spectra of molecules.
3. To understand the thermodynamic properties of real gases and to apply phase rule to three component systems.
4. To understand the advanced concepts involved in kinetics
5. To study reactions in photochemistry and radiation chemistry.

UNIT I: Quantum Chemistry-I **(18 hours)**

Inadequacy of classical mechanics - Black body radiation, Planck's concept - Wave -particle dualism - Uncertainty Principle - Inadequacy of old quantum theory. Schrodinger equation – Postulatory basis of quantum mechanics - Operator algebra: operator, linear and hermitian, eigen functions and eigen values, angular momentum operator, commutation relations. Application of wave mechanics to simple systems - particle in a box, one- and three-dimensional - distortion of the box and Jahn-Teller effect - quantum numbers - Orthogonalisation and normalization.

UNIT II: Molecular Spectroscopy – I **(18 hours)**

Einstein coefficient of absorption and transition probabilities - basis of selection rules - Representation of spectra - the width and intensity of spectral transitions oscillator strength. Electronic spectra - electronic spectra of molecules - Born Oppenheimer approximation - vibrational coarse structure - Franck-Condon principle - dissociation energy - Fortrat diagram - Pre-dissociation - various types of transitions - solvent effect on spectra. Infra red spectra - vibrational spectra - selection rules - harmonic and anharmonic oscillators - vibration and rotation spectra of diatomic molecules - vibration spectra of polyatomic molecules - normal vibration and normal coordinates - Influence of rotation on the spectra of polyatomic molecules - parallel and perpendicular bands - FTIR.

UNIT III: Classical Thermodynamics **(18 hours)**

Thermodynamic properties of real gases - Fugacity - definition - methods of determination of fugacity - variation of fugacity with temperature and pressure

- activity and activity coefficient - definition - Standard states for gases, liquids, solids and component of solutions - determination of activity and activity coefficient from freezing point - EMF and solubility measurements. Phase rule - Application of phase rule to the three component systems - systems of three liquids - solid-liquid system (Eutectic systems - two salts and water).

UNIT IV: Chemical Kinetics: (18 hours)

Theories of reaction rate - Absolute reaction rate theory (ARRT) - significance of reaction coordinate - Potential energy surfaces - Kinetic isotopic effect - Principle of microscopic reversibility - Steady-state approximation. - explosions and hydrogen – oxygen reactions. Factors influencing reaction rates in solution - application of ARRT to solution kinetics - effect of solvent and ionic strength, influence of pressure on rates in solution - significance of volume of activation. Acid-base catalysis - Hammett's acidity function - Bronsted relation

UNIT V: Techniques in Chemical Kinetics, Photochemistry and Radiation Chemistry (18 hours)

Fast reaction techniques: Flow methods: Stopped flow technique – Relaxation methods - Flash photolysis - Shock tube method - molecular beam method. **Photochemistry:** Photo physical process in electronically excited molecules – Jablonski diagram – Stern-Volmer equation - Chemical Actinometers - Lasers and their applications. **Radiation chemistry:** Sources of high energy radiation - radiolysis of water – solvated electrons - Scavenging techniques - Applications of radiation chemistry.

Course Outcomes:

The students will be able to

1. Apply quantum mechanics to simple chemical systems.
2. Interpret rotational, vibrational and electronic spectra of molecules.
3. Understand the thermodynamic properties of real gases and to apply phase rule to three component systems.
4. Understand the advanced concepts involved in kinetics and apply the same in the laboratory.
5. Acquire knowledge on photochemistry and radiation chemistry

Text Books:

1. A. K. Chandra, "*Introductory Quantum Chemistry*", 4th Ed., Tata McGraw Hill Ed., **1994**. (**UNIT I**).

2. R. K. Prasad, *Quantum Chemistry*, 2^{nd} Ed., New Age International Publishers (**2000**), (**UNIT I**).
3. N. Levine, *Quantum Chemistry*, 4^{th} Ed., Prentice Hall of India Pvt. Ltd., (**1994**), (**UNIT I**).
4. D. A. McQuarrie, *Quantum Chemistry,* University Science Books (**1998**), (**UNIT I**)
5. S. Glasstone, Introduction to Theoretical Chemistry, Affiliated East-West Press (**UNIT I & II**).
6. G. N. Barrow, Introduction to Molecular Spectroscopy, International McGraw Hill Ed., (**1993**) (**UNIT II**)

A. P. Straughan and S. Walker, Spectroscopy, Vol. I to III, Chapman Hall, London (**1976**) (**UNIT II**)

7. C.N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy' Tata- McGraw-Hill Education, 4^{th} Ed., **1994**. (**UNIT II**)
8. S. Glasstone, Thermodynamics for Chemists, East-west Affiliated Pvt., Ltd, New Delhi (**1969**), (**UNIT III**)
9. R. P. Rastogi and R. R. Misra, An Introduction to Chemical Thermodynamics Vikas Publishing House Pvt Ltd., (**1992**) (**UNIT III**)
10. Klotz and P. M. Rosenberg, Chemical Thermodynamics: Basics Theory and Methods, 3^{rd} ed., W. A. Benjamin, NY (**1974**) (**UNIT III**)
11. K.J.Laidler, Chemical Kinetics, 2^{nd} Ed., Tata McGraw Hill, **1975**, (UNIT IV)

A. A. Frost and R. G. Pearson, Kinetics and Mechanisms, John Wiley & Sons (**1953**). (**UNIT IV**)

12. J. C. Kuriacose and J. Rajaram, Kinetics and Mechanisms Transformations, Macmillan & Co., (**1993**). (**UNIT IV**)
13. P. W. Atkins, Advanced Physical Chemistry, 7^{th} Ed., Clarendon (**2002**) (**UNIT V**)
14. K. K. Rohatgi and Mukerjee, Fundamentals of Photo Chemistry, Wiley Eastern Ltd (**1986**). (**UNIT V**)
15. G. Hughes, Radiation Chemistry, Oxford University Press (**1973**) (**Unit V**)

Reference Books:

1. Peter Atkins and Julio de Paula, "*Atkin's Physical Chemistry*", Oxford Publishers, **2014**.

REACTION MECHANISM IN COORDINATION AND ORGANOMETALLIC CHEMISTRY - P19CH7

Semester: II | **Course Course: V**

Instructions Hours per Week: 6 | **Credits: 5**

Objectives:

1. To understand the principles and reaction mechanisms of coordination chemistry
2. To learn the biological role and mechanism of bioinorganic complexes
3. To study the various types of organometallic reactions and role of organometallic catalysts

UNITI: Coordination Chemistry Principles (18 hours)

Nomenclature of mono and polynuclear coordination compounds - valence bond theory - formation of octahedral complexes on the basis of VBT - limitations of VBT - crystal field theory (CFT) - shapes of d-orbitals in octahedral symmetry - CFSE - strong field and weak field splitting - calculation of CFSE - splitting in tetrahedral symmetry - only weak field - tetragonal symmetry - differences between tetrahedral and tetragonal symmetry - Jahn-Teller distortions - splitting pattern in various symmetries - factors affecting the magnitude of splitting (10 Dq) - Spectrochemical series - Jorgenson's relation - evidences for CFT - magnetism and colour of transition metal ions - LFT. MO theory – octahedral and tetrahedral complexes - π -bonding and MO theory - ligands having filled and empty π-bonds - effect of 10 Dq - evidences for -π- bonding from X-ray crystallography, IR and photoelectron spectroscopy - Nephelauxetic effect.

