

**M. Sc Chemistry Programme**  
**Under**  
**Learning Outcomes based Curriculum Framework**  
**(LOCF)**

**(For those students admitted during the Academic Year**  
**2022-23 and after)**

**SYLLABUS**



Since 1919

**POST GRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY**  
**(DST-FIST Sponsored Department)**

**NATIONAL COLLEGE (Autonomous)**

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

**College with Potential for Excellence by UGC,**

**DBT-STAR & DST-FIST Sponsored College**

**Tiruchirappalli-620 001**

## **Post Graduate and Research Department of Chemistry**

### **College**

**Vision:** To offer quality higher education to the younger generation, especially from rural India, who are economically and socially backward, to liberate themselves from prejudice, oppression and ignorance and to gain knowledge for their bright future.

### **Mission:**

- ❖ To ignite the young minds with lofty ideals and inspire them to achieve excellence in the chosen field.
- ❖ To facilitate individual growth of students, with accent on character building, through co- curricular and extra-curricular activities.
- ❖ To encourage the students to take up research and help them reach global standards.
- ❖ To provide a congenial atmosphere to study and to learn with infrastructural facilities of high standards.
- ❖ To instill in the minds of the students, a sense of Nationalism and to train them in social awareness.

### **Department**

#### **Vision:**

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.
- ❖ To create a better everyday life for the students and we help the students to realize their full potential.

#### **Mission:**

- ❖ 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.
- ❖ 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.
- ❖ To make the present day students who are the citizens of tomorrow more productive and successful by eliminating the barriers to opportunities.
- ❖ To make the students use the information gained in the classroom in their practical life, which is always challenging, by helping them to develop their skills.
- ❖ To shape the minds of the students so that they create a new future.
- ❖ To make the future teachers disseminate the educational content effectively and globally.
- ❖ To set the standards of excellence by helping them reach their full potential.

**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.

**Programme Educational Objectives (PEOs)**

1. Graduates will be able to accomplish professional standards in the global environment.
2. Graduates will be able to uphold integrity and human values.
3. Graduates will be able to appreciate and promote pluralism and multiculturalism in working environment.

**National College (Autonomous), Tiruchirappalli**  
**(PG Programme Outcomes)**  
**Master of Science (M.Sc.) Chemistry**

**On completion of this programme,**

- PO1:** Graduates will have good personal, professional, able to analyze and interpret data to create and design new **knowledge** in their respective disciplines and to take the society to the path of progress.
- PO2:** Graduates will be able to engage in innovative and socially relevant research and effectively **communicate** the findings and to allow them to contribute to the advancement of knowledge.
- PO3:** Graduates will get enhanced career prospects, improved **problem solving** and decision making skills. They will be able to use the information to deduce facts and determine the outcomes.
- PO4:** **Reflective thinking** is essential; the graduates will be able to choose and enact solutions that are most logical and advantages. They will be able to navigate a challenging period.
- PO5:** Graduates will have the ability to apply **professional ethics**, accountability, and equity in all their endeavors. They will be able to obey the rules of the firm/company/Institution where they work and also they will be responsible, accountable and they will have the trust and mutual respect for their colleagues in their work place.
- PO6:** Graduates will have the ability to understand, appreciate and interact with people whose **cultures** are different from their own. The students will be able to take initiative by themselves, choosing and implementing appropriate learning strategies and evaluating learning outcomes. They will be able to qualify in **NET/SET/JRF/CSIR** and other academic competitive examinations.

**M.Sc., Chemistry**

**Programme Specific Outcomes**

On successful completion of M.Sc. Chemistry programme, the students would have

- PSO1:** Learnt, understood and applied the **fundamental knowledge** of the basic principles in various fields of Chemistry to solve every day problems like softening of hard water, cleaning, purification of water, etc.
- PSO2:** Acquired the ability to **communicate** the advanced concepts in chemistry in a clear and concise manner. Confidently expressed the ideas of science to the society.
- PSO3:** **Critical thinking** helped them by applying the background of organic reaction mechanisms, complex chemical structures, instrumental methods of

chemical analysis, molecular rearrangements and separation techniques.

**PSO4:** Graduates gathered **knowledge** of advanced tools in chemistry and carried out experiments in the area of organic analyses, estimation, separation, derivative process, inorganic semi micro analyses, preparation, conductometric and potentiometric analyses.

**PSO5:** Adopted the principles of green chemistry for designing experimental techniques to mitigate **environmental pollution**. Demonstrated the ability to identify the **ethical issues** related to one's work, avoided **unethical behavior** such as fabrications, misrepresentations of data and/or committing plagiarism.

**PSO6:** **Trained themselves** to confidently appear for competitive examinations such as **NET, GATE, SET, UPSC, TNPSC, BARC, ONGC** etc, and also to become entrepreneur Contributed to the nation in the capacity of chemist and/or as innovator by taking up research career.

#### **GRADUATE ATTRIBUTES:**

1. **Academic Excellence:** They will have a promising career in academics, research institutes both in India and abroad.
2. Students will be able to apply very well their knowledge in the design and manufacture of compounds and become entrepreneurs.
3. **Communication skills:** Assignment writing develop all sorts of skills including critical thinking, creativity, and written communication.
4. Students will be able to communicate very well about their scientific findings both orally and written and in ICT formats.
5. **Critical Thinking:** They will be able to think rationally and draw logical conclusions.
6. **Problem Solving:** Students can become leaders of associations, which require finding solutions to problems faced by public.
7. **Analytical Reasoning:** The student will be able to discover trends in quantitative data, which they measure in the laboratory. Flaws and holes in the theory proposed ability to evaluate.
8. **Design and Development skills:** Able to design and develop new techniques in the field taken.
9. **Individual and teamwork:** Able to carry out individual and teamwork in qualitative and quantitative analytical field. This effect facilitate the teamwork efficiently.
10. **Technology, competency:** Able to increase the capacity to extrapolate from the technology gained in the thermodynamics and apply their competency to solve any non-familiar problem.
11. **Morals and Ethics:** Helps the students to acquire the ability to identify ethical issues and avoid unethical behavior in any trained practical field.

12. **Global citizenship:** Able to promote global citizenship by gaining and applying their skills in the fundamental and fast developing fields.
13. **Environmental and sustainability:** Able to provide environmental and sustainability from the exposure of teaching and evaluating methods (project base for PG learning) collaborative learning contribution from guest speakers, inter-disciplinary, multi-disciplinary working in the subject area selected.
14. **Lifelong learning:** Ability to acquire knowledge and skills that are necessary for participating in learning activities throughout life.
15. Students will learn the application of modern tools and techniques in a multidisciplinary environment.
16. Volunteering demonstrates dedication, time management and civic-mindedness.
17. They can defend their ideas in dialogue with peers, respect others' views and perspectives.
18. Participating in individual and team sports builds leadership and team working skills.
19. Students will be to mix with a broad set of people, which will prove to be particularly useful whenever they are required to work within, and manage a fairly diverse team.
20. Submitting the assignment notebooks, practical notebooks, record notebooks in time illustrates the ability to prioritise tasks and manage their time effectively.
21. Organizing association meetings and delivering talks to groups shows the ability to communicate clearly and present ideas confidently and confidence. It also helps in developing organisation and interpersonal skills.
22. Group practical offers the chance to gain teamwork skills like negotiation, compromise and cooperation.

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PG & RESEARCH DEPARTMENT OF CHEMISTRY

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**BLOOM'S TAXONOMY BASED ASSESSMENT PATTERN**

K1 - Remember; K2 - Understanding; K3 - Apply; K4 - Analyze; K5 - Evaluate

**1. Theory Examination - Part I, II & III**

**CIA Test Question Pattern:**

<b>Knowledge Level</b>	<b>Section</b>	<b>Marks</b>	<b>Description</b>	<b>Total Marks</b>
K1, K2 Q1 to Q10	A (MCQ)	10 X 1 = 10	Objective Multiple Choice Questions (4 Questions from each unit)	50
K2, K3 Q11 to Q16	B (4 out of 6)	4 X 5 = 20	Descriptive Answers	
K2, K3 & K4 Q17 to Q19	C (2 out of 3)	2 X 10 = 20	Detailed Answers	

**End Semester Examination Question Pattern:**

<b>Knowledge Level</b>	<b>Section</b>	<b>Marks</b>	<b>Description</b>	<b>Total Marks</b>
K1, K2 Q1 to Q20	A (MCQ)	20 X 1 = 20	Objective Multiple Choice Questions (4 Questions from each unit)	75
K2, K3 Q21 to Q25	B (Either/or type) ONE question from each unit	5 X 5 = 25	Descriptive Answers (Either/or type) (1 question from each unit)	
K2, K3 & K4 Q26 to Q30	C (3 out of 5)	3 X 10 = 30	Detailed Answers (1 Question from each unit)	

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**Course Structure (2022 onwards)**

SEM	PART	COURSE	COURSE TITLE	INS HOURS / WEEK	CREDIT	EXAM HRS	MARKS			TOTAL
							CIA	EXTERNAL		
								W	O	
I		CORE COURSE-CC1 (P22CH1)	SYNTHETIC AND STRUCTURAL INORGANIC CHEMISTRY	6	5	3	25	75	-	100
		CORE COURSE-CC2 (P22CH2)	ORGANIC CHEMISTRY-I	6	5	3	25	75	-	100
		CORE COURSE-CC3 (P22CH3P)	INORGANIC CHEMISTRY PRACTICALS -I	6	-	-	-	-	-	-
		CORE COURSE-CC4 (P22CH4P)	ORGANIC CHEMISTRY PRACTICAL-I	6	-	-	-	-	-	-
		ELECTIVE COURSE-I (P22CH5E)	ADVANCED TECHNIQUES AND COMPUTER APPLICATIONS IN CHEMISTRY	6	4	3	25	75	-	100
		<b>TOTAL</b>		<b>30</b>	<b>14</b>				-	<b>300</b>
II		CORE COURSE-CC V (P22CH6)	QUANTUM CHEMISTRY, GROUP THEORY AND CHEMICAL KINETICS	6	5	3	25	75	-	100
		CORE COURSE-CC VI (P22CH7)	REACTION MECHANISM IN COORDINATION AND ORGANOMETALLIC CHEMISTRY	6	5	3	25	75	-	100
		CORE COURSE-CC3 (P22CH3P)	INORGANIC CHEMISTRY PRACTICALS -I	6	5	6	25	75	-	100
		CORE COURSE-CC7 (P22H8P)	INORGANIC CHEMISTRY PRACTICAL-II	6	5	6	25	75	-	100
		CORE COURSE-CC4 (P22CH4P)	ORGANIC CHEMISTRY PRACTICAL-I	6	5	6	25	75	-	100
		CORE COURSE-CC8(P22CH9P)	ORGANIC CHEMISTRY PRACTICAL-II	6	5	6	25	75	-	100
		ELECTIVE COURSE-II (P22CH10E)	GREEN AND ENVIRONMENTAL CHEMISTRY	6	4	3	25	75	-	100
			<b>TOTAL</b>		<b>30</b>	<b>34</b>				-
III		CORE COURSE-C9(P22CH11)	ORGANIC CHEMISTRY-II	6	5	3	25	75	-	100
		CORE COURSE-CC10 (P22CH12)	ELECTROCHEMISTRY AND SPECTROSCOPY	6	5	3	25	75	-	100
		CORE COURSE-CC11 (P22CH13P)	PHYSICAL CHEMISTRY PRACTICAL-I	6	-	-	-	-	-	-
		CORE COURSE-CC14E ELECTIVE COURSE -III (P22CH14E)	SPECTRAL TECHNIQUES IN INORGANIC COMPOUNDS	6	4	3	25	75	-	100
		ELECTIVE COURSE - IV (P22CH15E)	BASIC STRATEGIES OF NANOMATERIALS AND SYNTHETIC ORGANIC CHEMISTRY	6	4	3	25	75	-	100
			<b>TOTAL</b>		<b>24</b>	<b>18</b>				-
IV		CORE COURSE-CC12 (P22CH16)	ORGANIC CHEMISTRY-III	6	5	3	25	75	-	100
		CORE COURSE-CC11 (P22CH13P)	PHYSICAL CHEMISTRY PRACTICAL-I	6	5	6	25	75	-	100
		CORE COURSE- 13(P22CH17P)	PHYSICAL CHEMISTRY PRACTICAL -II	6	5	6	25	75	-	100
		ELECTIVE COURSE - V (P22CH18E)	APPLICATIONS OF QUANTUM CHEMISTRY AND THERMODYNAMICS	6	4	3	25	75	-	100
		PROJECT P22CHP22	PROJECT-CHEMISTRY	12	5	3	25	75		100
		<b>TOTAL</b>		<b>36</b>	<b>24</b>					<b>500</b>
		<b>GRAND TOTAL</b>		<b>120</b>	<b>90</b>					<b>1900</b>



