SIKKIM UNIVERSITY

(A Central University Established by an Act of Parliament of India, 2007)

LEARNING OUTCOME - BASED CURRICULUM

M.Sc. (CHEMISTRY) CURRICULUM

(With effect from Academic Session 2023-24)

DEPARTMENT OF CHEMISTRY

SIKKIM UNIVERISTY

6TH MILE, TADONG - 737102

GANGTOK, SIKKIM, INDIA

VICE-CHANCELLOR'S MESSAGE

Sikkim University stands at the forefront of embracing the transformative National Education Policy (NEP) 2020. In alignment with NEP 2020's vision and the guidelines of the Learning Outcomes-based Curriculum Framework (LOCF) mandated by the UGC, we have undertaken a comprehensive revision of our curriculum across all departments. This initiative ensures a holistic educational experience that transcends traditional knowledge delivery, emphasizing the practical application of knowledge in real-world scenarios.The shift towards LOCF marks a pivotal change from teacher-centric to learner-centric education, fostering a more active and participatory approach to learning. Our updated curriculum clearly defines Graduate Attributes, Programme Learning Outcomes (PLOs), and Course Learning Outcomes (CLOs), setting clear objectives for our students to achieve. This revision is designed to enable a teaching-learning environment that supports the attainment of these outcomes, with integrated assessment methods to monitor and encourage student progress comprehensively.

A key innovation in our curriculum is the mandatory integration of Massive Open Online Courses (MOOCs) through the SWAYAM platform, enhancing accessibility and the breadth of learning opportunities for students. Our approach encourages multidisciplinary studies through the curriculum while allowing for specialization. The curriculum embodies the policy's core principle of flexibility by enabling mobility for students, thereby allowing the exit and entry of students in the program.

I extend my heartfelt gratitude to our faculty, the Head of the Department, the Curriculum Development Committee members, the NEP coordinators, and the dedicated NEP Committee of Sikkim University for their relentless dedication to updating our curriculum. I appreciate Prof. Yodida Bhutia, the Chairperson, and all dedicated NEP Committee members for their thorough review and integration of LOCF and NEP components into our curriculum.

To our students, I convey my best wishes as we embark on this journey with our updated and inclusive curriculum, aiming not only to enrich their academic knowledge but also to nurture their personal growth, critical thinking, and ability to adapt and innovate in an ever-changing world.

Best wishes,

Prof. Avinash Khare
Vice Chancellor
Sikkim University

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1. Vision

To establish a Centre of Excellence for teaching, research and innovation in the field of chemistry

2. Mission

- To impart high-quality teaching in the fundamental and advanced areas of chemistry.
- To engage in cutting-edge research in fundamental and applied chemistry.
- To equip students with practical experience in utilizing advanced experimental and instrumentation techniques.
- To enhance students' abilities to excel in competitive exams.
- To inculcate leadership qualities, teamwork spirit, and managerial skill among students.

3. Preamble

The two-year M.Sc. program has been designed to provide a comprehensive and intellectually rigorous learning experience that cultivates a liberal and genuine scientific approach in exploring and understanding the latest advancements in the field of chemistry.

4. The Broad Aims of Master's Degree (M.Sc.) Programme in Chemistry

4.1. To provide students with a comprehensive and in-depth understanding of chemistry, encompassing both fundamental principles and advanced knowledge in specialized areas of the field.

4.2. To develop students' analytical and problem-solving skills, enabling them to effectively address diverse challenges within the field of chemistry. This includes preparing them for further academic and research pursuits as well as interdisciplinary collaborations. Additionally, to foster an entrepreneurial mindset, equipping students with the ability to identify opportunities for self-employment and innovation.

4.3. To create a stimulating learning environment that promotes the holistic cognitive development of students, nurturing their critical thinking abilities, enhancing communication skills, and fostering core competencies. The aim is to cultivate well-rounded individuals who are capable of adapting to the evolving demands of the field and who contribute responsibly to society.

4.4. To actively support and guide students in their preparation for various competitive examinations, such as the UGC-CSIR NET and UPSC Civil Services Examination. The goal is to expand their future career opportunities and prospects, opening doors to advanced research positions, academic positions, and other professional roles.

5. Post Graduate Attributes

5.1. Core Competency/Disciplinary Knowledge: Chemistry postgraduates should possess a solid understanding of fundamental concepts in chemistry and applied chemistry, as well as a working knowledge of advancements in the field.

5.2. Communication Skills: They should be adept at effectively commu nicating and actively participating in scientific discussions. Additionally, they should be able to present their research findings and observations convincingly, with clarity and comprehension.

5.3. Critical Thinking: Chemistry postgraduates should be familiar with the basics of cognitive biases, mental models, logical fallacies, scientific methodology, and constructing coherent scientific arguments.

5.4. Psychological Skills: Postgraduates should demonstrate psychological resilience to face challenging situations, as well as the ability to interact effectively with individuals from diverse sociocultural, economic, and educational backgrounds.

5.5. Problem-Solving: They should possess strong problem-solving skills to identify and address unknown problems effectively.

5.6. Analytical Reasoning: Chemistry postgraduates should have developed strong analytical skills that can be applied across various domains.

5.7. Research Skills: They should have acquired sound research acumen through their research projects and possess the skills necessary to tackle complex problems.

5.8. Teamwork: Chemistry postgraduates should be able to work collaboratively and harmoniously as part of a research group, contributing positively as team members.

5.9. Digital Literacy: Postgraduates should be proficient in digital literacy, utilizing e-learning resources such as MOOCs, SWAYAM, and other digital tools for lifelong learning. They should also possess the ability to discern data fabrication and identify fake news through rational skepticism and analytical reasoning.

5.10. Moral and Ethical Awareness: Chemistry postgraduates are expected to be responsible individuals with a strong sense of moral and ethical values. They should be well-versed in scientific ethics, including the prevention of misconduct such as plagiarism. They are expected to be exemplary citizens of their country and the world.

5.11. Leadership Readiness: They should have developed leadership skills to effectively lead a team and function as competent team leaders.

6. Program Outcomes (POs)

PO 1	Core Competency: Students will acquire a strong foundation in Chemistry, as well as in allied subject areas.
PO 2	Problem Analysis: Students will develop the ability to identify, formulate, review research literature, and analyse complex problems within the field of science.
PO 3	Investigation of Research Problems: Students will utilize research-based knowledge, research methods, and innovative approaches to explore and provide solutions for various problems.
PO 4	Environment and Sustainability: Students will gain an understanding of the societal and environmental implications of scientific solutions, demonstrating their knowledge of and appreciation for the importance of sustainable development.
PO 5	Ethics: Students will apply ethical principles, uphold professional ethics, and embrace the responsibilities and norms of scientific practice.
PO 6	Individual and Teamwork: Students will demonstrate the ability to function effectively both as individuals and as members or leaders in diverse teams and multidisciplinary settings.
PO 7	Communication: Students will develop effective communication skills to articulate scientific problems to the scientific community and society as a whole. They will be able to deliver impactful presentations and reports to effectively convey their findings and ideas.
PO 8	Life-long Learning: Students will recognize the importance of continuous learning and possess the necessary preparation and skills to engage in independent and life-long learning within the ever-evolving landscape of scientific advancements.
PO 9	Societal Responsibility: Students will demonstrate a commitment to using their knowledge for the betterment of society, applying their skills and expertise to address social challenges and contribute positively to the well-being of communities.

7. Program Learning Outcomes (PLOs)

7.1. Students will have a solid foundation in the fundamentals and applications of Inorganic, Organic, and Physical Chemistry.

7.2. Students will be able to design and conduct scientific experiments, accurately record, and analyze the results of such experiments.

7.3. Students will possess skills in problem-solving, critical thinking, and analytical reasoning as they apply to scientific problems.

7.4. Students will be able to clearly communicate the results of scientific work in oral, written, and electronic formats to both scientists and the general public.

7.5. Students will be able to explore new areas of research in chemistry and related fields of science and technology.

7.6. Students will understand and appreciate the central role of chemistry in our society. They will utilize this knowledge as a foundation for ethical behavior, demonstrating an understanding of safe chemical handling, environmental issues, as well as key issues related to energy, health, and medicine.

7.7. Students will be able to explain why chemistry is crucial in addressing social, economic, and environmental problems.

7.8. Students will be capable of functioning as members of interdisciplinary problem-solving teams.

8. Qualification Descriptors

8.1. Comprehensive Knowledge: Demonstrate a comprehensive understanding of chemistry, including current research, scholarly literature, and advanced learning areas within the field.

8.2. Specialization and Current Updates: Develop skills and proficiency in utilizing knowledge effectively within specialized areas of chemistry, keeping up with the latest advancements and updates in the subject.

8.3. Job and Self-Employment Opportunities: Identify and utilize subject-related skills to explore employment opportunities and potentially engage in self-employment ventures.

8.4. Effective Communication: Communicate research findings and study outcomes within the academic field of chemistry, using key concepts, constructs, and techniques.

8.5. Practical Application in Daily Life: Apply subject knowledge to solve societal problems by understanding the practical applications of chemistry in day-to-day life.

8.6. Sustainable and Environmentally Friendly Initiatives: Apply subject knowledge to contribute to sustainable and environmentally friendly initiatives, promoting green practices and addressing environmental challenges.

8.7. Research and Technological Advancements: Apply subject knowledge to engage in new research endeavors and contribute to advancements in technology within the field of chemistry.