UNIT II: Coordination Chemistry and Reaction Mechanism (18 hours)

Stability of coordination compounds - detection of complex formation in solution - stability constants - step-wise and overall formation constants - pH metric, and photometric methods of determination of formation constants - factors affecting stability - statistical and chelate effects - forced configuration.

Kinetics and mechanism of reactions - labile and inert complexes - ligand displacement reactions - hydrolysis and anation reactions in octahedral and square planar complexes-trans effect - theory and applications - electron transfer reactions - complementary and non complementary types - inner sphere and outer sphere processes -isomerisation and racemisation - reactions of coordinated ligands - template effects - synthesis of macrocyclic ligands.

UNIT III: Bioinorganic Chemistry (18 hours)

Biological role of metal ions – Gold compounds and Rhematoid arthritis- anti cancer drugs- characterization of K^+, Na^+, Ca^{2+} and Mg^{2+} complexes of alkali and alkaline earth metal ions with macrocycles - ion channels - ion pumps. Oxygen transport (Hb and Mb) and storage - carbonic anhydrase - carboxypeptidases - iron-sulphur proteins and non-heme iron cytochromes of electron transport chain - cytochrome P-450 enzymes.

UNIT IV: Organometallic Reactions (18 hours)

Ligand association and dissociation reactions-oxidative addition and reductive elimination reactions. Hapticity - ligand classification - synthesis and structure - uses of typical organometallics in organic synthesis - such as metal alloys and organomercuric compounds in medicine. Metal carbenes - carbynes - metal clusters.Complexes of -acceptor ligands - carbonyls - 18 electron rule - applications and limitations - isolobal concept - applications to structure - carbonyl hydrides - nitrosyl complexes - bridging and terminal nitrosyls - bent and linear nitrosyls - dinitrogen complexes - dioxygen complexes – molecular orbitals of metallocenes.

UNIT V: Reaction and Catalysis by Organometallic Compounds (18 hours)

Catalysis by organometallic compounds - hydrogenation of olefins - hydroformylation of olefins - oxidation of olefins to aldehydes and ketones - polymerization of alkenes- Tolman catalytic loops- cyclooligomerisation of acetylene - Fischer-Tropsch synthesis - epoxidation - metathesis - carbonylation of methanol.

Course Outcomes:

By learning the basic principles of coordination chemistry and the reaction mechanism in organometallics, a student can improve his knowledge to predict the mechanism in coordination and organometallic reactions.

References:

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, "*Inorganic Chemistry – Principles of Structure and Reactivity*", Harper Collins College Publishers, 4^{th} Ed., **1993**.
2. F. A. Kettle, "*Physical Inorganic Chemistry - A Coordination Approach*", Spectrum Academic Publishers, Oxford University Press, **1996**.
3. P. Powell, "*Principles of Organometallic Chemistry*", 2^{nd} Ed., Chapman and Hall, London.

4. K. F. Purcel and J. C. Kotz, "*Inorganic Chemistry*", W. G. Saunder's Company, Philadelphia.
5. W. U. Malik, G. P. Tuli and R. D. Madan, "*Selected Topics in Inorganic Chemistry*", 6th Ed., **2001**, S. Chand & Company Ltd., New Delhi.
6. Gurdeep Raj, "*Advanced Inorganic Chemistry*", Vol. II, 8th Ed., **2002**, Goel Publishing House, Meerut.
7. W. Kaim and B. Schewederski, "*Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*", John-Wiley and sons, New York.

Reference Books:

1. G. L. Miessler and D.A. Tarr, "*Inorganic Chemistry*", Pearson, Prentice Publishers, Delhi, **2009**.
2. Cotton F A and Wilkinson G, "*Inorganic Chemistry A Comprehensive Text*", Inter science Publishers, New York, 5th Ed., **1988**.
3. Purcell K F and Kotz J C, "*Inorganic Chemistry*", W B Saunders Company, Philadelphia, **1977**.
4. B. Douglas, D.H. McDaniel and Concepts and Models of J.J. Alexander, "*Inorganic Chemistry*", John Wiley and Sons, New Delhi, **2001**.

INORGANIC CHEMISTRY PRACTICAL -II P19CH8P

Semester: II **Course Course : V**

Instructions Hours per Week: 6 **Credits: 5**

Objectives:

1. To learn the separation of ions in a mixture.
2. To learn the volumetric estimation of some inorganic cations.
3. To learn the gravimetric techniques.
4. To know the preparation of coordination complexes.

Titrimetry (V) and Gravimetry (G)

A mixture of solution(s) should be given for estimation

Cu (V) and Ni (G)
Cu (V) and Zn (G)
Fe (V) and Zn (G)
Fe (V) and Ni (G)
Zn (V) and Cu (G)

Preparation of the following compounds

a) Tetramminecopper (II) sulphate.
b) Potassium trioxalatochromate (III).
a) Potassiumtrioxalatoaluminate (III).
b) Trithioureacopper (I) chloride.
c) Trithioureacopper (I) sulphate.

Preparation of coordination complexes and their characterization by magnetic susceptibility measurements and Infrared, UV / Vis spectroscopic techniques.

Course Outcomes:

1. Students learn the estimation of ions by separating them in a mixture.
2. Students get skill in preparation of coordination compounds.

Text Book:

1. Inorganic Semi-Micro Qualitative Analysis, V.V. Ramanujam, The National Publishing House, Chennai, **1990**.

Reference Books

1. W.G. Palmer, "*Experimental Inorganic Chemistry*", Cambridge University Press, Cambridge, **1965**.
2. V.I. Posypaiko and N.A. Vasiua, "*Analytical Chemistry in Metallurgy*", Mir Publisher, Moscow, **1984**.
3. G.H. Jaffery, J. Bassett, J. Mendhan and R.C. Deeny, "*Vogel's Text book of quantitative Chemical analysis*", ELBS, **1997**.

ORGANIC CHEMISTRY PRACTICAL II – P19CH9P

Semester : II **Core Course: V**

Instruction Hours/Week: 6 **Credit: 5**

Objectives:

1. To learn quantitative analysis in organic chemistry.
2. To get hands on experience on the double stage preparation of organic compounds.
3. To learn the interpretation of UV and IR spectra of organic compounds.

Quantitative analysis of Organic Compounds

Estimation of phenol, aniline, ketone, glucose

Preparation of Organic Compounds (Double Stage)

a) *p*-bromo acetanilide from aniline (acetylation and bromination).
b) acetyl salicylic acid from methyl salicylate (hydrolysis and acetylation)
c) 1,3,5-tribromobenzene from aniline (bromination, diazotization and hydrolysation).
d) p-nitroaniline from acetanilide (nitrogen and hydrolysis).
e) benzilic acid from benzoin (rearrangement).
f) benzanilide from benzophenone (rearrangement).
g) *p*-bromoaniline from acetanilide (bromination and hydrolysis).
h) *m*-nitroaniline from nitrobenzene.
i) 1,2,4-triacetoxy benzene from hydroquinone (oxidation and acylation)

- Separation of organic compounds using thin layer and column chromatographic techniques.
- Characterization of organic compounds using infrared and *UV-Vis* spectroscopic techniques.

Course Outcomes:

1. Students understand the quantitative analysis in organic chemistry.
2. Students know the estimation of organic compounds.
3. Students understand the double stage organic preparations.
4. Students get to know the chromatographic techniques.

Text Books:

1. Dey and Sitaraman, "*Laboratory Manual of Organic Chemistry*", Allied Publishers, **1992**.
2. N. S. Gnanaprakasam, G. Ramamurthy, "*Organic Chemistry Lab Manual*", S. Viswanathan Printers and Publishers Pvt. Ltd., **2015**.