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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH1	SYNTHETIC AND STRUCTURAL INORGANIC CHEMISTRY		1
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I	5	90

**Course 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 theory and applications in inorganic photochemistry.
5. 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  $Cp_2TiS_5$ . Uses of carboranes and polythiazyls.

**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-Landé 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. Different techniques for the study of solid state reactions.

**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, liquid crystals types and applications. X-ray diffraction by crystals - function of crystals - transmission grating and reflection grating - Bragg's equation (No derivation) - diffraction methods - rotating crystal, oscillation and Weissenberg 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. Solar energy harvesting.

**UNIT V: Supramolecular Chemistry**

**(18 hours)**

Concepts and languages of supramolecular chemistry - hydrogen bonds - C-H...X interactions - halogen bonds -  $\pi$  -  $\pi$  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 - organometallic receptors - 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 Learning Outcomes:**

1. Describe the types, structures, and reactions of cyclic boron, sulphur, and nitrogen compounds.
2. Know the various structures of ionic compounds and solid state reaction mechanisms.
3. Learn the essential concepts of several crystal systems using X-ray diffraction techniques.
4. Recognize the concept and applications of inorganic photochemistry.
5. Have a solid understanding of the key ideas and list a few applications for supramolecular chemistry.

**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", 4th edn., 1993, Harper Collins College Publishers.
3. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry" 5th edn., 1988, Wiley- Interscience Publication, New York.
4. L. W. Azaroff, "Introduction to Solids", 2017, Tata Mcgraw hill publishing company, USA.
5. N. B. Hannay, "Solid State Chemistry", 1976, Printice Hall, New Delhi.

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7. F. C. Philips, "An Introduction to Crystallography", 3rd edn., 1963, Longmans, London.
8. K. F. Purcel and J. C. Kotz, "Inorganic Chemistry", 1982, W. G. Saunder's Company, Philadelphia.
9. Philadelphia.
10. D. F. Shriver, P.W. Atkins and C.H. Langford, "Inorganic Chemistry", ELBS. 6th edn., 1990, Oxford University press, England.
11. J. Ferraudi, "Elements of Inorganic Photochemistry", 1988, Wiley, New York.
12. W. Adamson and P. D. Fleischauer, "Concepts of Inorganic Photochemistry", 1975, Wiley, New York.
13. J. L. Atwood and J. W. Steed, "Supramolecular Chemistry: A concise Introduction", 2<sup>nd</sup> edn., 2009, John Wiley & Sons Ltd., UK.
14. J. M. Lehn, "Supramolecular Chemistry: Concepts and Perspectives", 1995, Wiley, VCH.

**Reference Books:**

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

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH2	ORGANIC CHEMISTRY-I		2
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I	5	90

**Course Objectives:**

1. To make the students to know about the nomenclature of organic compounds 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 students to understand and appreciate the importance of carbohydrates, antibiotics and steroids.

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

**1.1 Nomenclature:** 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.

**1.2 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.

**1.3 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)**

**2.1 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.**

**2.2 Correlation Analysis:** Linear Free Energy Relations - Hammett 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 -

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)**

**4.1 Geometrical isomerism:** Geometrical isomerism - E, Z - determination of configuration of geometrical isomers (cyclisation, converting into compounds of known configuration, dipole moment, 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.

**4.2 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.

**UNIT V: Natural Products (18 hours)**

**5.1 Carbohydrates:** Polysaccharides - structure of starch and cellulose, configuration of carbohydrates - photosynthesis.

**5.2 Antibiotics & Steroids:** Chemotherapy - definition LD<sub>50</sub> - Structural elucidation and synthesis of penicillin, streptomycin - cephalosporin-C. Classification-structural elucidation of cholesterol (synthesis not required), structural elucidation and synthesis of Vitamin D, estrone, progesterone, ergosterol.

**5.3 Alkaloids:** Biological importance of alkaloids- structural elucidation of Morphine and Reserpine - Vincristine, Adrenaline and Atropine (structure only)

**Course Learning Outcomes:**

1. Students learn bonding in organic molecules and the structural implications on properties
2. Students understand the importance of stereochemical aspects of structure and properties
3. Students get to know the chemical reactions and the mechanisms *via* different intermediates
4. Students learn the techniques of studying the mechanisms of reactions
5. Students get to know the structure and importance of carbohydrates, antibiotics and steroids and alkaloids

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**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*", 2<sup>nd</sup> 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*", 2<sup>nd</sup> 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, 5<sup>th</sup> Ed., (2006).

**Reference Books:**

1. Structure and Mechanisms, F. Carey, R. Sundberg, "*Advanced Organic Chemistry. Part-A*". 4<sup>th</sup> Ed., Kluwer Publishers, 2000.
2. Michael B. Smith, J. March, "*March's Advanced Organic Chemistry*", John Wiley & Sons, 6<sup>th</sup> 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<sup>th</sup> Ed., 2000.
5. M. B. Smith, "*Organic Synthesis*", Academic Press, Elsevier, 3<sup>rd</sup> Ed., 2010.
6. E.L. Eliel, "*Stereochemistry of Carbon Compounds*", McGraw Hill Book Company, New York, 1975.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH3P	INORGANIC CHEMISTRY PRACTICAL – I		3
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I & II	5	90

**Course Objectives:**

1. To learn and identify the inorganic cation in a mixture.
2. To know the colourimetric techniques for estimation of ions.

**Inorganic Qualitative Analysis:**

1. Semi-micro qualitative analysis of a mixture containing two common and two rare cations.

**Inorganic Quantitative Analysis:**

1. Estimation of Copper, Ferric, Nickel, Chromium and Manganese using photoelectric colorimeter.

**Course Learning 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**.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH4P	ORGANIC CHEMISTRY PRACTICAL – I		4
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I & II	5	90

**Course 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. Mixture containing all functional groups including halogens (nuclear, side chain).

**Preparation of Organic Compounds (Single Stage)**

- (a) Methyl-m-nitrobenzene from methyl benzoate (nitration)
- (b) Glucose penta acetate from glucose (acetylation)
- (c) Resacetophenone from resorcinol (acetylation)
- (d) Phenyl-azo-2-naphthol from aniline (diazotization)
- (e) 2-Naphthylmethylether from 2-Naphthol (methylation)
- (f) Dibenzalacetone from benzaldehyde

**Course Learning 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*", 5<sup>th</sup> Ed., Longman Scientific & technical, England, **1989**.



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SUBJECT	TITLE OF THE PAPER		ELECTIVE
P22CH5E	ADVANCED TECHNIQUES AND COMPUTER APPLICATIONS IN CHEMISTRY		1
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I	4	90

**Course 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; to use C language and to apply it to chemistry.
5. To learn the basics of modeling chemical systems.

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

**1.1 Error:** Various types of Error - accuracy, Precision, significant figures – Standard deviation - Correlation and regression - Fitting of linear equations – Multiple linear regression analysis.

**1.2 Spectroscopy: Atomic absorption spectroscopy:** Basic principle of AAS, Instrumentation (flame and flameless atomization) - Atomizers, Burners and Furnace, properties of Flame, Resonance line source, Hollow Cathode lamp and electrochemical radiation sources, detectors – Spectral and Chemical Interferences, applications of AAS. Flame Photometry – Theory, Instrumentation and a few important applications.

**UNIT II: Chromatography(18 hours)**

**2.1. Principles:** Solvent extraction - Basic principle of chromatographic techniques - Principles of ion exchange, paper, thin layer and column Chromatography techniques - Columns, adsorbents, methods. Significance of Partition Ratios in chromatography ( $K_d$ ) & Retention Time ( $t_R$ ) and relation between them (no derivation) – Definition and significance of Retention Factor  $R_f$  (Capacity Factor) and selectivity factor.

**2.2 Gas-liquid Chromatography:** Principles, Instrumentation (Carrier Gas, Inlet System- Types of Columns, Pre-packed columns, Pre-conditioning of columns, Stationary Phase, Detectors – Thermal Conductivity, Flame Ionization) and applications of GLC - GC-MS techniques: methods, principles and uses.

**2.3 High Performance Liquid chromatography:** Basic principle, instrumentation (Pumping Systems, Columns, Column packing, Detector) and applications.

**UNIT III: Thermoanalytical Methods and Molecular Luminescence Spectrometry (18 hours)**

**3.1 Thermoanalytical methods:** Comparison of Thermogravimetric analysis (TGA) and Differential Thermal analysis (DTA) - Differential Scanning Calorimetry (DSC). Principle and instrumentation-Thermometric titrations.

**3.2 Molecular Luminescence Spectrometry:** Instrument for measuring Fluorescence and Phosphorescence - Components of Fluorometers and Spectrofluorometer - block diagram instrument standardization. - Flow cytometry- applications. XRD-Principles, applications and Instrumentation only.

**UNIT IV: Computer Applications in Chemistry (18 hours)**

**4.1 Introduction to C language:** 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.

**4.2 Applications:** 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 ORIGINLAB 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 Learning Outcomes:**

**The students will be able to**

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

**Text Books:**

1. Willard, Merrit, Dean and Settle, *Instrumental methods of Analysis*

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- CBS Publishers and Distributors, 6<sup>th</sup> Ed., **1986. (UNIT I)**
2. Skoog, D. A. West, D. M. Holler. P. J. "*Fundamentals of Analytical Chemistry*" 7<sup>th</sup> 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, 2<sup>nd</sup> 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 ANSIC*", Tata McGraw Hill, 2<sup>nd</sup> Ed., New Delhi, **1999. (UNIT IV)**
  7. R. Leach, "*Molecular Modelling Principles and Applications*", 2<sup>nd</sup> 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)**.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH6	QUANTUM CHEMISTRY, GROUP THEORY AND CHEMICAL KINETICS		5
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I & II	5	90

**Course Objectives:**

1. To learn to the origin of quantum mechanics and its applications.
2. To learn in detail the applications of group theory to chemistry.
3. To understand the advanced concepts involved in kinetics.
4. To study reactions in photochemistry and radiation chemistry.
5. To study surface phenomena and micelles.