9. Course Structure of Two-Year M.Sc. programme

Code	Course Name	Credit	In-Sem Marks	End-Sem Marks	Total Marks
First Semester					
CHE-C-501	Inorganic Chemistry I	4	50	50	100
CHE-C-502	Organic Chemistry I	4	50	50	100
CHE-C-503	Physical Chemistry I	4	50	50	100
CHE-V-504	Contribution of Indians in Chemistry	4	50	50	100
CHE-S-505	Chemistry Software & Analytical Tools	2	25	25	50
CHE-P-506	Chemistry Practical-I	4	50	50	100
	Total	22	275	275	550
Second Semester					
CHE-C-551	Inorganic Chemistry II	4	50	50	100
CHE-C-552	Organic Chemistry II	4	50	50	100
CHE-C-553	Physical Chemistry II	4	50	50	100
CHE-C-554	Instrumental Techniques I	4	50	50	100
CHE-V-555	Cyber Security	2	25	25	50
CHE-P-556	Chemistry Practical-II	4	50	50	100
	Total	22	275	275	550
Third Semester					
CHE-C-601	Instrumental Techniques II	4	50	50	100
Elective I (Choose any one course from E-602 – E 604)					
CHE-E-602	Organometallic Chemistry	4	50	50	100
CHE-E-603	Advanced Topics in Organic Chemistry	4	50	50	100
CHE-E-604	Advanced. Statistical Thermodynamics	4	50	50	100
Elective II (Choose any one course from E-605 – E 608)					
CHE-E-605	Chemistry of Inorganic Materials	4	50	50	100
CHE-E-606	Instrumental Techniques for Organic Chemistry	4	50	50	100
CHE-E-607	Nanochemistry	4	50	50	100
CHE-E-608	Chemicals in Industry	4	50	50	100
CHE-S-609	Mathematical Techniques in Chemistry	2	25	25	50
CHE-S-610	Scientific Writing and Communication	2	25	25	50
CHE-O-611	Biochemistry	2	25	25	50
Elective Practical (One specialization specific practical from P-612 to P-614)					
CHE-P-612	Inorganic Elective Practical	4	50	50	100
CHE-P-613	Organic Elective Practical	4	50	50	100
CHE-P-614	Physical Elective Practical	4	50	50	100
	Total	22	275	275	550

Fourth Semester					
Elective III (Choose any one course from E-651 – E-653)					
CHE-E-651	Magneto Chemistry	4	50	50	100
CHE-E-652	Advances in Organic Synthesis	4	50	50	100
CHE-E-653	Advanced Quantum Chemistry	4	50	50	100
Elective IV (Choose any one course from E-654 – E-656)					
CHE-E-654	Bio-inorganic chemistry	4	50	50	100
CHE-E-655	Natural Product	4	50	50	100
CHE-E-656	Non-equilibrium thermodynamics and Statistical Mechanics	4	50	50	100
Elective V (Choose any one course from E-657 – E-658)					
CHE-E-657	Solid State Chemistry	4	50	50	100
CHE-E-658	Analytical Chemistry	4	50	50	100
CHE-S-659	Modern Synthetic Techniques	2	25	25	50
CHE-R-660	Project Work	8	100	100	200
	Total	22	275	275	550
	Grand Total (I-IV Sem)	88	1100	1100	2200

C – Core Courses; E – Elective Courses; O – Open Courses; R – Research;

S – Skill Enhancement Courses; V – Value Added Courses

Students may earn up to 40 percent of the total credits of the programme from MOOCs (Massive Open Online Courses) Courses offered on SWAYAM (Study Webs of Active–Learning for Young Aspiring Minds). The selection of the course(s) from SWAYAM is subject to the availability, no. of credit and the 75 percent similarity of content with the existing courses in the department. The credits and the grade earned by the students in the particular course will be transferred and added in their mark statement.

Mapping of Course with Program Outcomes (POs)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9
CHE-C-501	X	X							
CHE-C-502	X	X	X						
CHE-C-503	X	X	X						
CHE-C-504	X	X	X	X	X	X	X	X	X
CHE-O-505	X	X	X				X		
CHE-P-506	X	X	X			X			
CHE-C-551	X	X	X						
CHE-C-552	X	X	X						
CHE-C-553	X	X							
CHE-O-554	X	X	X				X		
CHE-S-555	X	X	X						
CHE-P-556	X	X					X		
CHE-O-601	X	X	X	X		X			X
CHE-E-602	X	X	X						
CHE-E-603	X	X	X		X	X	X		
CHE-E-604	X	X	X	X					
CHE-E-605	X	X	X						
CHE-E-606	X	X	X				X		
CHE-E-607	X	X	X	X					
CHE-E-608	X	X	X						
CHE-S-609	X	X	X						
CHE-S-610	X	X	X						
CHE-O-611	X	X	X						
CHE-P-612	X	X							
CHE-P-613	X	X							
CHE-P-614	X	X	X		X		X		
CHE-E-651	X	X	X			X			X
CHE-E-652	X	X	X		X	X	X		
CHE-E-653	X	X	X		X	X	X		
CHE-E-654	X	X	X		X	X	X		
CHE-E-655	X	X	X						
CHE-E-656	X	X	X						
CHE-E-657	X	X	X						
CHE-E-658	X	X	X						
CHE-S-659	X	X	X						
CHE-R-660	X	X	X						

11. Courses (All Semesters)

SEMESTER I

Course Name: Inorganic Chemistry I **Code:** CHE-C-501

Semester: I **Course Level: 500** **Total Marks: 100**

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): On completion of course, students will be able to

1. Formulate the shape and stereochemistry of molecules and ions.
2. Determine ions as acids or bases and predict trends of acidity or basicity within a group. Also, be able to predict the formation of stable salts and adducts.
3. Determine the symmetry point group of known and unknown molecules.
4. Construct a character table for a given point group and identify vibrational modes, translational modes, and rotational modes.
5. Construct CF (Crystal Field) splitting and MO (Molecular Orbital) diagrams for various geometries and predict the stability of the complexes.
6. Construct a Tanabe-Sugano diagram for d^n electronic configurations and predict the number and magnitude of transitions.

Course Description

This course provides a comprehensive understanding of the principles and theories underlying the stereochemistry, bonding, and spectroscopy of inorganic compounds. It covers a wide range of topics, from the shapes of molecules and ions to the electronic spectra of transition metal complexes. Students will gain knowledge of fundamental concepts and learn to apply them in the analysis and interpretation of chemical structures and properties.

Course Outline

Unit1: Stereochemistry and bonding in Main group compounds

Valence Shell Electron Pair Repulsion model, stereochemical rules and explanation of the shapes of molecules and ions of non-transition elements with 2-7 valence shell electron pairs. Walsh Diagram. Bent's rule and energetics of hybridization.

HSAB: Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardnessand softness; Lewis-acid base reactivity approximation; Group Characteristic of Lewis acids & base(group13,14,15,16,17 and s-block) donor and acceptor numbers, E and C equation; applications of HSAB concept.

Unit 2: Group Theory and Symmetry of molecules

Group Theory: Definition of group, symmetry, point groups, representation of group, Abelian group,Group multiplication table, Groups, sub-groups and classes, Point group, classification and symmetry number. Orthogonality theorem, irreducible representation, character table, Point group symmetry and optical activity, dipolemoment, vibrational spectroscopy and bonding.

Unit 3: Metal-Ligand Bonding in Transition Metal Complexes

Crystal field splitting in diverse geometrical structures ; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory of octahedral complexes, brief introduction to Angular Overlap Model.

Unit 4: Electronic spectra of Transition Metal Complexes

Spectroscopic ground states; Orgel diagram and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral Co(II) and Ni(II) complexes and calculation of ligand-field parameters. Russell-Saunders coupling for d states. Splitting of electronic levels of d^n system in Octahedral and Tetrahedral environment . Correlation diagram. The method of descending symmetry, selection rules. Spectral transition probability, vibronic coupling,non-centrosymmetric complexes, polarization of allowed transitions

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Learning Outcomes (CLOs) with Program Outcome (POs)

CLO1	formulate the shape and stereochemistry of molecules and ions.	[PO1]
CLO2	determine ions as acids or bases and predict trends of acidity or basicity within a group. Also, be able to predict the formation of stable salts and adducts.	[PO1][PO2]
CLO3	determine the symmetry point group of known and unknown molecules.	[PO1]
CLO4	construct a character table for a given point group and identify vibrational modes, translational modes, and rotational modes.	[PO1][PO2]
CLO5	construct CFT (Crystal Field Theory) and MO (Molecular Orbital) diagrams for various geometries and predict the stability of the complexes.	[PO1]
CLO6	Construct a Tanabe-Sugano diagram for d n electronic configurations and predict the number and magnitude of transitions.	[PO1][PO2]

Performance Indicators (PIs)

1. Identify the shapes of molecules and ions by applying the principles of VSEPR.

2. Apply the concept of electron-electron repulsion to determine the stereochemistry of molecules.
3. Classify ions as acids or bases using the HSAB principle and Lewis concept.
4. Predict the formation of stable acid-base adducts using the HSAB principle.
5. Calculate trends in acidity or basicity for molecules within the same groups.
6. Identify symmetry elements and apply symmetry operations to determine their relationships.
7. Classify molecules based on the number and type of symmetry elements they possess.
8. Apply the orthogonality theorem to construct character tables for various molecules.
9. Ability to generate reducible and irreducible representations and determine translational, vibrational, and rotational modes present in a molecule.
10. Calculate the Crystal Field Stabilization Energy (CFSE) for various d n configurations and predict its impact on different properties of the molecule.
11. Apply the concept of π-bonding to predict the magnitude of spectral transitions and magnetic properties.
12. Construct Molecular Orbitals (MO) for various geometries and predict the magnitude of electronic transitions.
13. Construct Orgel and Tanabe-Sugano diagrams for various electronic configurations and determine the number of electronic transitions in the presence of both strong field and weak field ligands.
14. Determine the ground state terms for different configurations and geometries.