References:

1. Furniss, S. B.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R. "*Vogel's Text Book of Practical Organic Chemistry*", 5th Ed., Longman Scientific & technical, England, **1989**.

GREEN AND ENVIRONMENTAL CHEMISTRY - P19CH10E

Semester : II **Elective Course: II**

Instruction Hours/Week: 6 **Credit: 4**

Objectives:

1. To learn the need and goals of green chemistry
2. To make the students to plan the synthesis of organic compounds in a greener approach.
3. To learn about the possible sources of agricultural pesticides its mode of transport and accumulation and its impacts on human health.
4. To improve their knowledge of basic information of radio active decay and permissiable radiation dose.

UNIT I: Introduction to Green Chemistry (18 hours)

Green chemistry - Introduction - need for green chemistry - goals of green chemistry- Anastas' twelve principles of green chemistry - Designing a green synthesis (tools) - choice of starting materials, solvents, catalysts, reagents, processes with suitable examples.

UNIT II Microwave, Ultrasound Assisted Organic Synthesis and Biocatalysts (18 hours)

Microwave activation - advantages of microwave exposure - Microwave assisted reactions, condensation reactions - oxidation, reduction reactions, multicomponent reactions. **Sonochemistry** - use of ultrasound in organic synthesis (alternate source of energy) - saponification - substitution, addition, oxidation reactions, reductions. **Biocatalysts** in green synthesis - use of biocatalysts in green chemistry - advantages - biochemical (microbial) oxidation and reduction reactions - Bakers yeast mediated bio-transformation - biocatalyst mediated Baeyer-Villiger reaction.

UNIT III: Ionic liquids - Phase Transfer Catalyst and Supercritical CO_2 in Green Synthesis (18 hours)

Ionic liquids - synthesis, physical properties of ionic liquids - applications in alkylation, epoxidation, Friedal-Crafts reaction - Diels-Alder reactions Knoevengal condensations and Wittig reactions. **PTC** - Definition - advantages, types of PTC reactions - synthesis of PTC, applications of PTC in organic synthesis Michael reaction - alkylation of aldehydes and ketones. Wittig, generation of dihalocarbene, elimination reaction. **Supercritical CO_2** - phase diagram - uses in extracting natural products, dry cleaning, bromination, Kolbe-Schmidt synthesis - Friedel-crafts reaction. Dimethyl carbonate as a methylating agent in green synthesis.

UNIT IV: Toxicity of pesticides and insecticides (18 hours)

Pesticides - General aspects of classification in terms of chemical nature and generation wise. Mode of action of insecticides - General aspects. Bio-accumulation and bio- magnification of pesticides - Fate of insecticides in environment and environmental hazards - Major disasters with pesticides and herbicides - Toxicity of DDT, gammexene and malathion - comparison of organochlorine, organophosphate and carbamate insecticides - Detoxification of pesticides and allied chemicals - Safer pesticides - IPM - Environmental hazards arising from fertilizers - Minimization of environmental problems caused by fertilizers.

UNIT V: Radioactive Pollution (18 hours)

Nature of radioactive emission - units - Radiation from natural sources and Man- made activities - Effects of radiation on human health -Permissible radiation dose - Comparative risk analysis of fossil fuel based power generation versus nuclear power generation - Radioactive fall out -Nuclear winter: atmospheric turbidity and effects - Radioactive pollution in land, atmosphere and water - Nuclear waste disposal: Nature, general principles and strategies - Causes and prevention of nuclear reactor accidents - Chernobyl disaster - Three Mile Island disaster.

Course Outcomes:

The student gained knowledge about

1. Twelve principles of green chemistry, eco-friendly synthesis using microwave, biocatalyst. PTC, ionic liquid and SCC.
2. Increase the use of environmentally friendly practices in reducing agricultural pollution.
3. The nuclear waste disposal prevention of nuclear reactor accidents, radioactive fall out.

References:

1. Paul T. Anastas and John C. Warner, "*Green Chemistry*", Oxford University Press, Indian Ed., **2008**.
2. V. K. Ahluwalia and M. Kidwai, "*New Trends in Chemistry*", Anamaya Publishers, 2nd Ed., **2007**.
3. V. Kumar, "*An Introduction to Green Chemistry*", Vishal Publishers, 1 Ed., **2007**.
4. V. K. Ahluwalia and R. S. Varma, "*Green Solvents*", for organic synthesis Narosa Publishing, 1st Ed., **2009**.
5. V. K. Ahluwalia and Renu Aggarwal, "*Organic Synthetic Special Techniques*", Narosa, 2nd Ed., **2009**.

6. V. K. Ahluwalia, "*Green Chemistry - Environmentally Benign Reactions*", Ane books, India, **2006**.
7. Rashmi Sanghi and N. M. Srivastava, "*Environment Friendly Alternatives*", Narosa Publishing House, **2003**.
8. D. K. Asthana and Meera Asthana, "*Environment - Problems and Solutions*", S. Chand & Co Ltd.
9. Benny Joseph, "Environmental Studies", Tata McGraw Hill publishing Company Ltd, New Delhi.1st Ed., **2009**.
10. Erach Bharucha, "*Text book of Environmental Studies*", University press 2nd Ed., **2013**.

Reference Books:

1. Green Chemistry-An Introductory Text; Mike Lancater; RSC publishers, **2011**.
2. Green Chemistry – Designing Chemistry for the Environment – edited by Paul T. Anastas & Tracy C. Williamson. 2nd Ed., **1998**.

ORGANIC CHEMISTRY II – P19CH11

Semester : III **Core course: IX**

Instruction Hours/Week: 6 **Credit: 5**

Objectives:

1. To appreciate the concept of substitution, addition and elimination reactions and their reaction mechanisms
2. To understand the path, feasibility and mechanism of a reaction
3. To understand the techniques involved in the determination of mechanism of reactions and applications of various molecular rearrangements
4. To enable the student to understand and appreciate the importance of biomolecules.

UNIT I: Nucleophilic Substitution Reaction (18 hours)

Aliphatic Nucleophilic Subsitution, Aromatic Nucleophilic Subsitution Subsitution and Aliphatic Electrophilic SubsitutionS_N1, S_N2, S_Ni mechanisms - stereochemical factors - effect of substrate structure, leaving group, attacking nucleophile and solvent - neighbouring group participation - substitution at allylic and vinylic carbons - ambident nucleophiles. S_N1, S_NAr, Benzyne mechanisms - orientation effect of substrate structure, leaving group, attacking nucleophile. SE^1, SE^2, SE^i, mechanisms - stark enamine reaction - decarboxylation of aliphatic acids - halogenation of aldehydes and ketones.

UNIT II: Aromatic Electrophilic Substitution and Aromaticity(18 hours)

Arenium ion mechanism - orientation and reactivity energy profile diagrams - the ipso attack - ortho/para ratio - substitution in thiophene - pyridine. Concept of aromaticity - Huckel's rule - effect of aromaticity on bond length, ring current - non-benzenoid aromatic compounds – aromatic character in three, five, seven and eight membered rings - anti aromaticity - system with 4, 8, 10 π electrons - annulene - sydnones - alternant and nonalternant hydrocarbons.

UNIT III:Addition Reactions and Addition to carbonyl group (18 hours)

Addition to carbon - carbon multiple bonds - electrophilic addition, nucleophilic and free radical additions - orientation and reactivity - birch reduction - hydroxylation - hydroboration - epoxidation - diels Alder reaction. Michael addition -ozonolysis, Clemmenson and Wolf-Kishner reductions. Mannich, Sobbe, Benzoin, Oppenauer oxidation - MPV reduction, Darzens Glycidic esters - Grignard reagents 1,2 and 1,4 addition - Gilman reagents - Wittig reaction.