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

**1.1 Origin of quantum theory:** Inadequacy of classical mechanics-Blackbody 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.

**1.2 Applications:** 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 Group Theory**

**(18 hours)**

**2.1 Introduction to group theory:** 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-

**2.2 Applications:** Applications of group theory for the determination of hybridization of atomic orbitals of nonlinear AX<sub>2</sub>, AX<sub>3</sub> and AX<sub>4</sub> molecules and linear molecules (CO<sub>2</sub>) - Determination of symmetries of vibrational modes in non-linear (H<sub>2</sub>O) and linear molecules(CO<sub>2</sub>)- Rules for IR and Raman Activity.

**UNIT III: Chemical Kinetics:**

**(18 hours)**

**3.1 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-Brønsted relation.**

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

**4.1 Fast reaction techniques:** Flow methods: Stopped flow technique–Relaxation methods - Flash photolysis - Shock tube method - molecular beam method.

**4.2 Photochemistry:** Photophysical process in electronically excited molecules–Jablonski diagram–Stern-Volmer equation–Chemical Actinometers - Lasers and their applications.

**4.3 Radiation chemistry:** Sources of high energy radiation - radiolysis of water – solvated electrons – Scavenging techniques–Applications of radiation chemistry.

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

**5.1 Adsorption:** Adsorption and free energy reaction at inter phase-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.

**5.2 Surface tension:** methods of measuring surface tension-Micelles and reverse micelles - solubilisation- microemulsion or micellar emulsions.

**5.3 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 Learning Outcomes:**

**The students will be able to**

1. Apply quantum mechanics to simple chemical systems.
2. Apply group theory to chemistry.
3. Understand the advanced concepts involved in kinetics and apply the same in the laboratory.
4. To acquire knowledge on fast reaction kinetics, photochemistry and radiation chemistry.
5. To study surface phenomena and micelles.

**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<sup>nd</sup> Ed., New Age International Publishers (**2000**), (**UNIT I**).
3. N. Levine, *Quantum Chemistry*, 4<sup>th</sup> 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**).

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6. F. A. Cotton, Chemical Applications of Group Theory, 2nd Ed., Wiley Eastern 1971. **(UNIT II)**
7. K. J. Laidler, Chemical Kinetics, 2nd Ed., Tata McGraw Hill, **1975, (UNIT III)**
8. A. Frost and R. G. Pearson, Kinetics and Mechanisms, John Wiley & Sons (**1953**). **(UNIT III)**
9. J. C. Kuriacose and J. Rajaram, Kinetics and Mechanisms Transformations, Macmillan & Co., (**1993**). **(UNIT III)**
10. P. W. Atkins, Advanced Physical Chemistry, 7<sup>th</sup> Ed., Clarendon (**2002**) **(UNIT V)**
11. K. K. Rohatgi and Mukerjee, Fundamentals of Photo Chemistry, Wiley Eastern Ltd (**1986**). **(UNIT IV)**
12. G. Hughes, Radiation Chemistry, Oxford University Press (**1973**) **(UNIT IV)**

**Reference Books:**

1. Peter Atkins and Julio de Paula, "*Atkin's Physical Chemistry*", Oxford Publishers, **2014**.
2. Alan Vincent, Molecular symmetry and group theory, John Wiley & Sons, New York, 1978.
3. Mool Chand Gupta , Atomic and Molecular Spectroscopy, New Age International Publishers, New Delhi, 2001.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH7	REACTION MECHANISM IN COORDINATION AND ORGANOMETALLIC CHEMISTRY		7
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	II	5	90

**Course Objectives:**

- To understand the key features and various theories of coordination compounds
- To describe the stability of metal complexes, types of isomers and reaction mechanism in
  - coordination compounds.
- To learn the biological role and mechanism of bioinorganic complexes.
- To study the various types of organometallic reactions.
- To provide an extensive knowledge of organometallic catalysts.

**UNIT I: 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 -  $\pi$ -bonding and MO theory - ligands having filled and empty  $\pi$ -bonds - effect of  $10 Dq$  - evidences for  $\pi$ -bonding from IR spectroscopy - higher coordination complexes - 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 - mixed valence complexes - reactions of coordinated ligands - template effects - synthesis of macrocyclic ligands.

**UNIT III: Bioinorganic Chemistry**

**(18 hours)**

Biological role of metal ions – Gold compounds and Rheumatoid 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 -superoxide and bovine superoxide dismutase - carbonic anhydrase - carboxypeptidases - iron-sulphur proteins and non-heme iron cytochromes of electron transport chain - cytochrome P-450 enzymes.

**UNIT IV: Organometallic Chemistry**

**(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 - nitrosyl complexes - bridging and terminal nitrosyls - bent and linear nitrosyls - dinitrogen complexes - dioxygen complexes - molecular orbitals of metallocenes. Classification of fluxional organometallic compounds.

**UNIT V: Catalysis by Organometallic Compounds**

**(18 hours)**

Hydrogenation of olefins - hydroformylation of olefins - gold-catalyzed addition of carboxylic acids to alkynes - 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 Learning Outcomes:**

1. Explain structure and bonding and magnetic properties of coordination compounds.
2. Discuss the properties and reaction mechanisms of coordination compounds.
3. Elucidate the binding and functions of inorganic elements in bioinorganic chemistry.
4. Identify bond-to-metal complexes and fundamental reactions in organometallic chemistry.
5. Establish the operating mechanisms in the catalytic processes via structure-activity relations.

**Text books:**

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, "Inorganic Chemistry - Principles of Structure and Reactivity", 4th edn., **1993**, Harper Collins College Publishers, New York.
2. F. A. Kettle, "Physical Inorganic Chemistry - A Coordination Approach", **1996**, Spectrum Academic Publishers, Oxford University Press.
3. P. Powell, "Principles of Organometallic Chemistry", 2<sup>nd</sup> edn., **1936**, Chapman and Hall, London.



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4. K. F. Purcel and J. C. Kotz, "Inorganic Chemistry", **1982**, W. G. Saunder's Company, Philadelphia.
5. W. U. Malik, G. P. Tuli and R. D. Madan, "Selected Topics in Inorganic Chemistry", 6<sup>th</sup> edn., **2001**, S. Chand & Company Ltd., New Delhi.
6. Gurdeep Raj, "Advanced Inorganic Chemistry", Vol. II, 8<sup>th</sup> edn., **2002**, Goel Publishing House, Meerut.
7. W. Kaim and B. Schewederski, "Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life", 4<sup>th</sup> edn. **2013**, John-Wiley and sons, New York.

**Reference Books:**

1. G. L. Miessler and D.A. Tarr, "Inorganic Chemistry", **2009**, Pearson, Prentice Publishers, Delhi.
2. F. A. Cotton and G. Wilkinson, "Inorganic Chemistry A Comprehensive Text", 5th edn., **1988**, Inter science Publishers, New York.
3. K. F. Purcell and J. C. Kotz, "Inorganic Chemistry", **1982**, W B Saunders Company, Philadelphia.
4. B. Douglas, D. H. McDaniel and Concepts and Models of J. J. Alexander, "Inorganic chemistry", **2001**, John Wiley and Sons, New Delhi.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH8P	INORGANIC CHEMISTRY PRACTICAL – II		7
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I & II	5	90

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

**Titrimetry (V) and Gravimetry (G)**

A mixture of solution(s) will be provided 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 trisoxalatochromate[III]
- a) Potassium trisoxalatoaluminate[III].
- b) Trithioureacopper[I] chloride.
- c) Trithioureacopper[I] sulphate.

**Course Learning Outcomes:**

1. Students learn the estimation of ions by separating them in a mixture.
2. Students get skill in preparation of coordination compounds, recording their infrared & electronic spectra and interpreting them.

**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**.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH9P	ORGANIC CHEMISTRY PRACTICAL – II		8
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	I & II	5	90

**Course 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 hydrolysis).
  - d) *p*-nitroaniline from acetanilide (nitrogen and hydrolysis).
  - e) benzoic 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 Learning 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", 5<sup>th</sup> Ed., Longman Scientific & technical, England, **1989**.

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SUBJECT CODE	TITLE OF THE PAPER		ELECTIVE
P22CH10E	GREEN AND ENVIRONMENTAL CHEMISTRY		2
YEAR	SEMESTER	CREDITS	LECTURE HOURS
I	II	4	90

**Course 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 understand the concepts and applications of ionic liquids, PTC and super critical CO<sub>2</sub>
4. To learn about the possible sources of agricultural pesticides its mode of transport and accumulation and its impacts on human health.
5. To improve their knowledge of basic information of radio active decay and permissible radiation dose.

**UNIT I: Introduction to Green Chemistry**

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**

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<sub>2</sub> in Green Synthesis**

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<sub>2</sub>**- phase diagram - uses in extracting natural products, dry

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cleaning, bromination, Kolbe-Schmidt synthesis -Friedel-crafts reaction. Dimethyl carbonate as a methylating agent in green synthesis.

**UNIT IV: Agriculture pollution and Waste management**

Pesticides - General aspects of classification in terms of chemical nature and generation wise. Bio-accumulation and bio- magnification of pesticides - Fate of insecticides in environment and environmental hazards - Toxicity of DDT, gammexene and malathion - Safer pesticides - IPM - Environmental hazards arising from fertilisers - Minimisation of environmental problems caused by fertilizers. Waste management Sources and types of waste - Waste treatment and disposal of waste - integrated waste management (IWM) - supercritical water oxidation (SCWO) of wastes - problems of e-waste and solution for e-waste.- Integrated waste management of plastics -illustration of 4R's.

**UNIT V: Radioactive Pollution**

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 learning Outcomes:**

**The student gained knowledge about**

1. Twelve principles of green chemistry.
2. Importance of eco-friendly synthesis using microwave and biocatalyst.
3. Synthesis and applications of PTC, ionic liquid and super critical CO<sub>2</sub>.
4. Increase the use of environmentally friendly practices in reducing agricultural pollution.
5. 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 Edition, **2008**.
2. V. K. Ahluwalia and M. Kidwai, "*New Trends in Chemistry*", Anamaya Publishers, 2<sup>nd</sup> Edition, **2007**.
3. V. Kumar, "*An Introduction to Green Chemistry*", Vishal Publishers, 1 Edition, **2007**.
4. V. K. Ahluwalia and R. S. Varma, "*Green Solvents*", for organic synthesis Narosa Publishing, 1<sup>st</sup> Edition, **2009**.
5. V. K. Ahluwalia and Renu Aggarwal, "*Organic Synthetic Special Techniques*", Narosa, 2<sup>nd</sup> Edition, **2009**.