Suggested Readings:

1. Cotton, F.A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6thEdn., John Wiley & Sons, New York.
2. Huheey, J.E., 1993, Inorganic Chemistry, 4thEd., Addison-Wesley Pub. Co., New York.
3. Drago, R.S., 1971 Physical Methods in Inorganic Chemistry, International Edn., Affiliated East-West Press, New Delhi.
4. Shriver, D.F. and Atkins, P.W.,1999, Inorganic Chemistry, 3rdEdn., ELBS, London.
5. Cotton, F.A., Wilkinson, G. and Gaus, P.L., Basic Inorganic Chemistry, 3rd Edition, John Wiley & Sons, New York.

6. Greenhood, 1976, Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
7. Lee, J.D.1999, Concise Inorganic Chemistry, Blackwell Science.
8. Purcell K.F. and Kotz J.C., 1987, Inorganic Chemistry, W. B. Sauders Com., Hong Kong.
9. Cotton, F.A. 1990, Chemical Application of Group Theory, 3rd Ed, Wiley- Blackwell

SEMESTER I

Course Name: Organic Chemistry I **Code:** CHE-C-502

Semester: I **Course Level:** 500 **Total Marks:**100 **L+T+P:**3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): On completion of the course, students will be able to:

1. Predict the principles and concepts of pericyclic reactions, including molecular orbital symmetry, Woodward-Hoffmann correlation diagrams, and the FMO and PMO approaches.
2. Classify pericyclic reactions and analyze their mechanisms, including electrocyclic reactions, cycloadditions, and sigmatropic rearrangements.
3. Explain the principles of photochemistry, including quantum yields, intersystem crossing, and energy transfer reactions.
4. Predict the photochemistry of olefins, carbonyl compounds, and aromatic compounds, including isomerization, additions, and substitutions, and demonstrate knowledge of specific synthetic methods and reactions, including the Paterno-Buchi reaction, di-pimethane rearrangement, Barton's reaction, and Photo-Fries rearrangement.
5. Utilize the principles of reagents in organic synthesis, including complex metal hydrides, Gilman's reagent, LDA, dicyclohexylcarbodiimide, and various other reagents for functional group transformations.
6. Write synthetic methods for heterocyclic compounds such as furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline, and indole, and predict their reactivity.
7. Predict the mechanisms and factors influencing esterification and hydrolysis of esters, including the evidence for tetrahedral intermediates and steric and electronic effects.

Course Description

This course delves into the key concepts of organic chemistry, providing students with a comprehensive understanding of pericyclic reactions, photochemistry, important reagents in organic synthesis, heterocyclic compounds and ester hydrolysis.

Course Outline:

Unit 1

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems. Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Unit 2

Photochemistry: Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries rearrangement.

Unit 3

Reagents in Organic Synthesis: Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

Unit 4

Esterification and Hydrolysis of Esters:Evidence for tetrahedral intermediate in BAc^2 and AAc^2 mechanisms, steric and electronic effects. The AAc^1 and other pathways involving alkylto-oxygen bond cleavage.

Heterocyclic Chemistry: Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Predict the principles and concepts of pericyclic reactions, including molecular orbital symmetry, Woodward-Hoffmann correlation diagrams, and the FMO and PMO approaches.	[PO1]
CLO2	Classify pericyclic reactions and analyze their mechanisms, including electrocyclic reactions, cycloadditions, and sigmatropic rearrangements.	[PO1][PO2]
CLO3	Explain the principles of photochemistry, including quantum yields, intersystem crossing, and energy transfer reactions.	[PO1][PO2]
CLO4	Predict the photochemistry of olefins, carbonyl compounds, and aromatic compounds, including isomerization, additions, and substitutions, and demonstrate knowledge of specific synthetic	[PO1][PO2] [PO3]

	methods and reactions, including the Paterno-Buchi reaction, di-pimethane rearrangement, Barton's reaction, and Photo-Fries rearrangement.	
CLO5	Utilize the principles of reagents in organic synthesis, including complex metal hydrides, Gilman's reagent, LDA, dicyclohexylcarbodiimide, and various other reagents for functional group transformations.	[PO3]
CLO6	Write synthetic methods for heterocyclic compounds such as furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline, and indole, and predict their reactivity.	[PO1][PO2][PO3]
CLO7	Predict the mechanisms and factors influencing esterification and hydrolysis of esters, including the evidence for tetrahedral intermediates and steric and electronic effects.	[PO1][PO2][PO3]

Performance Indicators (PIs)

1. Correctly identify the symmetry characteristics and predict reaction outcomes based on Woodward-Hoffmann correlation diagrams.
2. Interpret phenomena related to photochemical reactions, including quantum yields and energy transfer processes.
3. Apply knowledge of reagents in organic synthesis to propose appropriate transformations and synthetic routes for specific functional group conversions.
4. Solve problems related to the mechanisms and reactions of esterification and hydrolysis of esters, considering steric and electronic effects.
5. Utilize the principles of aromatic substitution and heterocyclic synthesis to propose synthetic routes for specific target molecules.
6. Communicate organic chemistry concepts and synthetic strategies effectively.
7. Demonstrate critical thinking skills by analyzing and evaluating the efficiency and selectivity of different synthetic methods and reactions.

Suggested Readings

Text Books:

1. I. Fleming, *Frontier Orbital and Organic Chemical Reactions* John Wiley, 1976.
2. W. Carruthers, *Some modern Methods of Organic Synthesis* Cambridge University Press, 1990.

3. T.W. Greene, *Protective Groups in Organic Synthesis* Wiley-VCH, 1999.
4. M.B. Smith & Jerry March, *March's Advanced Organic Chemistry*, 5th Edition (2001), John Wiley & Sons, New York.
5. J. A. Joule and K. Mills, *Heterocyclic Chemistry:* (4th Ed) Wiley-Blackwell
6. J. Cleydon, N. Greeves, S. Warren, P. Wolthers, *Organic Chemistry:* Oxford (2001)

Reference Books:

1. Modern Heterocyclic Chemistry by L. A. Paquette, W.A. Benjamin, Inc.,1968.
2. Organic Chemistry by I. L. Finar, Vol II, ELBS, 1968.
3. Heterocyclic Chemistry by T. R. Gilchrist, Longman,1989.
4. Selectivity in Organic Synthesis by Ward, Wiley-VCH, 1999.
5. Advances in Heterocyclic Chemistry: Ed. A. R. Kartritzky, Acad. Press

SEMESTER I

Course Name: Physical Chemistry I **Code:** CHE-C-503

Semester: I **Course Level: 500** **Total Marks: 100**

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs)

1. Apply thermodynamic principles to analyze chemical systems and calculate partial molar quantities.
2. Analyze non-equilibrium thermodynamic processes and their implications in various systems.
3. Understand the theory of electrolytes, including metal/electrolyte interfaces and electrochemical cells.
4. Evaluate micelles and colloids, including their stability and electro-kinetic phenomena.
5. Comprehend the properties and behaviour of polymers, including molecular mass determination and polymer processing.
6. Apply the learned concepts to solve real-world problems in thermodynamics, electrochemistry, micelles and colloids, and polymers.

Course Description:

This course covers key topics in Thermodynamics, Electrochemistry, Micelles and Colloids, and Polymers. Each unit provides a detailed exploration of the underlying principles and their applications.

Course Outline:

Unit 1

Thermodynamics: Review of Laws of Thermodynamics. Entropy, free energy and chemical potential. Partial molar properties and their significance. Fugacity: its concept and determination. Properties of ideal solutions; non-ideal systems-deviations (negative and positive) from ideal behaviour, excess functions for non-ideal solutions, calculations of partial molar quantities, determination of partial molar volume and partial molar enthalpy.

Non equilibrium Thermodynamics Thermodynamic criteria for non-equilibrium process, Entropy production and entropy flow, Entropy balance equations for heat flow, chemical reactions etc., Transformations of the generalized fluxes and forces, Nonequilibrium stationary states, Generalized flux and forces, Phenomenological equations, Onsager reciprocal relations, Principle of detailed balance, Electro kinetic phenomenon, Diffusion, Electric conduction, Transport number and electrochemical cells, Irreversible thermodynamicc for biological systems

Unit 2

Electrochemistry:Theory of electrolytes, Ion-electron theory; Debye Huckel Limiting law, Activity Coefficients, Metal/Electrolyte interface: Outer Helmholtz Potential (OHP) and Inner Helmholtz Potential (IHP), potential profile across double layer region, potential difference across electrified interface; Structure of the double layer: Helmholtz-Perrin, Gouy-Chapman (Poisson-Boltzmann equation), and Stern models. Butler-Volmer equation under near equilibrium and non- equilibrium conditions, exchange current density, Tafel plot. Polarizable and non-polarizable interfaces. Electrochemical cells and Batteries.

Unit 3

Micelle and Colloids: Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsions, reverse micelles. Colloids: Multimolecular, macromolecular and associated colloids. Stability of collids. The zeta potential. Kinetic, optical and electrical properties of colloids. Electrokinetic phenomena: Electrophoresis, electroosmosis, sedimentation potential and streaming potential. Donnan membrane equilibrium. Collodal quntum dots, Metal nanoparticles and magnetic nanoparticles. Size dependent optical and electrical properties. Supermagnetic limit.