UNIT IV: Rearrangements and Elimination Reactions (18 hours)

Classification - mechanisms of the following rearrangements - Wagner, Meervein, Dienone-phenol, Wolff, Favorski, Steven, Sommelet Hauser, Demjenov, Von-Richer, Schmidt, Pummerer rearrangements. Mechanisms of E^1, E^2, E^1CB - stereochemistry of elimination -competition between elimination and substitution pyrolytic cis elimination - chugaev reactiondehydration - dehydrohalogenation - hofmann degradation - cope elimination, Bredt's rule with examples.Saytzeff's rule and Hofmann rule.

UNIT V: Proteins, Nucleic Acids and Heterocyclic Compounds(18 hours)

Proteins classification – 1^o, 2^o, 3^o and quaternary structure of proteins - denaturation of proteins - biosynthesis of proteins. Nucleotides and Nucleosides - DNA - 1^o and 2^o structure- replication of DNA - RNA (*m*-RNA, *t*-RNA and *r*-RNA) genes - genetic code and informational theory - determination of base sequence of DNA - polymerase chain reactions. Synthesis and reactions of pyrazoles, oxazoles, thiazole, imidazole, pyridazine, pyrimidine, purines and pyrazines.

Course Outcomes:

1. Students learn the techniques of studying the mechanisms of reactions and to understand the nucleophilic substitution reactions shown by organic molecules.
2. Students get to know the mechanistic pathways of those nucleophilic substitution reactions.
3. Students understand the structural and stereochemical implications on Nucloephilic substitution reactions.
4. Students learn the characteristic features of electrophilic substitutions and understand the different kinds of electrophilic mechanisms in both aromatic and aliphatic compounds.
5. Students learn the addition reactions in carbon-carbon unsaturated bonds and carbon-hetero atom multiple bonds.
6. Students have sufficient knowledge on the mechanisms of elimination reactions and their name reactions.
7. Students get to know the classifications, mechanisms and applications of various molecular rearrangements.

Text Books:

1. Jerry March, "*Advanced Organic Chemistry (Reactions, Mechanisms and Structure)",* - Wiley, **2005**.
2. Thomas H. Lowry and K. S. Richardson, "*Mechanism and Theory in Organic Chemistry*" Addisson-Wesley, **1988**.

3. V. K. Ahluwalia and R. K. Parashar, *"Organic Reaction Mechanism"*, Narosa, **2006**.
4. Raj K. Bansal, *"Heterocyclic Chemistry (Synthesis, Reactions and Mechanism)",* Wiley- Eastern Limited **1999**.
5. J. H. Weil, "*General Bio-chemistry"* - New Age International, **1997**.
6. M. Badger, "*Aromatic Character"*, Cambridge University Press, **1969**.
7. I. L. Finar, "*Organic Chemistry*", Volume-II, 5th Ed., (**2006**).

Reference Books:

1. Structure and Mechanisms, F. Carey, R. Sundberg, "*Advanced Organic Chemistry. Part-A*". 4th Ed., Kluwer Publishers, **2000**.
2. Michael B. Smith, J. March, "*March's Advanced Organic Chemistry*", John Wiley & Sons, 6th Ed., **2007**.
3. J. Clayden, N. Greeves, P. Wothers, "*Organic Chemistry*", Oxford University Press, **2001**.
4. J. Mc. Murry, "*Organic Chemistry*", Brooks/Cole publisher, 5th Ed., **2000**.
5. M. B. Smith, "*Organic Synthesis*', Academic Press, Elsevier, 3rd Ed., **2010**.

PHYSICAL CHEMISTRY II - P19CH12

Semester: III **Core Course: X**

Instruction Hours/Week:6 **Credits : 5**

Objectives:

1. To learn in detail the applications of group theory to chemistry
2. To learn the advanced concepts in quantum chemistry
3. To study the concepts involved in NMR and ESR spectroscopy
4. To understand electrode-electrolyte equilibrium
5. To get knowledge about electro kinetic phenomena and corrosion

UNIT I: Group Theory **(18 hours)**

Elements of Group theory - Classes - group multiplication tables - properties of group, subgroup and isomorphism groups - symmetry elements and operations - point groups of molecules - Matrix representation of geometric transformation - Consequences of great orthogonality theorem and construction of character tables - reducible and irreducible representations and their relations- direct product – Applications of group theory for the determination of hybridization of atomic orbitals of non linear AX_2. AX_3 and AX_4molecules and linear molecules(CO_2) - Determination of symmetries of vibrational modes in non-linear(H_2O) and linear molecules(CO_2)- Rules for IR and Raman Activity.

UNIT II: Quantum Chemistry-II **(18 hours)**

Application of SWE to simple harmonic oscillator (Hermite polynomial, eigen functions, eigen values) - rigid rotator with free axis (SWE in polar coordinates, separation of angular functions and their solutions- selection rules for rotational and vibrational transitions - Bohr's correspondence principle - hydrogen atom and hydrogen like systems electron spin - Exactly solvable nature of systems - approximation methods - Variation method - application to hydrogen and helium atom - pertubation method to non -degenarate systems –Hartree Fock Self consistent field methods- Many electron atoms - wave function – one electron orbital - Pauli principle and Slater determinant.

UNIT III: Molecular Spectroscopy-II **(18 hours)**

NMR: Spin and applied magnetic field - Larmor precession - Relaxation processes – PMR chemical shifts – spin-spin interaction - FT NMR - multiple pulse NMR - ^{13}C NMR – Chemical exchange

ESR: Basic principles - Zero field splitting and Kramer's degeneracy - Factors affecting the '*g*' value - hyperfine splitting - spin Hamiltonian, spin densities and McConnell relationship, Measurement technique and applications.

Laser Raman spectra: Rotational Raman spectra of linear molecules - vibrational Raman spectra – rotational fine structure - Fermi resonance.

UNIT IV: Electrochemistry-I (18 hours)

Ionics: Debye-Huckel theory - radius of ionic atmosphere and its calculation – Debye-Huckel-Onsager equation and its modifications - asymmetry and electrophoretic effects – Debye Falkenhagen and Wien's effects - Activity of ions in solutions - Debye Huckel limiting Law. Electrode - electrolyte equilibrium: concentration cells - liquid junction potentials - Thermodynamic quantities from EMF data. Electrochemical energy - Storage system - Primary and secondary batteries –H_2-O_2 and Hydrocarbon - Oxygen fuel cells.

UNIT V: Electrochemistry-II (18 hours)

Electro kinetic Phenomena: Theories of electrical double layer - Theory of multiple layers at electrode electrolyte interface - electro kinetic phenomena. Processes at electrodes - the rate of charge transfer - current density – Butler-Volmer equation - Taft equation. Electro chemical corrosion - construction and use of Pourbaix and Evans diagram -prevention of corrosion - electro chemical oxidation and reduction.

Course Outcomes:

The students will be able to

1. Apply group theory to chemistry.
2. Gain knowledge on advanced concepts in quantum chemistry
3. Understand the theoretical background of NMR and ESR spectroscopy
4. Apply electrochemical principles in practical experiments.
5. Acquire knowledge on electrical double layers and on corrosion prevention.