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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. 1<sup>st</sup> Edition **2009**.
10. Erach Bharucha, "*Text book of Environmental studies*", University press 2<sup>nd</sup> Edition , **2013**.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH11	ORGANIC CHEMISTRY-II		9
YEAR	SEMESTER	CREDITS	LECTURE HOURS
II	III	5	90

**Course Objectives:**

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

**UNIT I: Nucleophilic Substitution Reaction (18 hours)**

Aliphatic Nucleophilic Substitution, Aromatic Nucleophilic Substitution and Aliphatic Electrophilic Substitution  $S_N1$ ,  $S_N2$ ,  $S_Ni$  mechanisms – stereo chemical 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  $\pi$  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, Meerwein, Dienone-phenol, Wolff, Favorski, Stevens, Sommelet Hauser, Demjenov, Von-Richter,

Schmidt, Pummerer rearrangements. Mechanisms of  $E^1$ ,  $E^2$ ,  $E^1CB$  - stereochemistry of elimination -competition between elimination and substitution pyrolytic cis elimination - chugaev reaction dehydration - 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 -  $1^\circ$ ,  $2^\circ$ ,  $3^\circ$  and quaternary structure of proteins, Chemistry of oxytocin- denaturation of proteins - biosynthesis of proteins. Nucleotides and Nucleosides - DNA -  $1^\circ$  and  $2^\circ$  structure- RNA (*m*-RNA, *t*-RNA and *r*-RNA) genes - genetic code and information storage-Replication of DNA, DNA damages, mutation and repair- determination of base sequence of DNA - polymerase chain reactions and RT-PCR. Synthesis and reactions of pyrazoles, oxazoles, thiazole, imidazole, pyridazine, pyrimidine, purines and pyrazines.

**Course Learning Outcomes:**

1. Students learn the techniques of studying the mechanisms of reactions and to understand the nucleophilic substitution and electrophilic substitution reactions shown by organic molecules.
2. Students learn the addition reactions in carbon-carbon unsaturated bonds and carbon-hetero atom multiple bonds.
3. Students have sufficient knowledge on the mechanisms of elimination reactions and their name reactions.
4. Students get to know the classifications, mechanisms and applications of various molecular rearrangements.
5. Students get to know about DNA, Genetic code, mutation, PCR and RTPCR

**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" Addison-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, 5<sup>th</sup> Ed., (**2006**).

**Reference Books:**

1. Structure and Mechanisms, F. Carey, R. Sundberg, "Advanced Organic Chemistry. Part-A". 4<sup>th</sup> Ed., Kluwer Publishers, **2000**.



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2. Michael B. Smith, J. March, "*March's Advanced Organic Chemistry*", John Wiley & Sons, 6<sup>th</sup> 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<sup>th</sup> Ed., **2000**.
5. M. B. Smith, "*Organic Synthesis*", Academic Press, Elsevier, 3<sup>rd</sup> Ed., **2010**.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH12	ELECTROCHEMISTRY AND SPECTROSCOPY		10
YEAR	SEMESTER	CREDITS	LECTURE HOURS
II	III	5	90

**Course Objectives:**

1. To understand Debye-Huckel theory, working of primary and secondary batteries and fuel cells.
2. To get knowledge about electro kinetic phenomena and corrosion.
3. To learn the concepts of polarographic and cyclic voltametric techniques.
4. To learn in detail rotational, vibrational and electronic spectra of molecules.
5. To study the concepts involved in NMR and ESR spectroscopy

**UNIT I: Electrochemistry-I**

**(18 hours)**

**Ionic:** 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<sub>2</sub>-O<sub>2</sub> and Hydrocarbon-Oxygen fuel cells.

**UNIT II :Electrochemistry-II**

**(18 hours)**

**Electrokinetic Phenomena:** Theories of electrical double layer-Theory of multiple layers at electrode electrolyte interface-electrokinetic phenomena. Processes at electrodes-the rate of charge transfer-current density-Butler-Volmer equation-Taft equation. Electrochemical corrosion-construction and use of Pourbaix and Evans diagram-prevention of corrosion-electrochemical oxidation and reduction.

**Unit III: 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 IV: 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. Infrared spectra-vibrational spectra-selection rules-harmonic

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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 V: 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 -<sup>13</sup>CNMR– 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.

**Course Learning outcomes:**

**The students will be able to**

1. Account for the interactions between the different ions, which are the primary cause of differences between the properties of dilute electrolyte solutions and those of so-called ideal solutions; the types of batteries and their applications;. cost effective and environmentally friendly solutions to improving our energy needs.
2. Understand electrophoresis, electro osmosis, streaming potential and similar electro kinetic phenomena; apply Taft equation to physical organic chemistry in the study of reaction mechanisms and in the development of quantitative structure–activity relationships for organic compounds; prevent corrosion.
3. Learn polarographic technique and cyclic voltammetric technique and to interpret the result; to study qualitative information about electrochemical processes under various conditions, such as the presence of intermediates in oxidation-reduction reactions, the reversibility of a reaction.
4. Learn to characterize and identify compounds that works by measuring the vibrations of compounds..
5. To study free radicals and other species by using ESR spectroscopy and NMR spectroscopy.

**Text Books:**

1. G. N. Barrow, Introduction to Molecular Spectroscopy, International Mc. Graw Hill Ed., (1993), **(UNIT IV & V)**
2. A. P. Straughan and S. Walker, Spectroscopy, Vol. I to III, Chapman Hall, London (1976), **(UNIT IV)**
3. C.N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy” Tata-McGraw-Hill Education, 4th Ed., 1994. **(UNIT IV & V)**

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4. P. W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford, 1983.(**ALL UNITS**)
5. A. S. Glasstone, Introduction to Electrochemistry, Affiliated East-West Press, 1968. (UNIT IV) R. Crow, Electrochemistry (**UNIT I, II & III**)

**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.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH13P	PHYSICAL CHEMISTRY PRACTICAL-I		11
YEAR	SEMESTER	CREDITS	LECTURE HOURS
II	III & IV	5	90

**Course Objectives:**

1. To understand the sequence of reactions and determine the reaction rates
2. To infer the composition, temperature of eutectic mixture applying phase rule.
3. To acquire knowledge of the extent of adsorption of carboxylic acid over charcoal.

**Experiments:**

1. Kinetics-Acid hydrolysis of ester-Comparison of strengths of acids.
2. Kinetics-acid hydrolysis of Ester-Determination of energy of activation ( $E_a$ ).
3. Kinetics-Saponification of Ester-Determination of  $E_a$  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.

**Course Learning Outcomes:**

After studying the principle and carrying out the practical the student will be able to

1. Understand the reaction kinetics, catalysis and influence of catalysts.
2. Evaluate the characteristic of various system based on phase rule.
3. Know about adsorption, extent of adsorption, quantitative determination of it various isotherms.

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**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*", 20<sup>th</sup> Ed., GOEL publishing House, Krishna Pakashan Media Ltd., (**2001**).
4. Findlay's "*Practical Physical Chemistry*" Revised and edited by B. P. Levitt 9<sup>th</sup> Ed., Longman, London, **1985**.
5. J. N. Gurtu and R. Kapoor, "*Advanced Experimental chemistry*", Vol. I. Chand & Co., Ltd, New Delhi.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
<b>P22CH14E</b>	<b>SPECTRAL TECHNIQUES IN INORGANIC COMPOUNDS</b>		<b>12</b>
<b>YEAR</b>	SEMESTER	CREDITS	LECTURE HOURS
<b>II</b>	<b>III</b>	<b>4</b>	<b>90</b>

**Course Objectives:**

1. To learn the theoretical aspects and applications 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  $\beta$  for octahedral complexes ( $Ti^{2+}$  and  $Ni^{2+}$  only) - application to transition, lanthanide and actinide complexes - 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) - spectra of gases - Applications of IR and Raman spectroscopy to coordination and organometallic complexes - 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 ( $^1H$ ,  $^{19}F$ ,  $^{31}P$ ,  $^{13}C$ ,  $^{29}Si$ ,  $^{119}Sn$ ,  $^{183}W$ ) - 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

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chemical exchange - study of fluxional behavior of molecules - an elementary treatment of second order spectra - spin tickling and spin decoupling - the nuclear overhauser effect and gated 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 McConnell 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-  $[\text{Cu}(\text{O}_2\text{C}_8\text{H}_7\text{O})_2(\text{H}_2\text{O})_2]$  - Multiple resonance in EPR.

**Magnetic properties:** Types of magnetism-Dia-para-ferro and antiferro magnetism. Magnetic properties of free ions - first order Zeeman effect - Second order Zeeman effect - states  $KT$  - states  $\ll KT$ - 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 - application of metamagnetism to coordination complexes.

**UNIT V: Mossbauer and NQR spectroscopy (18 hours)**

**Mossbauer Spectroscopy:** Isomer shift - Doppler effect - magnetic interactions Mossbauer emission spectroscopy - application to  $^{57}\text{Fe}$ ,  $^{119}\text{Sn}$ ,  $^{197}\text{Au}$  and  $^{129}\text{I}$  compounds - Mossbauer spectrum of iron carbonyl compound and  $[\text{Fe}_4(\mu_4\text{-O})(\mu\text{-MeO})_4(\text{bisi})_4](\text{ClO}_4)_2 \cdot 4\text{MeOH}$ . Time and temperature-dependant effects.

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

**Course Learning Outcomes:**

1. Investigate the theoretical background and applications of electronic spectroscopy.
2. Examine the structure of inorganic molecules using IR and Raman spectroscopy.
3. Reveal the structure of coordination and organometallic complexes by learning about the NMR of various nuclei.
4. Understand the principles and uses of EPR and magnetic characteristics.
5. Convey knowledge of NQR and Mossbauer spectroscopy for certain inorganic compounds.

**Text Books:**

1. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd edn., **1965**, Wiley Eastern company, London.
2. R. S. Drago, Physical Methods in Chemistry, **1977**, W.B. Saunders Company, Philadelphia, USA.



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3. F. A. Cotton and G. Wilkinson, "Advanced Inorganic Chemistry" 5th edn., **1990**, Wiley- Interscience Publication, New York.
4. Nakamoto, "Infrared Spectra of Inorganic and coordination compounds, 2nd edn., **1970**, Arnold, London.
3. E. A. V. Ebsworth, D. W. H. Rankin, S. Cradock, "Structural methods in Inorganic Chemistry", 1st edn., **1988**, ELBS Great Briton.
4. C. N. Banwell, Fundamentals of molecular spectroscopy, 3rd edn., **1983**, TMH, New Delhi.
5. J. Lewis and R. G. Wilkins, "Modern Coordination Chemistry – Principles and Methods", **1960**, Interscience Publishers, New York.
6. P. J. Wheatley, "The Determination of Molecular Structure", **1970**, Clarendon, Oxford.
7. G. M. Barrow, "Introduction to Molecular Spectroscopy," **1962**, McGraw-Hill Book, New York.
8. A. E. Gillan and E. S. Stern, "Electronic Absorption spectroscopy of inorganic compounds", Wiley, New York.
9. J. D. Roberts, "High Resolution Nuclear Magnetic Resonance", McGraw- Hill, New York.
10. T. P. Das and E. L. Hahn, "Nuclear Quadrupole Resonance Spectroscopy", **1958**, Academic Press, New York.
11. H. E. Duckworth, "Mass Spectroscopy", 2<sup>nd</sup> edn., **1990**, Cambridge University Press, New York.
12. B. N. Figgis and J. Lewis, "The Magnetic properties of transition metal complexes" in Progress in Inorganic Chemistry", Vol. 6, edn. Interscience, Publication, New York.
13. L. M. Epstein, J. Chem. Phys., 36 (**1962**) 2731.
14. B. Kozlevcar et al., Croat. Chem. Acta, 81 (**2008**) 369.
15. R. Pettinari et al., Dalton Trans., 44 (**2015**) 20523.

**Reference Books:**

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

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SUBJECT CODE	TITLE OF THE PAPER		ELECTIVE
P22CH15E	BASIC STRATEGIES OF NANOMATERIALS AND SYNTHETIC ORGANIC CHEMISTRY		4
YEAR	SEMESTER	CREDITS	LECTURE HOURS
II	IV	4	90

**Course 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, Classifications and types of nanomaterials as nano particles and 1D 2D 3D nanomaterials. Concept of bulk versus nanomaterials. Introduction to 'Top down' vs. 'Bottom up' approach of synthesis with suitable examples.