Unit 4

Polymers: Definition, types of polymers, liquid crystal polymers. Molecular mass-number and mass average molecular mass, determination of molecular mass (osmometry, visCLOsity, light scattering methods, Gel Permeation chromatography). Thermodynamics of polymer solutions – Florry Higgins theory. Microstructure of polymer chains, crystallinity in polymers, Glass transition temperature, rheological properties. Degradation of polymers. Polymer reactions. Polymer additives. Polymer Processing. Kinetics of Polymer Growth.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Learning Outcomes (CLOs) with Program Outcomes (POs)

CLO1	Apply thermodynamic principles to analyze chemical systems and calculate partial molar quantities.	[PO1]
CLO2	Analyze non-equilibrium thermodynamic processes and their implications in various systems.	[PO1][PO2]
CLO3	Understand the theory of electrolytes, including metal/electrolyte	[PO1]

	interfaces and electrochemical cells.	
CLO4	Evaluate micelles and colloids, including their stability and electrokinetic phenomena.	[PO1][PO2]
CLO5	Comprehend the properties and behavior of polymers, including molecular mass determination and polymer processing.	[PO1]
CLO6	Apply the learned concepts to solve real-world problems in thermodynamics, electrochemistry, micelles and colloids, and polymers.	[PO2][PO3]

Performance Indicators (PIs)

1. Demonstrate the ability to apply the laws of thermodynamics to solve numerical problems related to ideal and non-ideal solutions, including the calculation of partial molar quantities and the determination of deviations from ideal behavior.
2. Analyze and interpret the entropy balance equations for non-equilibrium processes, including heat flow and chemical reactions, and calculate entropy production and entropy flow.
3. Apply the concepts of ion-electron theory and activity coefficients to evaluate and predict the behavior of electrolytes, including the calculation of potential profiles across metal/electrolyte interfaces.
4. Analyze and interpret electrochemical cells and batteries using the Butler-Volmer equation under near equilibrium and non-equilibrium conditions, including the determination of exchange current density and the construction of Tafel plots.
5. Evaluate and interpret the factors affecting critical micellar concentration (cmc) and apply thermodynamic models to explain phase separation and mass action in micelles.
6. Analyze and interpret the properties and behavior of colloids, including the determination of zeta potential and the understanding of electrophoresis, electroosmosis, and sedimentation potential.
7. Apply the principles of polymer chemistry to determine molecular mass using osmometry, visCLOsity, light scattering, and gel permeation chromatography techniques.
8. Analyze and interpret the thermodynamics of polymer solutions using the Flory-Higgins theory, including the understanding of crystallinity, glass transition temperature, and rheological properties.
9. Evaluate and analyze the degradation, reactions, and additives of polymers, and understand their impact on polymer properties and performance.

10. Apply the knowledge of polymer processing techniques and analyze the kinetics of polymer growth in various scenarios.
11. Successfully solve complex problems and exercises related to thermodynamics, electrochemistry, micelles and colloids, and polymers, demonstrating a deep understanding of the underlying principles and their applications.
12. Apply the learned concepts and principles to real-world scenarios and propose appropriate solutions or strategies for addressing practical challenges in the field.

Suggested Readings:

1. Bockris J.O'M., and Reddy, A. K. N. 1998 Modern Electrochemistry, Vol. 1 & Vol. 2 AB, Second Edition, Plenum Press, New York.

2. Castellan G. W., Physical Chemistry, Addison-Wesley Publishing Company, Reading, MA.

3. Atkins, P. W. , 2002 Physical Chemistry, Seventh Edition, Oxford University Press, New York.

4. Levine, I. N. 2002 Physical Chemistry, 5th Edition, Tata McGraw Hill Pub. Co. Ltd., New Delhi.

5. Ram J. Raja and KuriaCLOse, J.C. 1993 Kinetics and Mechanism of Chemical Transformations, MacMillan Indian Ltd., New Delhi.

6. Barrow, G.M. Physical chemistry, 3rd Ed., International Student Edition, McGraw-Hill

7. Glasstone. S. 1940, Text - book of physical 1940. Publisher: Van Nostrand.

8. Pilling M. J. and Seakins, P. W. 1995 Reaction Kinetics, Oxford University Press, 1995

9. Moore, W. J. 1972, Physical Chemistry, Prentice Hall College Div; 4th edition

10. Engel T. and Reid P., Physical Chemistry, Pearson Education

SEMESTER I

Course Name: Contribution of Indians in Chemistry **Code:** CHE-V-504

Semester: I **Course Level:** 500 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 3 hrs; Tutorial = 1 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): By the end of the course, students will be able to:

1. Demonstrate a comprehensive understanding of the historical and contemporary contributions of Indian chemists to various fields of chemistry.
2. Apply critical thinking skills to evaluate the scientific, social, and economic impact of Indian chemists and their work.
3. Analyze the challenges and opportunities faced by Indian chemists throughout history.
4. Develop research and analytical skills through the study of Indian chemistry and its historical context.
5. Communicate effectively, both orally and in writing, about the contributions and significance of Indians in chemistry.

Course Description: The course explores the contributions of Indian scientists to the field of chemistry. It provides an in-depth examination of significant Indian chemists, their discoveries, and their impact on various areas of chemistry. Students will gain an understanding of the historical and cultural context in which these scientists worked and how their work has shaped the development of chemistry. It also examines the challenges faced by Indian chemists and the growth of the chemical industry in India.

Course Outline:

Unit 1

Ancient and medieval Indian techniques of glass making, pottery, cement, paper, soap, paints, weaponry, gold mining, medicine, dyeing of clothes and tanning of leather. Review of the work of Nagarjuna and Kanada. Chemistry in Dhatukriya (Dhatumanjari), Aurveda and Chemistry. Some of the important reactions discovered by Indians: Baker–Venkataraman rearrangement, Junjappa–Ila aromatic and Heteroaromatic Annulation reaction, Ramachary Reductive Coupling, Ramachary-Bressy-Wang cycloaddition, Ramachary Base Induced, Ring Opening (BIRO) Reaction, Green synthesis of β-diketones-$Mn(acac)_3$ and $Fe(acac)_3$ by M. K. Chaudhuri, Green Synthesis of dihydropyrimidinone -a three components coupling by B. C. Ranu.

Unit 2

Review of the Nobel wining work of Venkatraman Ramakrishnan. C. V. Raman and the Discovery of the Raman Effect and its applications in chemistry. Contribution of CNR Rao to the solid-state chemistry. Work of Prafulla Chandra Ray on nitrites. Work of Yellapragada Subba Rao on adenosine triphosphate (ATP) and drug discovery.

Unit 3

Notable Indian women in Chemistry: bibliography and their contribution to the field. Kamala Sohonie Asima Chatterjee and Darshan Ranganathan

Unit 4

History of Indian Chemical Industry: Bengal Chemical of Pharmaceutical Works Ltd. (Estd. 1901), Alembic Chemical Works (Estd. 1909), Alkali industry (Estd. 1937), Tata Chemicals (Estd. 1939). Case studies of dye industry in India before the discovery of synthetic indigo.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Outcome (CLOs) with Program Outcome (POs):

CLO1	Demonstrate a comprehensive understanding of the historical and contemporary contributions of Indian chemists to various fields of chemistry	[PO1]
CLO2	Apply critical thinking skills to evaluate the scientific, social, and economic impact of Indian chemists and their work.	[PO2],[PO3]
CLO3	Analyze the challenges and opportunities faced by Indian chemists throughout history.	[PO1],[PO2],[PO3]
CLO4	Develop research and analytical skills through the study of Indian chemistry and its historical context.	[PO2],[PO3]
CLO5	Communicate effectively, both orally and in writing, about the contributions and significance of Indians in chemistry.	[PO7]

Performance Indicators (PIs):

1. Successfully identify and discuss key contributions made by Indian chemists in various fields of chemistry.
2. Provide examples and evidence to support the understanding of the historical and contemporary significance of Indian chemists.
3. Apply critical thinking skills to evaluate the scientific, social, and economic impact of Indian chemists and their work
4. Present well-reasoned arguments and analyses that demonstrate an understanding of the broader implications of Indian chemists' contributions.
5. Analyze and articulate the challenges and opportunities faced by Indian chemists throughout history.
6. Identify and discuss factors that influenced the progress and achievements of Indian chemists in their respective fields.
7. Demonstrate research and analytical skills through the study of Indian chemistry and its historical context.
8. Conduct independent research to gather relevant information about Indian chemists and their work.
9. Communicate effectively, both orally and in writing, about the contributions and significance of Indians in chemistry.
10. Present clear and organized presentations or written reports that convey the scientific, societal, and cultural importance of Indian chemists' contributions.

Suggested Readings:

1. Praphulla Chandra Roy, 1903, A History of Hindu Chemistry, Volume-1, Second Edition, The Bengal Chemical & Pharmaceutical Works, Limited
2. Sreebrata Goswami and Samaresh Bhattacharya, Chemical Research of Sir Prafulla Chandra Ray, Resonance, January 2001, 42-49.
3. (a) Foil A. Miller, George B. Kauffman, C. V. Raman and the Discovery of the Raman Effect, Journal of Chemical Education, Volume 66 No.10 October 1989, 795-801.

   (b) SIR C HANDRASEKHARA V. RA M A N, The molecular scattering of light, Nobel Lecture, December 11, 1930.