Text Books:

1. F. A. Cotton, *Chemical Applications of Group Theory*, 2nd Ed., Wiley Eastern **1971**. (**UNIT I**)
2. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Ed., Tata McGraw Hill, **1994**. (**UNIT II**)
3. R. K. Prasad, *Quantum Chemistry*, 2nd Ed., New Age International Publishes (2000). (**UNIT II**)
4. D. A. Mcquarrie, *Quantum Chemistry*, University Science Books, **1983**. (**UNIT II**)
5. J. P. Lowe, *Quantum Chemistry*, Academic Press, **1978**. (**UNIT II**)
6. I. N. Levine, *Quantum Chemistry*, Allyn and Bacon, **1983**. (**UNIT II**)
7. G. N. Barrow, Introduction to Molecular Spectroscopy, International Mc. Graw Hill Ed., (**1993**), (**UNIT III**)

8. A. P. Straughan and S. Walker, Spectroscopy, Vol. I to III, Chapman Hall, London (**1976**), (**UNIT III**)
9. C.N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy' Tata-McGraw-Hill Education, 4th Ed., **1994**. (**UNIT III**)
10. P. W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford, **1983**.(**UNITS II, III, IV & V**)
11. A. S. Glasstone, Introduction to Electrochemistry, Affiliated East-West Press, **1968**. (UNIT IV) R. Crow, *Electrochemistry* (**UNIT V**)

Reference Books:

1. Peter Atkins and Julio de Paula, "*Atkin's Physical Chemistry*", Oxford Publishers, **2014**.
2. Allen J. Bard and Larry R. Faulkner, "*Electrochemical Methods Fundamentals and Applications*", 2nd Ed., John Wiley and Sons, **2004**.

PHYSICAL CHEMISTRY PRACTICAL-I - P19CH13P

Semester : III & IV **Core Course: XI**

Instruction Hours/Week: 6 **Credit : 5**

Any **ten** experiments (to be decided by the course teacher) out of the following Experiments:

1. Kinetics - Acid hydrolysis of ester- Comparison of strengths of acids.
2. Kinetics - acid hydrolysis of Ester- Determination of energy of activation (Ea).
3. Kinetics - Saponification of Ester- Determination of Ea by conductometry.
4. Kinetics - Persulphate- Iodine reaction- Determination of order, effect of ionic strength on rate constant.
5. Determination of molecular weight of substance by Transition Temperature method.
6. Study of phase diagram of two compounds forming a compound.
7. Study of phase diagram of three components system.
8. Determination of integral and differential heat of solutions by colorimetry.
9. Polymerization- Rate of polymerization of acrylamide.
10. Distribution law- Study of association of benzoic acid in benzene.
11. Adsorption - Oxalic acid/Acetic acid on charcoal using Freundlich isotherm.
12. Polarimetry – Inversion of cane sugar.

Text Books:

1. Senior Practical Physical Chemistry, D.D. Khosala, A. Khosala, V.C. Gard, R.Chand& Co., New Delhi, 1975.
2. Practical Physical Chemistry B. Viswanathan and P.S. Raghavan, Viva Books Pvt. Ltd., New Delhi, 2008.

Reference Books

1. Experimental Physical Chemistry Ed., by E. Daniels, International Student Ed., McGraw Hill,**1970**.
2. Experimental Physical Chemistry, G. Peter Mathews, Oxford Science Publications, **1985**.
3. J. B. Yadav, "*Advanced Practical Physical chemistry*", 20th Ed., GOEL publishing House, Krishna Pakashan Media Ltd., (**2001**).
4. Findlay's "*Practical Physical Chemistry*" Revised and edited by B. P. Levitt 9th Ed., Longman, London, **1985**.
5. J. N. Gurtu and R. Kapoor, "*Advanced Experimental chemistry*", Vol. I. Chand & Co., Ltd, New Delhi.

SPECTRAL TECHNIQUES IN INORGANIC COMPOUNDS - P19CH14E

Semester: III & IV **Core Course : XI**

Instruction Hours/Week: 6 **Credit : 5**

Objectives:

1. To learn the theoretical aspects and application of electronic spectroscopy.
2. To study the structural elucidation of inorganic compounds by IR and Raman spectroscopy.
3. To learn NMR of different nuclei and apply to find the structure of coordination and organometallic complexes.
4. To know the theory and application of EPR and magnetic properties.
5. To impart the knowledge of Mossbauer and NQR spectroscopy for selected compounds.

UNIT I: Electronic Spectroscopy **(18 hours)**

Microstates, terms and energy levels for d^1 - d^9 ions in cubic and square fields - intensity of bands - group theoretical approach to selection rules - effect of distortion and spin - orbit coupling on spectra - Orgel and Tanabe-Sugano diagrams - Evaluation of 10 Dq and β for octahedral complexes (Ti^{2+} and Ni^{2+} only) - application to simple coordination compounds - Charge transfer spectra-electronic spectra of $[Ru(bpy)3]^{2+}$ and $[Cu(phen)_3]^{2+}$ complexes.

UNIT II: Infrared and Raman Spectroscopy **(18 hours)**

Effect of isotopic substitution on the vibrational spectra of molecules - Vibrations in simple molecules (H_2O, CO_2) and their symmetry rotation for molecular vibrations - group vibrations and their limitations - combined uses of IR and Raman spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^- - effect of coordination on ligand vibrations - uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide - Vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment) – Applications of Raman Spectroscopy - Resonance Raman Spectroscopy.

UNIT III: NMR Spectroscopy **(18 hours)**

Examples for different spin systems - chemical shift and coupling constants (spin-spin coupling) involving different nuclei (^1H, ^{19}F, ^{31}P, ^{13}C) - interpretation and applications to inorganic compounds - ^{31}P NMR spectrum of $[Cp^*Rh(curc)(PTA)][SO_3CF_3]$ - effect of quadrupolar nuclei (^2H, ^{10}B, ^{11}B) on the ^1H NMR spectra – effect of low abundance isotopes on NMR- satellite spectra.

Systems with chemical exchange - study of fluxional behavior of molecules - an elementary treatment of second order spectra – spin tickling and spin decoupling- NMR of paramagnetic molecules – chiral and prochiral non-equivalence coincidences- Lanthanide shift reagents.

UNIT IV Electron Paramagnetic Resonance spectroscopy and magnetic properties (18 hours)

EPR spectroscopy: Theory of EPR spectroscopy - spin densities and McConell relationship - factors affecting the magnitude of g and A tensors in metal species - Zero-field splitting and Kramer's degeneracy - spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II), and Cu(II) complexes – EPR spectrum of cis-$[Cu(O_2C_8H_7O)_2(H_2O)_2]$ –Multiple resonance in EPR. **Magnetic Properties**: Types of magnetism-Dia-para-ferro and antiferrro magnetism. Magnetic properties of free ions - first order Zeeman effect - Second order Zeeman effect - states KT - states<<KT- Anomalous magnetic moments- equilibrium between two spin states-magnetically non equivalent sites- solute-solvent, solute-solute interaction- temperature independent paramagnetism.- spin pairing and Spin crossover in coordination compounds.

UNIT V: Mossbauer and NQR spectroscopy (18 hours)

Mossbauer Spectroscopy: Isomer shift - Doppler effect - magnetic interactions Mossbauer emission spectroscopy - application to Iron and Tin compounds – Mossbauer spectrum of iron carbonyl compound and $[Fe_4(\mu4\text{-}O)(\mu\text{-}MeO)_4(bisi)_4](ClO4)_2$ 34MeOH. Mossbauer spectrum of organic compounds.

NQR spectroscopy - characteristics of quadrupolar nucleus - effects of field gradient and magnetic field upon quadrupolar energy levels - NQR transitions - application to NQR spectroscopy.

Course Outcomes:

By learning the theoretical concepts and application of spectroscopic techniques a student can analyse the structure of inorganic complexes.