**Chemical Routes for synthesis of Nanomaterials:** Sol-gel synthesis, and Microwave heating synthesis. **Physical Routes for synthesis of Nanomaterials:** Bottom up-Ball Milling, Physical vapour deposition and Electrochemical approaches. Spin coating - Thin films - Epitaxy Quantum Dots. **Applications of nanomaterials:** Applications of nano-biotechnology in early medical diagnostics, in energy sector and in ceramics industries.

**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, **Pressure effects in Nanotubes** 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

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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 retrosynthetic analysis and disconnection approach - relay and convergent synthesis- linear synthesis- Synthesis of amines 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, Protecting groups for carbonyl compounds( aldehydes and ketones- Acyclic acetals, ketals and cyclic ketals as protecting groups for carbonyl compounds. C-C disconnections – Diels-Alder reaction and Robinson annulation – chemoselectivity (guidelines).

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

**Oxidation reactions:** CrO<sub>3</sub>, PDC, PCC, KMnO<sub>4</sub>, MnO<sub>2</sub>, SeO<sub>2</sub>, Pb(OAc)<sub>4</sub> Swern, OsO<sub>4</sub>, m-CPBA, O<sub>3</sub>, **Reduction reactions:** Catalytic Hydrogenation, LAH, NaBH<sub>4</sub>, LiAlH(OBu)<sub>3</sub>, NaCNBH<sub>3</sub>, Bu<sub>3</sub>SnH, LDA, Me<sub>2</sub>CuLi, MPV, H<sub>2</sub>/Pd-C, [(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>P]<sub>3</sub>RhCl, NH<sub>2</sub>NH<sub>2</sub>, DIBAL-H.

**Course Learning 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 Scientific series in nano science and Nanotechnology, Nanotechnology, Vol 12, 2nd Edn Jan **2011**. Imperial 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**)
6. T. Pradeep, Nano: The Essentials, McGraw Hill Education, 3rd Ed., **2009** (**Unit-I & Unit III**)
7. H. S. Nalwa, Handbook of Nanostructures: Materials and Nanotechnology,

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- Vol 1-5, Academic Press, Bostan, Oct **1999**, 1st Ed., (**Unit-I**)
8. M. Reza Mozafari, nanomaterials and nanosystems for biomedical applications, Springer, **2013**. (**Unit-II**)
  9. David S. Goodsell, Bionanotechnology, Wiley-Sciences, **2013** (**Unit-II**)
  10. H. Gleiter, Nanostructured Materials: Basic Concepts, Microstructure and Properties **2000**. (**Unit-II**)
  11. T. Tang and P. Sheng (Eds): Nano Science and Technology Novel Structures and Phenomena, Taylor & Francis, New York, 1<sup>st</sup> Ed., **2004**. (**Unit-II**)
  12. C. N. R. Rao, A. Muller, A. K. Cheetam (Ed.), The Chemistry of Nanomaterials, Vol. 1,2 Wiley- VCH, Weinheim, **2014** (**Unit-III**)
  13. Carbon Nanotubes: Properties and Applications- Michael J. O'Connell, 1<sup>st</sup> Ed., **2006**.
  14. Nanotubes and Nanowires- CNR Rao and A Govindaraj RCS Publishing
  11. Nanoscale materials -Liz Marzan and Kamat **2011**.
  15. Stuart Warren, Organic synthesis - The disconnection Approach, John Wiley & sons, **2004** (**Unit-IV**).
  16. Raymond K. Mackie & David M. Smith, Guidebook to Organic synthesis, **1994** (**Unit - IV**)
  17. Jagdamba Singh and L. D. S. Yadav, Organic Synthesis, Pragati Prakashan, **2011** (**Unit - IV**)
  18. W. Carothers, Some modern methods of organic synthesis, Cambridge University Press, **1993** (**Unit - IV**)
  19. H. O. House, Modern Synthetic Reactions, Allied Publishers, **1985** (**Unit - V**)
  20. V. K. Ahluwalia 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, 6<sup>th</sup> Ed., **2007**.
4. J. Clayden, N. Greeves, P. Wothers, "Organic Chemistry", Oxford University Press, **2001**.

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SUBJECT CODE	TITLE OF THE PAPER		CORE
<b>P22CH16</b>	<b>ORGANIC CHEMISTRY-III</b>		<b>12</b>
<b>YEAR</b>	SEMESTER	CREDITS	LECTURE HOURS
<b>II</b>	<b>IV</b>	<b>5</b>	<b>90</b>

**Course Objectives:**

1. To understand the principle behind pericyclic reactions and the concept of ORD\_CD
2. To know the importance of photochemical reactions and ESR spectroscopy
3. To learn about the applications of NMR and CMR of organic compounds
4. To understand the applications of UV, IR and Mass spectrometry.
5. To study the structure of the organic compounds and about the importance of terpenes.

**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 electrocyclic reactions ( $4n$  and  $4n+2$ ) system and cycloaddition reactions ( $2+2$  and  $4+2n$  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- $\pi$ -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 ( $C_6H_6^-$ ,  $p$ -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<sub>2</sub>) - Nuclear Overhauser Effect 2-D techniques (COSY, NOESY and ROSY).

<sup>13</sup>C 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 <sup>13</sup>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 -  $\alpha$ - $\beta$ - 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 Terpenes (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-Carbonyl compounds 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, **Terpenes:** Definition, Classification, isoprene rule, isolation and UV quantification of terpenoids, - biological activity- structure elucidation of zingiberin, camphor.

**Course Learning Outcomes:**

1. Students understand applications of pericyclic reactions.
2. Students understand the structural and stereochemical implications on photochemical reactions.
3. Students learn the principles, techniques and applications the of ESR and NMR spectroscopy for the structural elucidations
4. Students learn concepts and applications of UV-Vis, IR and Mass spectroscopy.
5. Students gains knowledge about classification, isoprene rule and biological activity of terpenes.

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**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**.
9. O. P. Agarwal, "*Chemistry of Organic Natural Products*", Volume I & II, Goel Publishers, **2014**.

**Reference Books:**

1. Structure and Mechanisms, F. Carey, R. Sundberg, "*Advanced Organic Chemistry. Part-A*". 4<sup>th</sup> Ed., Kluwer Publishers, **2000**.
2. Michael B. Smith, J. March, "*March's Advanced Organic Chemistry*", John Wiley & Sons, 6<sup>th</sup> 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<sup>th</sup> Ed., **2000**.
5. M. B. Smith, "*Organic Synthesis*", Academic Press, Elsevier, 3<sup>rd</sup> Ed., **2010**

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SUBJECT CODE	TITLE OF THE PAPER		CORE
P22CH17P	PHYSICAL CHEMISTRY PRACTICAL-II		13
YEAR	SEMESTER	CREDITS	LECTURE HOURS
II	III & IV	5	90

**Course Objectives:**

1. To study the various types of titrations conductometrically.
2. To determine the dissociation constants of organic acids.
3. To carry out various titrations potentiometrically.
4. To determine the solubility of sparingly soluble salts via conductometric and potentiometric methods.

**Experiments:**

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

**Course Learning Outcomes:**

The students will gain experience and will

1. Understand the salient features and merits of conductometric titrations
2. Determine the dissociation constants of organic acids.
3. Analyse the solubility of sparingly soluble salts.



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4. Appreciate the advantages of conductometric and potentiometric methods over conventional methods of estimations.

**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<sup>th</sup> Ed., GOEL publishing House, Krishna Pakashan Media Ltd., (**2001**).
4. Findlay's "*Practical Physical Chemistry*" Revised and edited by B. P. Levitt 9<sup>th</sup> Ed., Longman, London, **1985**.
5. J. N. Gurtu and R. Kapoor, "*Advanced Experimental chemistry*", Vol. I. Chand & Co., Ltd, New Delhi.

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SUBJECT CODE	TITLE OF THE PAPER		ELECTIVE
P22CH18E	APPLICATIONS OF QUANTUM CHEMISTRY AND THERMODYNAMICS		5
YEAR	SEMESTER	CREDITS	LECTURE HOURS
II	IV	4	90

**Course Objectives:**

1. To learn the advanced concepts in quantum chemistry.
2. To learn the basics of photoelectron spectroscopy and to apply ESCA and Auger spectroscopy.
3. To understand the thermodynamic properties of real gases and to apply phase rule to three component systems.
4. To learn the concept of partition functions.
5. To study partition functions and non-equilibrium thermodynamics.

**UNIT I: 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 - perturbation method to non-degenerate systems-Hartree Fock Self Consistent Field methods-Many electron atoms-wave function-one electron orbital-Pauli principle and Slater determinant.

**Unit II : Quantum Chemistry and Photoelectron Spectroscopy (18 hours)**

MO and VB treatment of hydrogen molecule-HMO model for systems like ethylene and butadiene - hybridization derivation of wave function 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 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).

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**Unit IV: Statistical Mechanics:**

Distinction between quantum mechanics, statistical mechanics and statistical thermodynamics- probability theorems in statistical thermodynamics- phase space-occupation number – microstate and macrostate -system, assembly and ensemble- the different types of ensembles- statistical equilibrium – thermodynamical probability- Boltzmann distribution law – partition function – physical significance of partition function-translational partition function- rotational partition function , vibrational partition function – electronic partition function – total partition function – partition functions and thermodynamic functions - - internal energy –heat capacity-entropy and probability- Boltzmann Planck’s equation – applications of partition functions to monoatomic gases and to diatomic molecules-statistical expression for equilibrium constant- equipartition of energy – limitations of Maxwell-Boltzmann statistics

**UNIT-V: IRREVERSIBLE THERMODYNAMICS AND QUANTUM STATISTICS**

**(18 hours)**

Introduction- Postulate of local equilibrium – entropy production – forces and fluxes- Onsager equations and applications - -linear law, Onsager reciprocal relations – application of Onsager relation-stationary states.

**QUANTUM STATISTICS:** Bose-Einstein statistics – applications of B-E statistics to photon gas and superfluidity of liquid helium - Fermi-Dirac statistics-Application of FD statistics to electron gas and thermionic emission.- Comparison of Maxwell-Boltzmann statistics, Bose-Einstein statistics and Fermi-Dirac statistics.

**Course Learning Outcomes:**

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

1. Gain knowledge on advanced concepts in quantum chemistry
2. Apply basics of photoelectron spectroscopy, ESCA and Auger spectroscopy.
3. Understand the thermodynamic properties of real gases and to apply phase rule to three component systems.
4. Understand in detail about Statistical thermodynamics, partition functions.
5. Acquire knowledge on irreversible thermodynamics and quantum statistics.