   (c) C V RAMAN, The Raman effect Investigation of molecular structure by light scattering, Trans. Faraday Soc. 25 781-792 (1929).
4. Gao, Y G, Selmer M, Dunham C M, Weixlbaumer A , Kelley A C, Ramakrishnan V, The structure of the ribosome with elongation factor G trapped in the post trans locational state. Science (New York, N.Y.), 2009, 326:694-9, DOI: 10.1126/Science.1179709.
5. Voorhees R M, Weixlbaumer A , Loakes D, Kelley AC, Ramakrishnan V. Insights into substrate stabilization from snapshots of the peptidyl transferase center of the intact 70S ribosome Nature Structural and Molecular Biology.2009, 16: 528-533. DOI: 10.1038/nsmb.1577.
6. (a) E. Venkata Rao, Visionary chemist – Dr Yellapragada Subba Row, Current Science, Vol. 109, No. 1, 10 July, 2015, 213.

   (b) Koscak Maruyama, The Discovery of Adenosine Triphosphate and the Establishment of Its Structure, Journal of the History of Biology, vol. 24, no. 1 (Springer 1991) 145-154.]
7. (a) J. Gopalakrishnan, C. N. R. Rao and the Growth of Solid State and Materials Chemistry as a Central Domain of Research, Z. Anorg. Allg. Chem. 2014, 640, (6), 1031–1041, (John Wiley) DOI: 10.1002/zaac.201300592.

   (b) A. K. Ganguli and T. V. Ramakrishnan, Living Legends in Indian Science, C. N. R. Rao, Current Science, Vol. 111, NO. 5, 10 September 2016.
8. Anirban Mitra, The Life and Times of Kamala Bhagvat Sohonie The Unsung Hero of Science in India, RESONANCE ¨ April 2016, 301-314.
9. Amrit Krishna Mitra, Asima Chatterjee, one of the brightest stars in the galaxy of organic chemistry, Current Science, Vol. 121, No. 7, 10 October 2021, 974-983.
10. Darshan Ranganathan, Designer Hybrid Cyclopeptides for Membrane Ion Transport and Tubular Structures, Acc. Chem. Res. 2001, 34, 919-930.

11. (a) Ila, H.; Junjappa, H.; Mohanta, P. K. Prog. Heterocycl. Chem. 2001, 13, 1;
    (b) Ila, H.; Junjappa, H.; Barun, O. J. Organomet. Chem. 2001, 624, 34.
12. J. J. Li, Name Reactions, A Collection of Detailed Mechanisms and Synthetic Applications Sixth Edition, Springer, page 13-15.
13. Guangyou Jiang,‡a Min Liu,‡a Dongmei Fang,b Ping Tan,a Min Huang,a Taiping Zhou,a Zhenju Jiang,a Zhihong Xu a and Zhouyu Wang, A base promoted one pot solvent free version of the Ramachary reductive coupling/alkylation reaction for the synthesis of 2,2-disubstituted ethyl cyanoacetates, RSC Adv., 2018, 8, 8961–8964.
14. Manoj Kumar Na,b , Satheesh Kumar Nukalaa , Narasimha Swamy Thirukovelaa , Rakesh Sreeramaa , Ramya Sucharitha Ea , Pavan Kamarajugadda b , Sirassu Narsimha, Journal of Molecular Structure 1262 (2022) 132975.
15. M.N. Bhattacharjee, M.K. Chaudhuri and D.T. Khathing, J. Chem. Soc., Dalton Trans.,1982, 669.
16. M. K. Chaudhuri and S.K. Ghosh, J. Chem. Soc. Dalton Trans., 1983, 839.\
17. B. C. Ranu, A. Hajra and S. S. Dey, Org. Proc. Res. Dev. 2002, 6, 817.

SEMESTER I

Course Name: Chemistry Software & Analytical Tools **Code:** CHE-S-505

Semester: II **Course Level:** 500 **Total Marks:** 50

L+T+P: 1+1+0 **=**2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Skill Enhancement

Course Learning Outcome (CLOs)

By the end of this course, students will be able to:

1. Demonstrate proficiency in using a variety of basic tools and analytical software commonly employed in chemistry, including MS Excel, MS PowerPoint, MS Word, and ChemDraw.
2. Utilize computational software and molecular modeling tools effectively, such as Gaussian, AutoDock Vina, Discovery Studio, PyMOL, and Mathematica, to solve chemical problems and perform molecular simulations.
3. Apply software tools like Mercury, Diamond, and Highscore plus to analyze X-ray diffraction data and generate structural information and crystallographic representations.
4. Process and analyze scientific images using ImageJ, including quantification, image enhancement, and data extraction techniques applicable to various chemical experiments and measurements.
5. Analyze X-ray photoelectron spectroscopy (XPS) data using CASA XPS and XPSPeak41 software, interpreting spectra and extracting chemical and electronic information from different types of samples.
6. Perform molecular modeling and computational chemistry calculations using software tools like Gaussian, AutoDock Vina, Discovery Studio, and PyMOL, applying appropriate methods to predict molecular properties, perform molecular dynamics simulations, and analyze chemical reactions.
7. Apply critical thinking and problem-solving skills to select and utilize the most appropriate software tool for a given chemical task or problem, considering factors such as accuracy, efficiency, and computational requirements.
8. Communicate scientific findings, results, and interpretations effectively using appropriate software tools, demonstrating clear and concise written and oral communication skills in the context of chemistry-related projects and presentations.

Course Description:

The Chemistry Software course introduces students to a wide range of software tools commonly used in the field of chemistry. Through practical hands-on exercises and projects, students will gain proficiency in utilizing various software applications for data analysis, molecular modeling, spectroscopy, crystallography, image processing, and computational chemistry.

Course Outline:

Unit 1

Basic analytical software and tools:MS Excel, MS Powerpoint, MS words, Origin, Chemdraw,Mercury, Diamond, MestReNova, ImageJ, CASA XPS, XPSPeak41, HighScore Plus. Basic understanding of errors in chemical analysis and statistical evaluation of data: Systematic and random errors, accuracy and precision, the correlation coefficient, mean, median and modes, variance, standard deviation and significant figures.

Unit 2

Advanced analytical tools, Computational software and molecular modeling:Gaussian, AutoDock Vina, Discovery Studio, Pymol, Mathematica, Matlab, OLEX

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of POs with CLOs

	Course Learning Outcome (CLOs)	(POs)
CLO1	1. Demonstrate proficiency in using a variety of basic tools and analytical software commonly employed in chemistry.	[PO1]
CLO2	2. Utilize computational software and molecular modeling tools effectively to solve chemical problems and perform molecular simulations.	[PO2]
CLO3	3. Apply software tools to analyze X-ray diffraction data and generate structural information and crystallographic representations.	[PO2]
CLO4	4. Process and analyze scientific images using ImageJ, including quantification, image enhancement, and data extraction techniques.	[PO2]
CLO5	5. Analyze X-ray photoelectron spectroscopy (XPS) data using CASA XPS and XPSPeak41 software, interpreting spectra and extracting chemical information.	[PO2]
CLO6	6. Perform molecular modeling and computational chemistry calculations, predict molecular properties, perform molecular dynamics simulations.	[PO2]
CLO7	7. Apply critical thinking and problem-solving skills to select the most appropriate software tool for a given chemical task or problem.	[PO2]
CLO8	8. Communicate scientific findings effectively using appropriate software tools, demonstrating clear and concise written and oral communication skills.	[PO7]

Performance Indicators (PIs)

1. Proficiently and accurately utilize computational software and molecular modeling tools.
2. Solve complex chemical problems using these tools effectively.
3. Perform molecular simulations with a high level of proficiency and accuracy.
4. Demonstrate a strong understanding of the application of computational tools in chemistry.
5. Achieve reliable and accurate results through the use of these tools.
6. Apply critical thinking and problem-solving skills while utilizing the software and tools.
7. Effectively analyze and interpret the outcomes of molecular simulations and chemical problem-solving.

Suggested Readings:

1. Martin, Mariano Martin. Introduction to Software for Chemical Engineers.
2. House, Dorothy. Microsoft Word, Excel, and PowerPoint: Just for Beginners.
3. Arsalan, Muhammad and Awais, Azka. Origin Software Complete Usage Instruction and Graph Representation: A complete Guide for new users.
4. Foresman, James B. Exploring Chemistry With Electronic Structure Methods: A Guide to Using Gaussian.
5. Cambridge Scientific Computing. Chem Draw 7.0: Chemical Structure Drawing Standard - User's Guide.
6. Ge, Wei Yong. OLEX2 software single crystal structure analysis and crystal visualization.
7. Northwestern University. Structure Solution and Refinement with Olex2.
8. Mavada, Vishal. Beginner's guide to Protein-Ligands Docking using AutoDockVina.

SEMESTER I

Course Name: Chemistry Practical **-I** **Code:** CHE-P-506

Semester: I **Course Level:** 500 **Total Marks:** 100

L+T+P: 0+0+4 = 4 Credits (Lecture = 0 hrs; Tutorial = 0 hrs; Practical = 60 hrs)

Type: Core Practical

Course Outcome (CLOs):

On completion of the course, students will be able to:

1. Apply critical thinking and scientific inquiry to perform, design, interpret, and document laboratory experiments.
2. Demonstrate proficiency in synthesizing coordination complexes in a laboratory setting.
3. Monitor the progress of a chemical reaction through observation and data analysis.
4. Employ methods to characterize coordination complexes.
5. Recognize the appropriate use of solvents and follow proper disposal procedures.
6. Execute targeted synthesis experiments, including the Diels-Alder reaction of anthracene and maleic anhydride, aspirin synthesis, Sandmeyer's reaction, Cannizzaro reaction, preparation of tribromobenzene, and acetoacetic ester condensation.
7. Predict the identity and purity of synthesized compounds by employing melting point determination and employing diverse spectroscopic methods.
8. Demonstrate Proficiency in physical experimental techniques and to acquire and analyze experimental data.
9. Collaborate effectively in a team environment.
10. Acquire knowledge and skills in laboratory reporting and following manuals.
11. Identify laboratory hazards and implement safety precautions.