Text Books:

1. R. S. Drago, *Physical Methods in Inorganic Chemistry*, 3rd Ed., Wiley Eastern company, London.
2. R. S. Drago, *Physical Methods in Chemistry*, W.B. Saunders Company, Philadelphia, USA.
3. F. A. Cotton and G. Wilkinson, "*Advanced Inorganic Chemistry*" 5th Ed., Wiley- Interscience Publication, New York, **1990**.
4. Nakamoto, "*Infrared Spectra of Inorganic and coordination compounds* , 2nd Ed., Arnold, London

5. E. A. V. Ebsworth, *Sructural methods in Inorganic chemistry*, 3rd Ed., ELBS Great Briton, **1987**.
6. C. N. Banwell, *Fundamentals of molecular spectroscopy*, 3rd Ed., TMH, New Delhi, **1983**.
7. Lewis and Wilkins, *Modern Coordination Chemistry*.
8. P. J. Wheatley, "*The Determination of Molecular Structure*", Clarendon, Oxford, **1970**.
9. G. M. Barrow, "*Introduction to Molecular Spectroscopy*," McGraw-Hill, New York.
10. A. E. Gillanand and E. S. Stern, "Electronic Absorption spectroscopy of inorganic compounds", Wiley, New York.
11. J. D. Roberts, "*High Resolution Nuclear Magnatic Resonance*", McGraw-Hill, New York.
12. T. P. Das and E. L. Hahn, "*Nuclear Quadrupole Resonance Spectroscopy*", Academic, New York.
13. H. E. Duckworth, "*Mass Spectroscopy*", Cambridge, New York.
14. B. N. Figgis and J. Lewis," *The Magnetic properties of transitition metal complexes*"' in Progress in Inorganic Chemistry", Vol. 6, ed. F. A. Cotton, Interscience, New York
15. L. M. Epstein, *J. Chem. Phys*., *36* (**1962**) 2731.
16. B. Kozlevcar et al., *Croat. Chem. Acta*, *81* (**2008**) 369.
17. R. Pettinari et al., *Dalton Trans.*, 44 (**2015**) 20523.

Reference Books:

1. F. A. Cotton and G. Wilkinson, "*Advanced Inorganic Chemistry*" 5th Ed., Wiley- Interscience Publication, New York, **1990**.
2. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, **1962**.

BASIC STRATEGIES OF NANOMATERIALS
AND SYNTHETIC ORGANIC CHEMISTRY - P19CH15E

Semester: III **Elective Course - IV**
Instruction Hours/Week: 6 **Credit: 4**

Objectives:

1. To Make the students learn about basis of nanomaterial science, preparation methods, types and application.
2. To learn the basic characterization techniques of nanomaterials.
3. To instruct the basic knowledge about carbon nanotubes, properties and applications.
4. To impart the knowledge of retro synthetic analysis and synthetic strategies.
5. To understand the different applications of reagents in oxidation and reduction process.

UNIT-I: Basic concepts and Synthesis of Nanomaterials (18 hours)

Introduction to nanoscale materials - atomic & molecular size. Scientific revolutions, Scope of nano science and technology, Quantum Dots. Nanostructures: Zero-, One-, Two- and Three- dimensional structures, Chemical Routes for synthesis of Nanomaterials: Sol-gel synthesis, Microwave heating synthesis and Sono chemical Synthesis. Physical Routes for synthesis of Nanomaterials: Bottom up-Ball Milling, Physical vapour deposition and Electrochemical approaches. Spin coating - Thin films – Epitaxy – Lithography. Applications of nanomaterials: Applications of nano-biotechnology in early medical diagnostics, in energy sector and in ceramics industries. **Organic nanomaterials**: Rotoxanes and Catenanes.

UNIT-II: Characterization Techniques and Methodologies (18 hours)

Techniques for characterization of nanoscale materials: Principles of Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) - Resolution and Scanning – Scanning Transition Electron Microscopy (STEM), Scanning Tunneling Microscopy (STM), Scanning Near field Optical Microscopy (SNOM). Nano carrier systems in biomedicine and drug delivery – Nano-biotechnology – Molecular modelling – Nano surveillance.

UNIT III: **Carbon Nanostructures & Functionalization (18 hours)**

Carbon nanotube (CNT) and its Applications: Carbon nanotube (CNT), structure of CNT, synthesis ,mechanism and functionalization of CNT, electronic, vibrational, mechanical and optical properties of CNT; applications of CNT and Fullerenes and graphenes. Chemically modified carbon nanotubes – doping - Functionalizing nanotubes – Properties of carbon nanotubes -

Applications of carbon nanotubes Nanowires: Synthetic strategies. Applications of carbon nanomaterials: In environment and Biology.

UNIT IV: **Retro Synthetic analysis and Strategy (18 hours)**

Disconnection Approach and Synthetic Strategies: Introduction to retro synthetic analysis and disconnection approach - relay and convergent synthesis- linear synthesis- Introduction to synthons, synthetic equivalents - target molecule - Umpolung - designing synthesis by disconnection approach-Functional group interconversions: The importance of the order of events in organic synthesis - protecting group - principle, preparation and properties of alcohol and amine. C-C disconnections – Diels-Alder reaction and Robinson annulation – chemoselectivity (guidelines)

UNIT V: Reagents for Oxidation and Reduction Reactions (18 hours)

Oxidation reactions: CrO_3, PDC, PCC, $KMnO_4$, MnO_2, Swern, SeO_2, $Pb(OAc)_4$, Pd-C, OsO_4, *m*-CPBA, O_3, $NaIO_4$. Reduction reactions: Catalytic Hydrogenation, LAH, $NaBH_4$, $LiAlH(OBu)_3$, $NaCNBH_3$, Bu_3SnH, LDA, Me_2CuLi, MPV, H_2/Pd-C, $[(C_6H_5)_3P]_3RhCl$, NH_2NH_2, DIBAL-H.

Course Outcomes:

On completion of the course the student shall be able to:

1. Explain general concepts and methods of synthesis of nanomaterials.
2. Define physical phenomena and characterization of nanomaterials relevance within the field of nano sciences.
3. Understand the mechanism, functionalization and applications of carbon nanotubes.
4. Describe and be able to predict retro synthetic analysis and strategy
5. Choose appropriate reagents for oxidation and reduction process.

Text Books:

1. Sulbha K. Kulkarni, Nanotechnology: Principles & Practicals, springer, Nov **2014**, 3rd Ed., Capital Publishing Co., New Delhi (**Unit-I**)
2. Guozhong Cao, Nanostructures & Nanomaterials Synthesis, Properties & Applications, world scientifics series in nano science and Nanotechnology, Nanotechnology, Vol 12, 2nd Edn Jan **2011**. Imperials College Press London (**Unit-I**)
3. Charles P. Poole, Frank J. Owens, "*Introduction to Nanotechnology*", Wiley Interscience, **2003**, 1st Ed., May 20 (**Unit-I**)
4. C. P. Poole Jr. and F. J. Owens, *Introduction to Nanotechnology*, Wiley Student Ed., **2014** (**Unit-I & Unit III**)
5. T. Pradeep, Nano: The Essentials, McGraw Hill Education, 3rd Ed., **2009** (**Unit-I & Unit III**)