**Text Books:**

1. G. Aruldhas, Molecular Structure and Spectroscopy, PHI Learning Private Limited, Delhi, , 2<sup>nd</sup> edition,2018.(**UNIT I**)
2. R.K. Prasad, Quantum Chemistry , New Age International Publishers,New Delhi, 2<sup>nd</sup> edition,2002(**UNIT I**).
3. I.N.Levine,*Quantum Chemistry*,AllynandBacon, **1983(UNITI)**
4. P.W.Atkins,*Physical Chemistry*,ELBSandOxfordUniversityPress,Oxford,**1983(U NITSII ,III,IV&V)**
5. J.RajaramandJ.C.Kuriacose,*ThermodynamicsforstudentsofChemistry-Classical*,

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- Statistical and Irreversible,* Shobhan Lal  
Nagin, New Delhi, **1981 (UNITS II & III)**
6. S. Glasstone, *Introduction to Electro Chemistry*, Affiliated East-west Press, **1968 (UNIT IV)**
  7. D. R. Crow, *Polarography of metal complexes*, Academic Press, New York **(UNITS IV & V)**
  8. Gurdeep Raj, "*Advanced physical chemistry*", Meerut publication **(UNIT IV)**
  9. D.N. Bajpai, *Advanced Physical chemistry*.
  10. F. A. Cotton, *Chemical Applications of Group Theory*, 2nd Ed., Wiley Eastern **1971. (UNIT I)**
  11. A. K. Chandra, *Introductory Quantum Chemistry*, 4th Ed., Tata McGraw Hill, **1994. (UNIT II)**
  12. R. K. Prasad, *Quantum Chemistry*, 2nd Ed., New Age International Publishes (2000). **(UNIT II)**
  13. D. A. Mcquarrie, *Quantum Chemistry*, University Science Books, **1983. (UNIT II)**
  14. J. P. Lowe, *Quantum Chemistry*, Academic Press, **1978. (UNIT II)**
  15. I. N. Levine, *Quantum Chemistry*, Allyn and Bacon, **1983. (UNIT II)**

Semester	Course code	Title of the Course	Hours	Credits
I	P22CH1	CORE 2: SYNTHETIC AND STRUCTURAL INORGANIC CHEMISTRY	6	5
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	On successful completion of this course, students will be able to			
CO-1	acquire the knowledge chemistry and structure of Boron, Sulphur and Nitrogen chain compounds			K1
CO-2	understand the structure of ionic compounds and mechanism of solid- state reactions			K2
CO-3	understand the crystal systems by X-ray diffraction methods			K2
CO-4	apply the essential concepts of several crystal systems using X-ray diffraction techniques.			K3
CO-5	analyze the various structures of ionic compounds and solid-state reaction mechanisms			K4
CO-6	evaluation the types of isomers, reaction mechanism and applications of coordination compounds			K5

Semester	Course code	Title of the Course				Hours	Credits
I	P22CH1	CORE 2: SYNTHETIC AND STRUCTURAL INORGANIC CHEMISTRY				6	5
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self- directed lifelong learning.	
CO1-K1- Remembering	9	9	9	9	9	9	
CO2-K2- Understanding	9	9	9	9	9	9	
CO3-K2- Understanding	9	9	9	9	9	9	
CO4-K3-Applying	9	3	9	9	3	3	
CO5-K4-Analyzing	9	9	3	3	3	3	
CO6-K5-Evaluating	9	3	3	3	3	3	
Weightage	54	42	42	42	36	36	
Mapping Correlation	Low		Medium		High		No Correlation
Level of Correlation	1		3		9		0

Semester	Course code	Title of the Course	Hours	Credits
I	P22CH2	CORE COURSE 2 ORGANIC CHEMISTRY – I	5	5
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	acquire the knowledge about IUPAC nomenclature, electronic effects, Reactive Intermediates, determining reaction mechanism, kinetic and non-kinetic methods and Correlation Analysis, organic stereochemistry - geometrical and Optical isomerism, dynamic Stereochemistry and about the importance of carbohydrates, antibiotics, steroids and alkaloids.			<b>K1</b>
<b>CO-2</b>	understand the basic concepts of electronic effects, reactive intermediates and its structure and stability, organic stereochemistry and isomerism -both geometrical and optical isomerism			<b>K2</b>
<b>CO-3</b>	apply the electronic effects and elucidate reaction mechanism ,categorize organic compounds as R & S notations, E & Z notations, sort out as cis and trans nomenclature of 3,4,6 membered substituted cyclic systems, decalins.			<b>K3</b>
<b>CO-4</b>	analyze and correlate the linear free energy relations, examine stereochemistry of overcrowded molecules, correlate between conformation and reactivity			<b>K4</b>
<b>CO-5</b>	evaluate kinetic and non-kinetic methods of reaction, spectroscopic studies and energy profile diagrams, Newmann, sawhorse and fisher projections, dipole moment, optical purity, neighbouring group participation			<b>K5</b>
<b>CO-6</b>	conceive the importance of carbohydrates, antibiotics, steroids and alkaloids			<b>K6</b>

Semester	Course code	Title of the Course				Hours	Credits
I	P22CH2	CORE COURSE 2 ORGANIC CHEMISTRY – I				5	5
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning.	
CO1-K1-Remembering	9	9	9	9	3	3	
CO2-K2-Understanding	9	9	9	9	1	3	
CO3-K3-Applying	9	9	9	9	9	3	
CO4-K4-Analyzing	9	9	9	9	3	3	
CO5-K5-Evaluating	9	9	9	9	1	9	
CO6-K6-Creating	9	3	3	3	3	9	
Weightage	54	48	48	48	20	36	
Mapping Correlation	Low		Medium		High		No Correlation
Level of Correlation	1		3		9		0



Semester	Course code	Title of the Course	Hours	Credits
I&II	P22CH3P	CORE 3: INORGANIC CHEMISTRY PRACTICAL - I	90	5
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	acquire the knowledge about cation, anion, and interfacial radicals			<b>K1</b>
<b>CO-2</b>	understand the basic concepts of qualitative analysis			<b>K2</b>
<b>CO-3</b>	understand the basic concepts of Quantitative analysis			<b>K2</b>
<b>CO-4</b>	apply the instrumentation concept in Photocolorimeter			<b>K3</b>
<b>CO-5</b>	analyze the various inorganic cation in a mixture			<b>K4</b>
<b>CO-6</b>	evaluation the amount of inorganic ions present in a sample			<b>K5</b>

Semester	Course code	Title of the Course			Hours	Credits
I&II	P22CH3P	CORE 3: INORGANIC CHEMISTRY PRACTICAL - I			90	5
Course Outcome (COs)	Programme Outcomes (POs)					
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning.
CO1-K1-Remembering	9	9	9	9	9	9
CO2-K2-Understanding	9	9	9	9	9	9
CO3-K2-Understanding	9	9	9	9	9	9
CO4-K3-Applying	9	9	9	9	9	9
CO5-K4-Analyzing	9	9	3	3	3	3
CO6-K5-Evaluating	3	3	3	3	3	3
Weightage	51	51	48	48	48	48
Mapping Correlation	Low		Medium		High	No Correlation
Level of Correlation	1		3		9	0

Semester	Course code	Title of the Course	Hours	Credits
I&II	P22CH4P	CORE COURSE-4 ORGANIC CHEMISTRY PRACTICALS-I	6	5
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	Separate the organic compounds from the binary mixtures			<b>K1</b>
<b>CO-2</b>	Specify the functional groups present on each of the organic compounds.			<b>K2</b>
<b>CO-3</b>	Examine the methods of qualitative analysis of an organic compounds			<b>K2</b>
<b>CO-4</b>	Determine the micro level analysis of an organic compounds			<b>K3</b>
<b>CO-5</b>	Develop steps to prepare single stage preparation of organic compounds			<b>K4</b>
<b>CO-6</b>	Formulate the derivatives of the organic functional groups.			<b>K5</b>

Semester	Course code	Title of the Course				Hours	Credits
I&II	P22CH4P	CORE COURSE-4 ORGANIC CHEMISTRY PRACTICALS-I				6	5
<b>Programme Outcomes (POs)</b>							
Course Outcome (COs)	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning	
CO1-K1-Remembering	9	9	9	9	9	9	
CO2-K2-Understanding	9	9	9	9	9	9	
CO3-K2-Understanding	9	9	9	9	9	3	
CO4-K3-Applying	9	9	9	3	3	9	
CO5-K4-Analyzing	9	9	9	3	3	3	
CO6-K5-Evaluating	9	3	9	1	3	3	
<b>Weightage</b>	54	48	54	34	36	36	
<b>Mapping Correlation</b>	<b>Low</b>		<b>Medium</b>		<b>High</b>		<b>No Correlation</b>
<b>Level of Correlation</b>	1		3`		9		0

Semester	Course code	Title of the Course	Hours	Credits
I	P22CH-5E	<b>ELECTIVE COURSE 1: ADVANCED TECHNIQUES AND COMPUTER APPLICATIONS IN CHEMISTRY</b>	90	4
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	acquire the knowledge of error analysis and instrumental methods			<b>K1</b>
<b>CO-2</b>	understand the separation and purification of organic and inorganic compounds			<b>K2</b>
<b>CO-3</b>	understand the concepts of thermal methods and fluorescence spectroscopy, comprehends the fundamental concepts of molecular modeling.			<b>K2</b>
<b>CO-4</b>	able to use computers for research in chemistry; to use C language and to apply it to chemistry			<b>K3</b>
<b>CO-5</b>	analysis the properties of materials by thermoanalytical method			<b>K4</b>
<b>CO-6</b>	evaluate the Retention Factor $R_f$ (Capacity Factor) and selectivity factor			<b>K5</b>

Semester	Course code	Title of the Course				Hours	Credits
I	P22CH-5E	<b>ELECTIVE COURSE 1: ADVANCED TECHNIQUES AND COMPUTER APPLICATIONS IN CHEMISTRY OR PRACTICAL-I-VOLUMETRIC ANALYSIS</b>				90	4
Course Outcome (COs)	<b>Programme Outcomes (POs)</b>						
	<b>PO1 Disciplinary Knowledge</b>	<b>PO2 Communication Skills</b>	<b>PO3 Critical Thinking, Problem Solving and Analytical Reasoning</b>	<b>PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.</b>	<b>PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.</b>	<b>PO6 Multicultural competency and Self- directed lifelong learning.</b>	
<b>CO1-K1- Remembering</b>	9	9	9	9	9	9	
<b>CO2-K2- Understanding</b>	9	9	9	9	9	3	
<b>CO3-K3-Applying</b>	9	9	9	9	3	3	
<b>CO4-K4-Analyzing</b>	9	9	9	3	3	3	
<b>CO5-K5-Evaluating</b>	9	9	3	3	3	3	
<b>CO6-K6-Creating</b>	9	3	3	3	3	3	
<b>Weightage</b>	54	48	42	36	30	24	
<b>Mapping Correlation</b>	<b>Low</b>		<b>Medium</b>		<b>High</b>		<b>No Correlation</b>
<b>Level of Correlation</b>	1		3		9		0

Semester	Course code	Title of the Course	Hours	Credits
II	P22CH6	QUANTUM CHEMISTRY, GROUP THEORY AND CHEMICAL KINETICS	6	5
Course Outcome (COs)	CO-Statement			Cognitive Level
	On successful completion of this course, students will be able to			(K-Level)
CO-1	acquire the knowledge about quantum mechanics, group theory, photochemistry and radiation chemistry			K1
CO-2	Understand the basics of chemical kinetics, its techniques and surface phenomena			K2
CO-3	Understand the fast reaction techniques and adsorption			K2
CO-4	Apply the group theory and find the hybridization of atomic orbitals			K3
CO-5	analyze the theories of reaction rate and factors influencing reaction rate in solution			K4
CO-6	evaluation of role of surface in catalysis by Langmuir-Hinshelwood, Langmuir-Rideal and Rideal-Eley mechanisms			K5