Course Description:

Chemistry Practical-I is a 4-credit course focused on conducting inorganic, organic and physical chemistry experiments. The course includes three main components: A Preparation and Characterization of Inorganic complexes, B) Synthesis and characterization of organic compounds & C) Physical experiments based on electrochemistry and kinetics. Through hands-on laboratory work, students will develop practical skills in analytical techniques, synthesis, and characterization.

Course Outline:

1. Preparation and Characterization of the following compounds (Any six) : Characterization includes microanalysis, magnetic susceptibility and conductance measurements and infrared, UV-Visible, NMR spectroscopy, XRD and cyclic voltammetry studies.

a) Tris (oxalate) manganese (III)
b) Tetrapyridinesilver (II) peroxidisulphate
c) Tris (acetylacetonato) iron (III)
d) Bis (N,N-diethyldithiocarbamato) nitrosyliron (I)
e) Optical isomers of tris (ethylenediamine) cobalt (III) chloride
f) Linkage isomers of nitro and nitritopentamminecobalt (III) chloride
g) Ferrocene or dibenzene chromium
h) Hydridochlorocarbonyl tris (triphenylphosphine) ruthenium (II)
i) Tris(2,2'-bipyridine)ruthenium (II) perchlorate
j) $[(p\text{-}(cymene)RuCl_2]_2$
k) Tris (acetylacetonato) manganese (III)
l) Copper(I) Thiourea complexes: $[Cu(Tu)_6]SO_4 . H_2O$

2. Synthesis of organic compounds, purification and characterization by chemical analysis, IR, UV-Vis, PL, NMR spectral analysis and mass spectral analysis: (Any three)

a) Synthesis of fluorescein, a classic fluorescent dye
b) Synthesis and chemiluminescence of luminol
c) Diels-Alder reaction of anthracene and maleic anhydride
d) Aspirin synthesis: Conventional and with microwave assistance
e) Sand Meyer's reaction: p-Chlorotoluene from p-chlorotoluidine.
f) Cannizzaro reaction using 4-chlorobenzaldehyde
g) Preparation of 1,3,5 tribromobenzene from analine
h) Acetoacetic ester condensation

3. Electrochemistry and Kinetics: (Any three)

a) Analysis of halide mixture by differential potentiometry
b) Degree of hydrolysis of urea hydrochloride by kinetics method.
c) Equilibrium constant of KI + I ↔ KI by distribution method.
d) Kinetics of the iodide-hydrogen peroxide clock reaction
e) An experiment to determine the energy of activation, Ea
f) Determination of the amount of calcium in milk powder by EDTA complexometry
g) Estimation of iodine in iodized common salt using iodometry
h) Determination of phosphoric acid in soft drinks
i)Antioxidant property of Tea (DPPH method).

Suggested Teaching-Learning Approaches:

1. Engaging Lectures: Employing interactive lectures coupled with live discussions and vivid demonstrations of laboratory skills and techniques.
2. Experiential Learning: Encouraging hands-on practice to actively engage students in real-life applications, fostering a deeper understanding of the subject matter.

3. Collaborative Learning: Facilitating group discussions, promoting active participation, and encouraging the exchange of ideas among students, leading to enhanced critical thinking and problem-solving skills.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Assignment	Oral Test, Viva-Voce, Presentation	Presentation
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: Teachers have the flexibility to select an appropriate mode of formative assessment based on the nature of the learning outcomes and its feasibility within the given context.

Mapping of Course Outcome (CLOs) with Program Outcome (POs):

CLO1	Apply critical thinking and scientific inquiry to perform, design, interpret, and document laboratory experiments.	[PO1][PO9]
CLO2	Analyze and select appropriate methods for estimating metal ions or compounds.	[PO1][PO2][PO3]
CLO3	Calculate the quantitative estimation of constituents in a mixture.	[PO1][PO2][PO3]
CLO4	Demonstrate proficiency in synthesizing organic molecule and coordination complexes in a laboratory setting.	[PO1][PO2][PO3]
CLO5	Monitor the progress of a chemical reaction through observation and data analysis.	[PO1][PO2][PO3]
CLO6	Employ methods to characterize synthesied complounds.	[PO1][PO2]
CLO7	Recognize the appropriate use of solvents and follow proper disposal procedures.	[PO5][PO7][PO8]
CLO8	Collaborate effectively in a team environment.	[PO6][PO7]
CLO9	Acquire knowledge and skills in laboratory reporting and following manuals.	[PO1][PO5][PO7]
CLO10	Identify laboratory hazards and implement safety precautions.	[PO1][PO4][PO5] [PO7]

Performance Indicators (PIs):

A. Ore, Alloy, and Commercial Product Analysis:

1. Accurately determine the concentrations of silica and manganese in pyrolusite through appropriate titration or spectrophotometric methods.
2. Quantify the copper and iron content in chalcopyrite using suitable analytical techniques, such as complexometric titration or atomic absorption spectroscopy.
3. Perform complexometric titration to determine the iron content in hematite.
4. Analyze solder samples to determine the concentrations of tin and lead using appropriate instrumental or titration methods.
5. Employ suitable methods to determine the iron and chromium content in mild steel samples.
6. Utilize UV-Vis spectrophotometry to quantify the iron content in hematite samples.
7. Apply appropriate methods to determine the phosphoric acid concentration in soft drinks.
8. Conduct comprehensive analysis of cement samples, including determining the composition and properties of cementitious materials.
9. Employ appropriate techniques to determine the fluoride concentration in toothpaste samples.

B. Preparation and Characterization of Inorganic Compounds:

1. Successfully synthesize and characterize tris(oxalate)manganese(III) and tetrapyridinesilver(II)peroxidisulphate compounds.
2. Prepare and characterize tris(acetylacetonato)iron(III) and bis(N,N-diethyldithiocarbamato)nitrosyliron(I) compounds.
3. Synthesize and characterize optical isomers of tris(ethylenediamine)cobalt(III) chloride and linkage isomers of nitro and nitritopentamminecobalt(III) chloride.
4. Prepare and characterize ferrocene or dibenzene chromium compounds.
5. Conduct synthesis and characterization of hydridochlorocarbonyl tris(triphenylphosphine)ruthenium(II) and tris(2,2'-bipyridine)ruthenium(II) perchlorate compounds.
6. Successfully synthesize and characterize [(p-(cymene)$RuCl_2$]$_2$ compound.
7. Prepare and characterize tris(acetylacetonato)manganese(III) compound.
8. Perform synthesis and characterization of copper(I) thiourea complexes: $[Cu(Tu)_6]SO_4 . H_2O$.

Suggested Readings:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.

2. A text book of Quantitative Inorganic Analysis – A. I. Vogel, Experimental Inorganic Chemistry - W. G. Palmer
3. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.
4. Chemistry experiments for Instrumental Methods by Donald T. Sawyer, William R. Heineman & Jalice M. Beebe , John Wiley & Sons ,1984.
5. Experimental Physical Chemistry by G. Peter Matthews, Clarendon Press, 1985.
6. Modern Experiments for Introductory Chemistry, compiled by Neidig and Strattom, 2nd Ed., Reprinted from Journal of Chemical Education,1990.
7. Handbook of Inorganic Synthesis: G. Brauer
8. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, Gregory Girolami, Thomas B. Rauchfuss and Robert J. Angelici. University Science Books.

SEMESTER II

Course Name: Inorganic Chemistry II **Code:** CHE-C-551

Semester: II **Course Level:** 500 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): By the end of this course, students will be able to:

1. Distinguish the difference in reactivity between non-transition elements and transition metals.
2. Determine the structure and reactivity of compounds such as boranes, carboranes, borazines, phosphazenes, thiazenes, silicates, and silicones.
3. Demonstrate the ability to differentiate between associative and dissociative reactions and identify the factors that influence reaction rates.
4. Utilize the concept of trans effect to develop strategies for synthesizing inorganic complexes.
5. Apply the concepts of CFT (Crystal Field Theory) to understand and predict the energetics of reactions.
6. Differentiate between outer sphere and inner sphere electron transfer.
7. Analyze the energetics involved in electron transfer and predict the mode of electron transfer.
8. Demonstrate the use of radiationless transitions and their influence on excited state chemistry.
9. Differentiate between different radiative transitions and assess the influence of various factors on emissive transitions.
10. Differentiate various quenching processes and assess their implications on radiative transitions.
11. Interpret and differentiate energy transfer reactions and their applications.

Course Description:

This course offers an advanced exploration of inorganic chemistry, focusing on the reactivity, structure, and properties of various compounds and elements. The curriculum encompasses a wide range of topics and concepts, enabling students to develop a comprehensive understanding of the field.

Course Outline:

Unit 1

Chemistry of non-transition elements: Non-transition metal chemistry. Synthesis, Properties, Structure and Bonding: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds; Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones.