6. H. S. Nalwa, Handbook of Nanostructures: Materials and Nanotechnology, Vol 1-5, Academic Press, Bostan, Oct **1999**, 1st Ed., (**Unit-I**)
7. M. Reza Mozafari, nanomaterials and nanosystems for biomedical applications, Springer, **2013**. (**Unit-II**)
8. David S.Goodsell, Bionanotechnology, Wiley-Sciences, **2013** (**Unit-II**)
9. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties **2000**. (**Unit-II**)
10. T. Tang and P. Sheng (Eds): Nano Science and Technology Novel Structures and Phenomena, Taylor & Francis, New York, 1st Ed., **2004**. (**Unit-II**)
11. C. N. R. Rao, A. Muller, A. K. Cheetam (Ed.,), The Chemistry of Nanomaterials, Vol. 1,2 Wiley- VCH, Weinheim, **2014** (**Unit-III**)
12. Carbon Nanotubes: Properties and Applications- Michael J. O'Connell, 1st Ed., **2006**.
13. Nanotubes and Nanowires- CNR Rao and A Govindaraj RCS Publishing 10. Nanoscale materials -Liz Marzan and Kamat **2011**.
14. Stuart Warren, Organic synthesis - The disconnection Approach, John Wiley & sons, **2004** (**Unit-IV**).
15. Raymond K. Mackie & David M. Smith, Guidebook to Organic synthesis, **1994** (**Unit - IV**)
16. Jagdamba Singh and L. D. S. Yadav, Organic Synthesis, Pragati Prakashan, **2011** (**Unit - IV**)
17. W. Carouthers, Some modern methods of organic synthesis, Cambridge University Press, **1993** (**Unit – IV**)
18. H. O. House, Modern Synthetic Reactions, Allied Publishers, **1985** (**Unit - V**)
19. V. K. Ahluwali and R. K. Parashar, *Organic Reaction Mechanism*, Narosa, **2006**. (**Unit-V**)

Reference Books:

1. J. Dutta, H.F. Tibbals and G.L. Hornyak, "*Introduction to Nanoscience*", CRC press, Boca Raton, **2008**.
2. T. Pradeep, "Nano: The Essentials: Understanding Nanoscience and Nanotechnology", McGraw-Hill Professional Publishing, **2008**.
3. Michael B. Smith, J. March, "*March's Advanced Organic Chemistry*", John Wiley & Sons, 6th Ed., **2007**.
4. J. Clayden, N. Greeves, P. Wothers, "*Organic Chemistry*", Oxford University Press, **2001**.

ORGANIC CHEMISTRY III – P19CH16

Semester : IV **Core Course: XII**

Instruction Hours/Week: 6 **Credit: 5**

Objectives:

1. To learn reagent less organic reactions
2. To understand the principle behind thermal and photochemical organic reactions
3. To know the importance of addition reactions in organic compounds.
4. To learn c-c bond formation reaction in organic synthesis.
5. To understand the applicability of the spectroscopic techniques
6. To study the structure of the organic compounds from the study of spectra

UNIT I: Pericyclic Reactions and Optical Rotatory Dispersion and Circular Dichorism **(18 hours)**

Characteristics - classification - molecular orbital symmetry - frontier orbitals ethylene,1,3-butadiene, 1,3,5-hexatriene and allyl systems - applications of frontier molecular orbital(FMO) and molecular orbital correlation diagram methods to eletrocyclic reactions (4n and4n+2) system and cycloaddition reactions (2+2 and 4+2π electron system) - Woodward Hofmann rules - sigmatropic rearrangement (1,3 and 1,5 hydrogen shift) cope and claisen rearrangement (3,3 carbon shift) - chelotropic reactions. Introduction to theory and terminology - circular birefringence – circular dichorism - cotton effect and ORD curves - comparison between ORD and CD and their inter relationship - axial haloketone rule and octant rule - applications to determine the absolute configuration of monocyclic ketones and steroids.

UNIT II: Organic Photochemistry and Electron Spin Resonance Spectroscopy **(18 hours)**

Fundamental concepts - Jablonski diagrams - photosensitization - photochemical reactions - photo reduction - photo oxidation, photo rearrangements - di-π-methane rearrangement, photo reactions of ketones and enones – Norrish type I and II reactions - Paterno Buchi reaction - barton reactions - photochemistry of alkenes, dienes - photo addition reactions, photo chemistry aromatic compounds.

ESR: Basic principles - comparison between ESR and NMR spectroscopy - hyperfine splitting - calculation of unpaired electron density on an atom in a delocalized system (C6H6 -, p-xylene anion, naphthalene radical ion) - structure of methyl radical, p-benzoquinone radical anion.

UNIT III: NMR and ^{13}C NMR Spectroscopy (18 hours)

^1H NMR spectroscopy - introduction - chemical shift, shielding, deshielding, chemical and magnetic non-equivalence of protons - spin-spin splitting - coupling constant - dependence of J on dihedral angle - vicinal and germinal coupling - karplus equation - factors influencing chemical shift - first and second order proton - simplification of complex. Spectra- double resonance techniques - contact shift reagents - chemical spin decoupling of exchangeable protons (OH, SH, COOH, NH, NH_2) - Nuclear Overhauser Effect 2-D techniques (COSY, NOESY and ROSY).

C^{13} NMR- Basic principles - FT - NMR relaxation - broad band decoupling - off resonance decoupling and calculation of chemical shift for simple aliphatic (olefin, alkynes, carbonyl carbon) and aromatic compounds - conformation and chemical shift correlation peak assignments. Importance of NOE phenomenon in ^{13}C spectroscopy.

UNIT IV: UV-Visible Spectroscopy and Mass Spectrometry (18 hours)

Basic principles of electronic transitions - applications of UV-visible spectroscopy - woodward-fiescher scott rules - applications to conjugated dienes, trienes, polyenes - α-β- unsaturated carbonyl compounds. Conjugated cyclic ketones and acetophenones - aromatic hydrocarbons and heterocyclic systems - differentiation of position isomers and cis-trans isomers. Mass spectroscopy : Introduction - ion production - factors affecting fragmentation, ion analysis - ion abundance - base peak, isotopic peak, meta stable peak, parent peak - fragmentation of organic compounds with respect to their structure determination of common functional groups - molecular ion peak - McLafferty rearrangements. Nitrogen rule - high resolution mass spectroscopy.

UNIT V: Infrared Spectroscopy and Combined Spectroscopic Techniques (18 hours)

Problems Molecular vibrations - stretching vibrations - symmetric and asymmetric - bending vibrations - rocking, scissoring, wagging and twisting - finger print region - 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, acids) - effect of hydrogen bonding (inter and intra molecular) and solvent effect on vibrational frequencies - overtones - fermi resonance. Calculation of double bond equivalents and its application in structural elucidation - problems involving combined UV, IR, NMR, CMR and mass spectra data.

Course Outcomes:

1. Students understand stereo chemical implications of pericyclic reaction in organic synthesis.
2. Students get to know the mechanistic pathways of DA, sigmatropic and electrocyclic reaction
3. Students understand the structural and stereochemical implications on photochemical reactions
4. Students learn the principles, techniques and applications the of ESR and NMR spectroscopy for the structural elucidations
5. Students learn concepts and applications of UV-Vis spectroscopy
6. Students get learnt the concept IR spectroscopy and are able to find out the IR stretching frequency of organic functional groups

Text Books:

1. "*Organic Photo Chemistry and Pericyclic reaction*", M.G. Arora.
2. *Organic Reactions and Orbital symmetry*, T.L. Gilchrist and R.C. Storr. Cambridge, **1979**.
3. *The Conservation of Orbital symmetry*, R.B. Woodward and R. Hoffmann, Academic Press, **1970**.
4. *Photochemistry and Pericyclic reactions*. Jagdamba Singh and Jaya Singh New Age International, **2005**.
5. *Organic Spectroscopy - Principles and Applications*, Jag Mohan -Narosa, **2009**.
6. *Elementary Organic Spectroscopy (Principles and Chemical Application)*. Y. R. Sharma, S. Chand, **2005**.
7. *Organic Spectroscopy*, William Kemp Macmillan, **2008**.
8. *Spectroscopy of Organic Compounds* - P.S. Kalsi - New Age International, **2012**.