Semester	Course code	Title of the Course			Hours	Credits	
II	P22CH6	QUANTUM CHEMISTRY, GROUP THEORY AND CHEMICAL KINETICS			6	5	
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning.	
CO1-K1-Remembering	9	3	9	3	3	9	
CO2-K2-Understanding	9	3	9	3	3	9	
CO2-K2-Understanding	9	3	9	3	9	9	
CO3-K3-Applying	9	3	3	3	3	3	
CO4-K4-Analyzing	9	3	9	3	3	9	
CO5-K5-Evaluating	3	1	3	0	1	1	
Weightage	48	16	42	15	22	40	
Mapping Correlation	Low		Medium		High		No Correlation
Level of Correlation	1		3		9		0



Semester	Course code	Title of the Course	Hours	Credits
II	P22CH7	<b>CORE COURSE-VI</b> Reaction Mechanism in Coordination And Organometallic Chemistry	6	5
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	acquire the knowledge about coordination compounds and organometallic compounds			<b>K1</b>
<b>CO-2</b>	understand the key features and various theories of coordination compounds			<b>K2</b>
<b>CO-3</b>	understand the biological role and mechanism of bioinorganic complexes			<b>K2</b>
<b>CO-4</b>	Identify bond-to-metal complexes and fundamental reactions in organometallic chemistry			<b>K3</b>
<b>CO-5</b>	analysis the stability of metal complexes, types of isomers and reaction mechanism in coordination compounds			<b>K4</b>
<b>CO-6</b>	evaluate the properties of inorganic and organic materials			<b>K5</b>

Semester	Course code	Title of the Course				Hours	Credits
II	P22CH7	CORE COURSE-VI Reaction Mechanism in Coordination And Organometallic Chemistry				6	5
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self- directed lifelong learning.	
CO1-K1- Remembering	9	9	9	9	9	9	
CO2-K2- Understanding	9	9	9	9	9	9	
CO2-K2- Understanding	9	9	9	9	9	9	
CO3-K3-Applying	9	9	3	3	9	9	
CO4-K4-Analyzing	9	9	3	3	3	9	
CO5-K5-Evaluating	9	3	3	3	3	3	
Weightage	54	48	36	36	42	48	
Mapping Correlation	Low		Medium		High		No Correlation
Level of Correlation	1		3		9		0

Semester	Course code	Title of the Course	Hours	Credits
I&II	P22CH8P	CORE 7: INORGANIC CHEMISTRY PRACTICAL - II	90	5
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
CO-1	acquire the knowledge about the separation of ions in a mixture			K1
CO-2	understand the volumetric estimation of some inorganic cations			K2
CO-3	understand the gravimetric techniques			K2
CO-4	apply the Infrared, UV / Vis spectroscopic techniques to characterization of coordination complexes			K3
CO-5	analyze the coordination compounds			K4
CO-6	estimation of ions by separating them in a mixture			K5

Semester	Course code	Title of the Course				Hours	Credits
I&II	P22CH8P	CORE 7: INORGANIC CHEMISTRY PRACTICAL - II				90	5
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self- directed lifelong learning.	
CO1-K1- Remembering	9	9	9	9	9	9	
CO2-K2- Understanding	9	9	9	9	9	9	
CO2-K2- Understanding	9	9	9	9	9	9	
CO3-K3-Applying	9	9	9	9	9	9	
CO4-K4-Analyzing	9	9	3	3	3	3	
CO5-K5-Evaluating	3	3	3	3	3	3	
Weightage	51	51	42	42	42	42	
Mapping Correlation	Low		Medium		High		No Correlation
Level of Correlation	1		3		9		0

Semester	Course code	Title of the Course	Hours	Credits
I & II	P22CH9P	<b>CORE COURSE 8: ORGANIC CHEMISTRY PRACTICAL-II</b>	6	5
<b>Course Outcome (COs)</b>	<b>CO-Statement</b>			<b>Cognitive Level (K -Level)</b>
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	describe the principles of quantitative analysis in organic chemistry.			<b>K1</b>
<b>CO-2</b>	understand the procedure for estimation of organic compounds.			<b>K2</b>
<b>CO-3</b>	apply the uses of chromatographic techniques for the synthesized organic compound.			<b>K3</b>
<b>CO-4</b>	prepare organic compounds via single and double stage method and able to carry out the recrystallization.			<b>K4</b>
<b>CO-5</b>	determine the amount of yield obtained.			<b>K5</b>
<b>CO-6</b>	interpret organic compounds using UV and IR spectra.			<b>K6</b>

<b>I &amp; II</b>	<b>P22CH9P</b>	<b>CORE COURSE 8: ORGANIC CHEMISTRY PRACTICAL-II</b>	<b>6</b>	<b>5</b>
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<b>Course Outcome (COs)</b>	<b>Programme Outcomes (POs)</b>					
	<b>PO1 Disciplinary Knowledge</b>	<b>PO2 Communication Skills</b>	<b>PO3 Critical Thinking, Problem Solving and Analytical Reasoning</b>	<b>PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.</b>	<b>PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.</b>	<b>PO6 Multicultural competency and Self-directed lifelong learning.</b>
<b>CO1-K1-Remembering</b>	9	9	9	9	9	9
<b>CO2-K2-Understanding</b>	9	9	9	9	9	3
<b>CO3-K3-Applying</b>	9	9	9	9	3	3
<b>CO4-K4-Analyzing</b>	9	9	3	3	3	3
<b>CO5-K5-Evaluating</b>	9	3	3	3	3	3
<b>CO6-K6-Creating</b>	9	3	3	3	3	3
<b>Weightage</b>	54	42	36	36	30	24
<b>Mapping Correlation</b>	<b>Low</b>		<b>Medium</b>		<b>High</b>	<b>No Correlation</b>
<b>Level of Correlation</b>	1		3		9	0

<b>Semester</b>	<b>Course code</b>	<b>Title of the Course</b>	<b>Hours</b>	<b>Credits</b>
<b>II</b>	<b>P22CH10E</b>	<b>GREEN AND ENVIRONMENTAL CHEMISTRY</b>	<b>6</b>	<b>4</b>
<b>Course Outcome (COs)</b>	<b>CO-Statement</b>			<b>Cognitive Level (K-Level)</b>
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	acquire the knowledge about green chemistry and its applications, the environmental hazards of agricultural and radioactive pollution , about waste management , problems of e-waste and 4Rs			<b>K1</b>
<b>CO-2</b>	Understand the goals and principles of green chemistry			<b>K2</b>
<b>CO-3</b>	apply the principles and experiment with microwave and ultrasound methods for organic synthesis, make use of the green techniques to solve the problems arising in synthetic organic chemistry			<b>K3</b>
<b>CO-4</b>	analyze the environmental hazards of agricultural pesticides and diagnose its impacts on human health			<b>K4</b>
<b>CO-5</b>	evaluate the causes of radioactive pollution and recommend new strategies for its prevention			<b>K5</b>
<b>CO-6</b>	create new strategies for reducing the pollution and radioactive hazards ,design methods to reduce waste and fabricate techniques to dispose waste			<b>K6</b>

Semester	Course code	Title of the Course				Hours	Credits
II	P22CH10E	GREEN AND ENVIRONMENTAL CHEMISTRY				6	4
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1	PO2	PO3	PO4	PO5	PO6	
	Disciplinary Knowledge	Communication Skills	Critical Thinking, Problem Solving and Analytical Reasoning	Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	Multicultural competency and Self-directed lifelong learning.	
CO1-K1-Remembering	9	9	3	3	9	9	
CO2-K2-Understanding	9	3	3	3	3	3	
CO3-K3-Applying	9	3	9	3	3	3	
CO4-K4-Analyzing	9	3	9	9	3	9	
CO5-K5-Evaluating	9	9	9	9	9	9	
CO6-K6-Creating	9	9	9	9	9	9	
Weightage	54	36	42	36	36	42	
Mapping Correlation	Low		Medium		High		No Correlation
Level of Correlation	1		3		9		0



Semester	Course code	Title of the Course	Hours	Credits
III	P22CH11	CORE COURSE 9: ORGANIC CHEMISTRY-II	6	5
Course Outcome (COs)	CO-Statement			Cognitive Level ( K -Level)
	On successful completion of this course, students will be able to			
CO-1	understand the criteria for aromaticity and differentiate the aromatic electrophilic and nucleophilic substitution reactions.			K1
CO-2	examine the mechanisms of nucleophilic substitution reactions and describe nucleophilic substitution on aromatic rings.			K2
CO-3	apply the knowledge of reaction mechanism to aliphatic substitution and elimination reactions			K3
CO-4	assess the concept of aromaticity and classify the reactions on aromatic rings.			K4
CO-5	identify the mechanism of preparation and reactions of heterocycles			K5
CO-6	design a detailed mechanism for rearrangement reactions, addition and elimination reactions			K6

Semester	Course code	Title of the Course				Hours	Credits
III	P22CH11	CORE COURSE 9: ORGANIC CHEMISTRY-II				6	5
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning.	
CO1-K1-Remembering	9	9	9	9	9	9	
CO2-K2-Understanding	9	9	9	9	9	9	
CO3-K3-Applying	9	9	9	9	3	3	
CO4-K4-Analyzing	9	9	3	3	3	3	
CO5-K5-Evaluating	9	3	3	3	3	1	
CO6-K6-Creating	9	1	3	3	3	3	
Weightage	54	40	36	36	30	30	
Mapping Correlation	Low		Medium		High	No Correlation	
Level of Correlation	1		3		9	0	

Semester	Course code	Title of the Course	Hours	Credits
III	P22CH14E	<b>CORE COURSE 11: ELECTROCHEMISTRY AND SPECTROSCOPY</b>	6	4
Course Outcome (COs)	CO-Statement			Cognitive Level ( K -Level)
	On successful completion of this course, students will be able to			
CO-1	memorize and retain the basics of various concepts of interactions between the different ions and implement the concepts of solubility products, common ion effects, relate electrode-electrolyte equilibrium and concentration cells			K1
CO-2	understand the underlying principles of electrodicts and spectroscopy.			K2
CO-3	execute the theories of electrode-electrolyte interfaces and kinetics of electrochemical reactions and implements the significance of over voltage and corrosion			K3
CO-4	analyze the intricacies of electrical double layer and evaluate its implications in real life.			K4 & K5
CO-5	correlate the concepts of NMR, ESR, and laser Raman spectroscopy			K5
CO-6	analyse and evaluate the experimental set up and applications of electro analytical techniques.			K5

<b>III</b>	<b>P22CH14E</b>	<b>CORE COURSE 11: ELECTROCHEMISTRY AND SPECTROSCOPY</b>	<b>6</b>	<b>4</b>
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<b>Course Outcome (COs)</b>	<b>Programme Outcomes (POs)</b>					
	<b>PO1 Disciplinary Knowledge</b>	<b>PO2 Communication Skills</b>	<b>PO3 Critical Thinking, Problem Solving and Analytical Reasoning</b>	<b>PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.</b>	<b>PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.</b>	<b>PO6 Multicultural competency and Self-directed lifelong learning.</b>
<b>CO1-K1-Remembering</b>	9	9	9	9	9	3
<b>CO2-K2-Understanding</b>	9	9	9	9	3	3
<b>CO3-K3-Applying</b>	9	9	9	9	3	3
<b>CO4-K4-Analyzing</b>	9	9	3	3	3	3
<b>CO5-K5-Evaluating</b>	9	3	3	1	3	3
<b>CO6-K6-Creating</b>	9	1	3	1	3	3
<b>Weightage</b>	54	40	36	32	24	18
<b>Mapping Correlation</b>	<b>Low</b>		<b>Medium</b>		<b>High</b>	<b>No Correlation</b>
<b>Level of Correlation</b>	1		3		9	0