Isopoly and Heteropoly Acids and Salts. Synthesis, structural principles and application of V, Nb, Ta, Cr, Mo and W polyacids

Unit 2

Kinetics and Mechanism of reactions of transition metal complexes. Energy profile of reactions, discussion on general reactivity of metal complexes, inert and labile complexes, different types of mechanisms (D, A, I_D and I_A). Techniques for experimental measurements of reaction rates, techniques for fast reaction. Substitution reactions: Application of CFT, mechanism of ligand substitution in octahedral complexes, mechanism of isomerization and racemization, Twist mechanism of racemization, substitution reactions in square planar complexes. Cis- and trans-effects.

Unit 3

Electron Transfer Reactions. Mechanism of redox reactions with reference to metal complexes. Electron transfer reactions – outer sphere and inner sphere, atom transfer, induced electron transfer reactions, two electron transfer reactions, non-complementary reactions, synthetic implications of electron transfer reactions, solid state electron transfer reactions. Electroprotic reactions, Marcus-Husch theory, correlation between thermal and optical electron transfer reactions; identification of intervalence transfer bands in solution

Unit 4

Photochemistry. Radiation less transitions, density of energy states, theory of unimolecular reactions, fluorescence emission, influence of structure and substituents, heteroaromatic molecules, Phosphorescence emission, influence of paramagnetic molecules, emission property and electronic configuration, photophysical kinetics of unimolecular process, E-type and P-type delayed fluorescence, photophysical kinetics of bimolecular process, fluorescence quenching, kinetics of collisional quenching, excimer and excited state dimers, quenching by added substances, Electronic energy transfer, long range and short range transfer, intramolecular energy transfer.

Suggested-teaching learning strategy

1.Lecture with interactive discussions and problem-solving activities.

2.Assignments and individual presentations.

3.Student-led classroom teaching.

4.Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs

CLO1	distinguish the difference in reactivity between non-transition elements and transition metals.	[PO1]
CLO2	determine the structure and reactivity of compounds such as boranes, carboranes, borazines, phosphazenes, thiazenes, silicates, and silicones.	[PO1] [P02]
CLO3	demonstrate the ability to differentiate between associative and dissociative reactions and identify the factors that influence reaction rates.	[PO1]

CLO4	utilize the concept of trans effect to develop strategies for synthesizing inorganic complexes.	[PO1][PO2] [PO3]
CLO5	apply the concepts of CFT (Crystal Field Theory) to understand and predict the energetics of reactions.	[PO1][PO2]
CLO6	differentiate between outer sphere and inner sphere electron transfer.	[PO1]
CLO7	analyze the energetics involved in electron transfer and predict the mode of electron transfer.	[PO1][PO2]
CLO8	demonstrate the use of radiationless transitions and their influence on excited state chemistry.	[PO1]
CLO9	differentiate between different radiative transitions and assess the influence of various factors on emissive transitions.	[PO1][PO2]
CLO10	differentiate various quenching processes and assess their implications on radiative transitions.	[PO1]
CLO11	interpret and differentiate energy transfer reactions and their applications.	[PO1]

Performance Indicators (PIs)

1. Demonstrate the ability to explain the reactivity difference between non-transition elements and transition group elements based on their structure and bonding characteristics.
2. Identify and discuss specific factors that contribute to the reactivity disparity.
3. Interpret and analyze the reactivity patterns of interhalogens, halogens, and pseudohalogens.
4. Provide explanations and examples to support the understanding of their reactivity trends.
5. Apply the principles of structure and bonding characteristics to predict the reactivity of molecules formed by main group elements.
6. Justify and support predictions with relevant scientific concepts and evidence.
7. Identify and describe the shapes and reactivity of Xenon-halide compounds.
8. Explain the relationship between their structures and their chemical behavior.
9. Identify and differentiate between associative and dissociative reactions.
10. Use various factors to determine the mechanism of a reaction and provide clear demonstrations of their application.
11. Interpret and classify data related to chemical reactions in order to predict their reaction mechanisms.

12. Apply analytical skills to analyze experimental or theoretical data and draw meaningful conclusions.
13. Demonstrate a clear understanding of the different factors that contribute to the trans effect.
14. Explain the impact of these factors on the properties and reactivity of metal complexes.
15. Utilize the concept of trans effect to explain the formation of products and develop synthetic strategies for the preparation of desired metal complexes.
16. Apply the understanding of trans effect to propose appropriate reaction conditions and techniques.
17. Use the concept of Crystal Field Theory (CFT) to predict the lability and inertness of a metal complex.
18. Justify predictions based on the coordination environment and the nature of the metal ion.
19. Predict the influence of coordination geometry and the nature of the metal ion on the rate and type of reaction mechanism.
20. Provide explanations and examples to support the predictions.
21.Demonstrate a clear understanding of outer sphere and inner sphere electron transfer.
22. Differentiate between these two types of electron transfer and explain their respective characteristics.
23. Ability to predict the type of electron transfer possible for a given electron transfer reaction.
24. Apply relevant principles and concepts to determine the feasibility and mechanism of electron transfer.
25. Utilize the theory of radiationless transitions to understand excited state chemistry.
26. Explain the role of radiationless transitions in determining the behavior and properties of excited states.
27. Assess the influence of different factors on radiationless transitions.
28. Analyze and explain how factors such as temperature, solvent, and molecular structure affect the rates and efficiency of radiationless transitions.
29. Distinguish between fluorescence and phosphorescence and identify various factors that affect radiative transitions.
30. Discuss the principles and mechanisms underlying these types of radiative transitions.
31. Differentiate between excimers and exciplexes and describe their influence on excited state chemistry.
32. Explain the formation and behavior of excimers and exciplexes in relevant systems.
33. Able to classify the influence of various quenching process and agents on the outcome of radiative transition.

34. Demonstrate ability to use Stern-Volmer equation to predict the kinetics of excited state processes.

35. Ability to distinguish long range energy transfer and short range energy transfer.

36. Able to assess the influence of different factors on the nature and magnitude of energy transfer.

Suggested Readings:

1. Huheey, J. 1993 E. Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York.
2. Cotton F. A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John- Wiley & Sons, New York.
3. Crabtree, R.H. 1988 The Organometallic Chemistry of the Transition Metals, 1st Edn., John-Wiley & Sons, New York.
4. Shriver , D. F. and Atkins, P. W. 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
5. Greenhood, 1976 Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
6. Cleydon, J. , Greeves, N. , Warren, S. and Wolthers, P. , 2001 Organic Chemistry: Oxford
7. Collman, J. P. , Hegedus, L. S. , Norton J. R and Finke, Richard G. 1987 Principles and Applications of Organotransition Metal Chemistry, 1st Edn., University Science Books, Mill Valley, California.
8. Elschenbroich, Ch. and. Salzer, A, 1991 Organometallics: A
9. Fundamentals of Photochemistry, K.K. Rohatgi-Mukherjee

SEMESTER II

Course Name: Organic Chemistry II **Code:** CHE-C-552

Semester: II **Course Level:** 500 **Total Marks:** 100

L+T+P: 3+1+0 = 4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): On completion of the course, students will be able to:

1. Predict the principles and concepts of pericyclic reactions, including molecular orbital symmetry, Woodward-Hoffmann correlation diagrams, and the FMO and PMO approaches.
2. Classify pericyclic reactions and analyze their mechanisms, including electrocyclic reactions, cycloadditions, and sigmatropic rearrangements.
3. Explain the principles of photochemistry, including quantum yields, intersystem crossing, and energy transfer reactions.
4. Predict the photochemistry of olefins, carbonyl compounds, and aromatic compounds, including isomerization, additions, and substitutions, and demonstrate knowledge of specific synthetic methods and reactions, including the Paterno-Buchi reaction, di-pimethane rearrangement, Barton's reaction, and Photo-Fries rearrangement.
5. Utilize the principles of reagents in organic synthesis, including complex metal hydrides, Gilman's reagent, LDA, dicyclohexylcarbodiimide, and various other reagents for functional group transformations.
6. Write synthetic methods for heterocyclic compounds such as furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline, and indole, and predict their reactivity.
7. Predict the mechanisms and factors influencing esterification and hydrolysis of esters, including the evidence for tetrahedral intermediates and steric and electronic effects.

Course Description

This course delves into the key concepts of organic chemistry, providing students with a comprehensive understanding of pericyclic reactions, photochemistry, important reagents in organic synthesis, heterocyclic compounds and ester hydrolysis.

Course Outline:

Unit 1

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems. Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Unit 2

Photochemistry: Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries rearrangement.

Unit 3

Reagents in Organic Synthesis: Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman’s reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson’s synthesis, Wilkinson’s catalyst, Baker yeast.

Unit 4

Esterification and Hydrolysis of Esters:Evidence for tetrahedral intermediate in BAc^2 and AAc^2 mechanisms, steric and electronic effects. The AAc^1 and other pathways involving alkylto-oxygen bond cleavage.