Reference Books:

1. Structure and Mechanisms, F. Carey, R. Sundberg, "*Advanced Organic Chemistry. Part-A*". 4^{th} Ed., Kluwer Publishers, **2000**.
2. Michael B. Smith, J. March, "*March's Advanced Organic Chemistry*", John Wiley & Sons, 6^{th} Ed., **2007**.
3. J. Clayden, N. Greeves, P. Wothers, "*Organic Chemistry*", Oxford University Press, **2001**.
4. J. Mc. Murry, "*Organic Chemistry*", Brooks/Cole publisher, 5^{th} Ed., **2000**.
5. M. B. Smith, "*Organic Synthesis*', Academic Press, Elsevier, 3^{rd} Ed., **2010**.

PHYSICAL CHEMISTRY PRACTICAL II - P19CH17P

Semester: III & IV **Core Course: XIII**

Instruction Hours/Week: 6 **Credit : 5**

Any **ten** experiments (to be decided by the course teacher) out of the following

Experiments:

2. Conductometry - Acid- alkali titrations.
3. Conductometry - Precipitation titrations.
4. Conductometry - Displacement titrations.
5. Conductometry - Determination of dissociation constant of weak acids.
6. Conductometry - Solubility product of sparingly soluble silver salts.
7. Conductometry- Verification of Onsager equation
8. Conductometry - Determination of degree of hydrolysis and hydrolysis constant of a substance.
9. Conductometry - To determine the relative strength of two acids.
10. Potentiometric titrations - Acid -alkali titrations.
11. Potentiometric titrations - Precipitation titrations.
12. Potentiometric titrations - Redox titrations.
13. Potentiometry - Determination of dissociation constant of weak acids.
14. Potentiometry - Determination of solubility of silver salts.
15. Potentiometry - Determination of activity and activity coefficient of ions.
16. Potentiometry - pH titration of orthophosphoric acid.
17. Potentiometry- To determine the pH of a buffer solution using quinhydrone electrode.

Text Books:

1. D.D. Khosala, A. Khosala, V.C. Gard, "*Senior Practical Physical Chemistry*", R. Chand & Co., New Delhi, **1975**.
2. B. Viswanathan and P.S. Raghavan, "*Practical Physical Chemistry*", Viva Books Pvt. Ltd., New Delhi, **2008**.

Reference Books

1. E. Daniels, "*Experimental Physical Chemistry*", International Student Ed., McGraw Hill, **1970**.
2. G. Peter Mathews, "*Experimental Physical Chemistry*", Oxford Science Publications, **1985**.
3. J. B. Yadav, "*Advanced Practical Physical chemistry*", 20^{th} Ed., GOEL publishing House, Krishna Pakashan Media Ltd., (**2001**).
4. Findlay's "*Practical Physical Chemistry*" Revised and edited by B. P. Levitt 9^{th} Ed., Longman, London, **1985**.
5. J. N. Gurtu and R. Kapoor, "*Advanced Experimental chemistry*", Vol. I. Chand & Co., Ltd, New Delhi.

PHYSICAL CHEMISTRY III - P19CH18

Semester : IV **Core Course: XIV**

Instruction Hours/Week: 6 **Credit : 4**

Objectives:

The students will be able

1. To learn the basics of photoelectron spectroscopy and to apply ESCA and Auger spectroscopy.
2. To understand in detail about Statistical mechanics and quantum statistics.
3. To study partition functions and non-equilibrium thermodynamics
4. To learn the concepts of polarographic and cyclic voltametric techniques
5. To study surface phenomena and micelles.

UNIT I: Quantum Chemistry and Spectroscopy (18 hours)

MO and VB treatment of hydrogen molecule - HMO model for systems like ethylene and butadiene - concept of bond order and charge density - hybridization derivation of wavefunction for sp, sp^2 and sp^3 hybrid orbitals.

Photoelectron spectroscopy: basic principles - UPES, XPES and AES - valence and core binding analysis, Koopman's theorem - ESCA and Auger spectroscopy to the study of surfaces.

UNIT II: Statistical Mechanics and Quantum Statistics (18 hours)

Statistical Mechanics: Basic concepts and classical statistics. Statistical Mechanics calculation of thermodynamic probability of system- phase space-ergodic hypothesis-definition of micro and macro states- different methods of counting microstates-distinguishable and indistinguishable particles- classical statistics-derivation of Maxwell's Boltzmann distribution law velocity and energy distribution.

Quantum Statistics: Bose-Einstein and Fermi-Dirac statistics- comparison of them with Boltzmann statistics- Application of BE statistics to photon gas and superfluidity of liquid helium- Application of FD statistics to electron gas and thermionic emission.

UNIT III: Statistical Thermodynamics (18 hours)

Partition functions: Translational, rotational, vibrational, electronic - calculation of enthalpy , internal energy, entropy and other thermodynamic functions - application of partition functions to mono and diatomic molecules. Heat capacity of solids: Einstein and Debye's treatments - concept of negative Kelvin temperature. Non-equilibrium thermodynamics: Thermodynamics of irreversible process - enthalpy production and entropy flow in open system - Onsager theory - phenomenological relations - Onsager reciprocal relations - steady state conditions.

UNIT IV: Electrochemistry-III **(18 hours)**

Principles and applications of Polarography -Instrumentation, Types of cells, advantages of dropping mercury electrode, interpretation of current voltage curves, determination of '*n*' value, polarographic maxima. Cyclic voltammetry, advantages over polarography techniques - test of reversibility of electron transfer reactions.

UNIT V: Surface Phenomena: **(18 hours)**

Adsorption and free energy reaction at interphase - potential energy diagram - Lennard-Jones plot - surface area determination – heat of adsorption - determination - adsorption from solution - Gibbs adsorption theorem - solid-liquid interface - Wetting and contact angle - solid-gas interfaces - soluble and insoluble films. **Surface tension:** methods of measuring surface tension - Micelles and reverse micelles- solubilisation - micro emulsion or micellar emulsions. **Role of surface in catalysis:** kinetics of surface reaction involving adsorbed species. Langmuir-Hinshelwood mechanism of bimolecular reaction - Langmuir-Rideal mechanism - Rideal-Eley mechanism.

Course Outcomes:

The students will be able to:

1. Apply basics of photoelectron spectroscopy, ESCA and Auger spectroscopy.
2. Understand in detail about Statistical mechanics and quantum statistics.
3. Acquire knowledge on statistical thermodynamics
4. Apply polarographic and cyclic voltametric techniques while doing research.
5. Understand the role of surface in catalysis.

Text Books:

1. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Ed., Tata McGraw Hill, **1994** (**UNIT I**)
2. I. N. Levine, *Quantum Chemistry*, Allyn and Bacon, **1983** (**UNIT I**)
3. P. W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford, **1983** (**UNITS II , III, IV & V**)
4. J. Rajaram and J. C. Kuriacose, *Thermodynamics for students of Chemistry-Classical, Statistical and Irreversible*, Shobhan Lal Nagin, New Delhi, **1981**(**UNITS II & III**)
5. S. Glasstone, *Introduction to Electro Chemistry*, Affiliated East-west Press, **1968** (**UNIT IV**)
6. D. R. Crow, *Polarography of metal complexes*, Academic Press, New York (**UNITS IV & V**)
7. Gurdeep Raj, *"Advanced physical chemistry"*, Meerut publication (**UNIT V**)

Reference Book:

1. Peter Atkins and Julio de Paula, "*Atkin's Physical Chemistry*", Oxford Publishers, **2014**.