Semester	Course code	Title of the Course	Hours	Credits
III & IV	P22CH13P	<b>CORE COURSE 11: PHYSICAL CHEMISTRY PRACTICAL-I</b>	6	4
Course Outcome (COs)	CO-Statement			Cognitive Level ( K -Level)
	On successful completion of this course, students will be able to			
<b>CO-1</b>	describe the principles of selected non-electrical experiments.			<b>K1</b>
<b>CO-2</b>	understand the theoretical concepts of each given non-electrical experiments.			<b>K2</b>
<b>CO-3</b>	construct and analyze the graphical output needed for the experiments.			<b>K3</b>
<b>CO-4</b>	predict the observed results and can correlate with their properties.			<b>K4</b>
<b>CO-5</b>	acquire the practical skills by following each steps in the given experiments.			<b>K5</b>
<b>CO-6</b>	create the innovation skills to the students to develop new techniques and apply for new systems in various physical chemistry field like chemical kinetics, surface chemistry, thermochemistry and thermodynamics.			<b>K6</b>

Semester	Course code	Title of the Course	Hours	Credits
III & IV	P22CH13P	CORE COURSE 11: PHYSICAL CHEMISTRY PRACTICAL-I	6	4

Course Outcome (COs)	Programme Outcomes (POs)					
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning.
CO1-K1-Remembering	9	9	9	9	9	9
CO2-K2-Understanding	9	9	9	9	9	3
CO3-K3-Applying	9	9	9	9	3	3
CO4-K4-Analyzing	9	9	3	3	3	3
CO5-K5-Evaluating	9	3	3	3	3	3
CO6-K6-Creating	9	1	3	1	3	3
Weightage	54	40	36	34	30	24
Mapping Correlation	Low		Medium		High	No Correlation
Level of Correlation	1		3		9	0

Semester	Course code	Title of the Course	Hours	Credits
III	P22CH14E	<b>ELECTIVE COURSE 3: SPECTRAL TECHNIQUES IN INORGANIC COMPOUNDS</b>	6	4
Course Outcome (COs)	CO-Statement			Cognitive Level ( K -Level)
	On successful completion of this course, students will be able to			
CO-1	describe the principle of the selected spectra in all units.			K1
CO-2	explain the concepts of the given spectral techniques.			K2
CO-3	apply the rules in the structural elucidation of metal complexes.			K3
CO-4	analyze the spectral data for both coordination and organometallic complexes.			K4
CO-5	support the modified structure from the reported one from the spectral data.			K5
CO-6	create the innovation skills to the students by interpreting the spectral data and adopting new techniques in research.			K6

<b>III</b>	<b>P22CH14E</b>	<b>ELECTIVE COURSE 3: SPECTRAL TECHNIQUES IN INORGANIC COMPOUNDS</b>	<b>6</b>	<b>4</b>
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<b>Course Outcome (COs)</b>	<b>Programme Outcomes (POs)</b>					
	<b>PO1 Disciplinary Knowledge</b>	<b>PO2 Communication Skills</b>	<b>PO3 Critical Thinking, Problem Solving and Analytical Reasoning</b>	<b>PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.</b>	<b>PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.</b>	<b>PO6 Multicultural competency and Self- directed lifelong learning.</b>
<b>CO1-K1- Remembering</b>	9	9	9	9	9	9
<b>CO2-K2- Understanding</b>	9	9	9	9	9	3
<b>CO3-K3-Applying</b>	9	9	9	9	3	3
<b>CO4-K4-Analyzing</b>	9	9	9	3	3	3
<b>CO5-K5-Evaluating</b>	9	3	3	3	3	3
<b>CO6-K6-Creating</b>	9	3	3	3	3	3
<b>Weightage</b>	54	42	42	36	30	24
<b>Mapping Correlation</b>	<b>Low</b>		<b>Medium</b>		<b>High</b>	<b>No Correlation</b>
<b>Level of Correlation</b>	1		3		9	0



Semester	Course Code	Title of the Course	Hours	Credits
III	P22CH15E	Elective Course-4 Basic Strategies of Nanomaterials and Synthetic Organic Chemistry	6	4
Course Outcome (COs)	CO- statement			Cognitive Level(K-Level)
CO-1	On successful completion of this course, Students will be able to Define nano materials, and their types, preparation methods and applications.			K1
CO-2	Illustrate the basic characterization techniques of nanomaterials.			K2
CO-3	Categorize nano materials' existence as carbon nano tubes.			K3
CO-4	Infer the usage of nano materials.			K4
CO-5	Elucidates the retro synthetic analysis and strategies of organic compounds			K5
CO-6	Compile the different applications of reagents in oxidation and reduction process in Organic chemistry			K6

Semester	Course Code	Title of the Course				Hours	Credits
III	P22CH15E	Elective Course-4 Basic Strategies of Nanomaterials and Synthetic Organic Chemistry				6	4
<b>Programme Outcomes (POs)</b>							
Course Outcome (COs)	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning	
CO1-K1-Remembering	9	9	9	9	3	3	
CO2-K2-Understanding	9	9	9	3	9	9	
CO3-K3-Applying	9	9	9	9	9	9	
CO4-K4-Analyzing	9	9	3	9	9	3	
CO5-K5-Evaluating	9	3	9	1	3	0	
CO6-K6-Creating	9	9	3	3	3	3	
<b>Weightage</b>	54	48	42	34	36	27	
<b>Mapping Correlation</b>	<b>Low</b>		<b>Medium</b>		<b>High</b>	<b>No Correlation</b>	
<b>Level of Correlation</b>	1		3`		9	0	

Semester	Course code	Title of the Course	Hours	Credits
IV	P22CH16	CORE COURSE CC-12: ORGANIC CHEMISTRY-III	5	5
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
CO-1	acquire the knowledge about pericyclic reactions and the concept of ORD_CD			K1
CO-2	Understand the structural and stereochemical implications on photochemical reactions			K2
CO-3	Understand the principles, techniques and applications of ESR and NMR spectroscopy for the structural elucidations			K2
CO-4	understand the concepts and applications of UV, IR and Mass spectrometry			K3
CO-5	analyze the structure of the organic compounds			K4
CO-6	Evaluate the isoprene rule along with the classification, and biological activity Terpenes.			K5

Semester	Course code	Title of the Course				Hours	Credits
IV	P22CH16	CORE 12: ORGANIC CHEMISTRY – III				5	5
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self-directed lifelong learning.	
CO1-K1-Remembering	9	9	9	9	9	9	
CO2-K2-Understanding	9	9	9	9	9	9	
CO3-K3-Applying	9	9	9	9	9	3	
CO4-K4-Analyzing	9	9	9	9	9	3	
CO5-K5-Evaluating	9	9	9	9	9	3	
CO6-K6-Creating	9	9	9	3	9	3	
Weightage	54	54	54	48	54	30	
Mapping Correlation		Low	Medium	High	No Correlation		
Level of Correlation		1	3	9	0		

Semester	Course code	Title of the Course	Hours	Credits
IV	P22CH17P	CORE COURSE 13: PHYSICAL CHEMISTRY -PRACTICAL-II	5	5
CO. No.	CO-Statement			Cognitive Level (K-Level)
	On successful completion of this course, students will be able to			
CO-1	Acquire the knowledge about the different types of conductometric titrations			K1
CO-2	Understand the different types of potentiometric titrations			K2
CO-3	Determine the dissociation constant of weak acids			K2
CO-4	Determine the activity coefficient of ions			K3
CO-5	Analyze the solubility of explicit salts			K4
CO-6	Evaluate the pH of a buffer solution			K5

Semester	Course code	Title of the Course				Hours	Credits
IV	P22CH17P	PRACTICAL-II: PHYSICAL CHEMISTRY				5	5
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self- directed lifelong learning.	
CO1-K1- Remembering	9	9	9	9	9	9	
CO2-K2- Understanding	9	9	9	9	9	9	
CO3-K3-Applying	9	9	9	9	9	9	
CO4-K4-Analyzing	9	9	9	9	9	9	
CO5-K5-Evaluating	9	9	9	9	9	9	
CO6-K6-Creating	9	9	9	9	9	3	
Weightage	54	54	54	54	54	48	
Mapping Correlation		Low	Medium	High	No Correlation		
Level of Correlation		1	3	9	0		

Semester	Course code	Title of the Course	Hours	Credits
IV	P22CH18E	APPLICATIONS OF QUANTUM CHEMISTRY AND THERMODYNAMICS	90	4
Course Outcome (COs)	CO-Statement			Cognitive Level (K-Level)
	<b>On successful completion of this course, students will be able to</b>			
<b>CO-1</b>	<p>Recall how the universe is connected to everything else through higher dimensions that our senses cannot comprehend, Show the connection between classical and quantum physics.</p> <p>Describe real quantum systems, as it turns out to be very difficult to find exact solutions to the Schrodinger equation for Hamiltonians of even moderate complexity.</p> <p>Calculate the energy levels of difficult quantum systems.</p>			K1,K2,K3
<b>CO-2</b>	<p>Determine the energies and shapes of n molecular orbitals in conjugated systems.</p> <p>Predict the distribution of electrons in a molecule which in turn can help predict molecular properties such as shape, magnetism and bond order.</p> <p>Investigate the properties of matter through the measurement of the orbital energies of electrons,</p> <p>Study the surface of solids.</p>			K2,K5,K6
<b>CO-3</b>	<p>Study how much a solution differs from an ideal solution.</p> <p>Study the relation between heat, work, temperature and energy.</p>			K4
<b>CO-4</b>	Apply statistical methods and probability theory to large assemblies of microscopic entities.			K3
<b>CO-5</b>	Understand quantum statistics which can explain many phenomena which classical statistic cannot explain.			K5
<b>CO-6</b>	Create reliable methodologies for optimizing performance and improving design of various power systems, analyse the foundation for heat engines, power plants, chemical reactions, refrigerators and many more concepts that the world we live in today relies on.			K6

Semester	Course code	Title of the Course				Hours	Credits
IV	P22CH18E	CORE COURSE-XIV APPLICATIONS OF QUANTUM CHEMISTRY AND THERMODYNAMICS				6	4
Course Outcome (COs)	Programme Outcomes (POs)						
	PO1 Disciplinary Knowledge	PO2 Communication Skills	PO3 Critical Thinking, Problem Solving and Analytical Reasoning	PO4 Reflective thinking and Scientific reasoning. Team work with leadership Qualities.	PO5 Moral and ethical awareness. Appreciating Environmental and Sustainability Issues.	PO6 Multicultural competency and Self- directed lifelong learning.	
CO1-K1- Remembering	9	3	3	3	3	3	
CO2-K2- Understanding	9	3	3	3	3	3	
CO3-K3-Applying	3	3	3	3	3	3	
CO4-K4-Analyzing	3	3	3	3	3	3	
CO5-K5-Evaluating	3	3	3	3	3	3	
CO6-K6-Creating	3	3	3	3	3	3	
Weightage	30	18	18	18	18	18	
Mapping Correlation	Low		Medium		High		No Correlation
Level of Correlation	1		3		9		0