Heterocyclic Chemistry: Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3.. Student-led classroom teaching.
4.Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Predict the principles and concepts of pericyclic reactions, including molecular orbital symmetry, Woodward-Hoffmann correlation diagrams, and the FMO and PMO approaches.	[PO1]
CLO2	Classify pericyclic reactions and analyze their mechanisms, including electrocyclic reactions, cycloadditions, and sigmatropic rearrangements.	[PO1][PO2]
CLO3	Explain the principles of photochemistry, including quantum yields, intersystem crossing, and energy transfer reactions.	[PO1][PO2]
CLO4	Predict the photochemistry of olefins, carbonyl compounds, and aromatic compounds, including isomerization, additions, and substitutions, and demonstrate knowledge of specific synthetic methods and reactions, including the Paterno-Buchi reaction, di-pimethane rearrangement, Barton's reaction, and Photo-Fries rearrangement.	[PO1][PO2][PO3]
CLO5	Utilize the principles of reagents in organic synthesis, including complex metal hydrides, Gilman's reagent, LDA, dicyclohexylcarbodiimide, and various other reagents for functional group transformations.	[PO3]
CLO6	Write synthetic methods for heterocyclic compounds such as furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline, and indole, and predict their reactivity.	[PO1][PO2][PO3]
CLO7	Predict the mechanisms and factors influencing esterificat ion and	[PO1][PO2][PO3]

	hydrolysis of esters, including the evidence for tetrahedral intermediates and steric and electronic effects.	

Performance Indicators (PIs)

1. Correctly identify the symmetry characteristics and predict reaction outcomes based on Woodward-Hoffmann correlation diagrams.
2. Interpret phenomena related to photochemical reactions, including quantum yields and energy transfer processes.
3. Apply knowledge of reagents in organic synthesis to propose appropriate transformations and synthetic routes for specific functional group conversions.
4. Solve problems related to the mechanisms and reactions of esterification and hydrolysis of esters, considering steric and electronic effects.
5. Utilize the principles of aromatic substitution and heterocyclic synthesis to propose synthetic routes for specific target molecules.
6. Communicate organic chemistry concepts and synthetic strategies effectively.
7. Demonstrate critical thinking skills by analyzing and evaluating the efficiency and selectivity of different synthetic methods and reactions.

Suggested Readings

Text Books:

1. I. Fleming, *Frontier Orbital and Organic Chemical Reactions* John Wiley, 1976.
2. W. Carruthers, *Some modern Methods of Organic Synthesis* Cambridge University Press, 1990.
3. T.W. Greene, *Protective Groups in Organic Synthesis* Wiley-VCH, 1999.
4. M.B. Smith & Jerry March, *March's Advanced Organic Chemistry*, 5th Edition (2001), John Wiley & Sons, New York.
5. J. A. Joule and K. Mills, *Heterocyclic Chemistry:* (4th Ed) Wiley-Blackwell
6. J. Cleydon, N. Greeves, S. Warren, P. Wolthers, *Organic Chemistry:* Oxford (2001)

Reference Books:

1. Modern Heterocyclic Chemistry by L. A. Paquette, W.A. Benjamin, Inc.,1968.
2. Organic Chemistry by I. L. Finar, Vol II, ELBS, 1968.
3. Heterocyclic Chemistry by T. R. Gilchrist, Longman,1989.
4. Selectivity in Organic Synthesis by Ward, Wiley-VCH, 1999.
5. Advances in Heterocyclic Chemistry: Ed. A. R. Kartritzky, Acad. Press

SEMESTER II

Course Name: Physical Chemistry II **Code:** CHE-C-553

Semester: II **Course Level:** 500 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs): By the end of this course, students will be able to:

1. Analyse thermodynamic properties through Statistical mechanics calculations.
2. Master principles of atomic stability and processes of molecule formation.
3. Evaluate the interaction between molecules and atoms with electromagnetic radiation.
4. Analyze and interpreting spectra of diverse molecules and atoms.
5. Understand the intricacies of chemical kinetics processes.
6. Discern and categorize kinetic pathways in transformations

Course Description:

This course delves into the principles and applications of statistical thermodynamics, quantum mechanics, group theory, molecular spectroscopy, electronic spectroscopy, and reaction dynamics. Students will develop a comprehensive understanding of these fundamental concepts and their implications in various areas of physical chemistry.

Course Outline:

Unit 1

Statistical Thermodynamics of ideal systems: Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical and microcanonical ensembles, Boltzmann distribution of particles.

Partition function: translational, rotational and vibrational partition functions, thermodynamic properties of ideal gases in terms of partition function.

Unit 2

Quantum Mechanics: Fundamentals.Review of essential mathematical concepts. Origin of the quantum theory. Postulates of quantum mechanics and Schrödinger equation; its application on some model systems viz., free- particle and particle in a box, tunneling, the harmonic oscillator, the rigid rotator, and the hydrogen atom. The variation theorem; linear variation principle;

Approximation Methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples. Variation method. Ground state of He atom. Time-dependent perturbation theory. Radiative transitions. Einstein coefficients.

Atomic Structure: Many electron wave functions. Pauli Exclusion principle. Helium atom. Atomic term symbols. The self-consistent field method. Slater-type orbitals.

Group Theory Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, derivation of projection operator

Unit 3

Molecular Spectroscopy: Selection rules. A review of MW and IR spectroscopy. Symmetry properties and nuclear spin effects. Raman effect: Rotational and vibration-rotational transitions. Polarization of Raman lines. Vibration of polyatomic molecules– normal coordinates.

Electronic Spectroscopy: Absorption and Emission of radiation. Selection rules. Line shapes and widths. Electronic spectroscopy of diatomic molecules. Franck-Condon factor. Dissociation and pre- dissociation. Rotational fine structure. Lasers and Laser spectroscopy.

Unit 4

Reaction Dynamics: Methods of determining rate laws, collision theory of reaction rates, Arrhenius equation and activated complex theory. Potential energy surfaces. Unimolecular reactions and their treatments (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRK], RRKM theory) Experimental Methods: Enzyme kinetics, studies of fast reactions by flow method, relaxation method, flash photolysis and NMR. Techniques: Flow techniques.

General consideration of gas and solution phase fast reactions: Gas phase and solution phase reactions, Reactions at microsecond and nanosecond scale, ultrafast reactions: reactions at piCLOseconds and femtoseconds scale.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Analyze thermodynamic properties through Statistical mechanics calculations.	[PO1]
CLO2	Master principles of atomic stability and processes of molecule formation.	[PO1][PO2]
CLO3	Evaluate the interaction between molecules and atoms with electromagnetic radiation.	[PO1]
CLO4	Analyze and interpreting spectra of diverse molecules and atoms.	[PO1][PO2]
CLO5	Understand the intricacies of chemical kinetics processes.	[PO2]
CLO6	Discern and categorizing kinetic pathways in transformations.	[PO1]

Performance Indicators (PIs):

1. Calculate and interpret thermodynamic properties, such as entropy, enthalpy, and free energy, using Statistical mechanics methods.

2. Apply Statistical mechanics principles to analyze and predict the behavior of systems in different thermodynamic conditions.

3. Demonstrate proficiency in utilizing statistical tools and mathematical techniques to determine thermodynamic properties accurately.

4. Explain the factors influencing atomic stability and their impact on the formation of stable molecules.

5. Apply knowledge of atomic stability principles to predict the stability of different molecular structures.

6. Analyze and compare the stability of various atoms and molecules based on their electronic configurations and bonding patterns.
7. Describe the interaction between molecules and atoms with electromagnetic radiation.
8. Demonstrate the ability to calculate and interpret the response of molecules and atoms to different wavelengths and intensities of electromagnetic radiation.
9. Utilize spectroscopic techniques to analyze experimental data and determine molecular and atomic properties.
10. Predict and interpret the spectra (UV-Vis, IR, NMR, etc.) of different molecules and atoms.
11. Identify the characteristic peaks and patterns in spectra and relate them to the molecular or atomic structure.
12. Correlate the spectroscopic data with the electronic and vibrational transitions occurring in the molecules and atoms.
13. Explain the fundamental principles and theories of chemical kinetics.
14. Analyze and interpret experimental data related to reaction rates and rate laws.
15. Predict the effect of various factors (temperature, concentration, catalysts) on the rate of chemical reactions.
16. Identify and differentiate between different kinetic pathways in chemical transformations.
17. Analyze and predict the reaction mechanisms based on kinetic data and theoretical models.
18. Design experiments to study and validate proposed kinetic pathways in chemical reactions.

Suggested Readings

1. Atkins, P. W. 2002 Physical Chemistry, 7th Edition, Oxford University Press, New York.
2. Maczek, A. Statistical Thermodynamics, Oxford University Press Inc., Ne
3. Reif, F, 1985 Fundamental of Statistical and Thermal Physics McGraw Hill, International edition.
4. Barrow, G. M. Introduction to Molecular Spectroscopy McGraw Hill
5. Pilar, F. L. 1990 Elementary Quantum Chemistry 2nd Edition, McGraw - Hill Publishing Company.
6. Atkins P. W. and Friedman, R. S, 1997, Molecular Quantum Mechanics 3rd Edition, Oxford Univ. Press.
7. Laidler, K. 1995 Chemical Kinetics Harper and Row.
8. Levine, I. N. 2002 Physical Chemistry, 5th Edition, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
9. Brouard, M. 1998 Reaction Dynamics, Oxford University Press, Oxford.

10. Levine R.D. and Bernstein, R.B. 1987 Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, Oxford.

SEMESTER II

Course Name: Instrumentation Techniques I **Code:** CHE-C-554
Semester: II **Course Level:** 500 **Total Marks:** 100
L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)
Type: Core Theory

Course Learning Outcomes (CLOs):

By the end of the Instrumentation Technique I course, students will be able to:

1. Demonstrate a comprehensive understanding of the principles and concepts underlying rotational and vibrational spectroscopy, including microwave spectroscopy, infrared spectroscopy, and Raman spectroscopy.
2. Apply their knowledge to analyze and interpret spectra of rigid diatomic molecules, non-rigid rotors, and polyatomic molecules using rotational and vibrational spectroscopy techniques.
3. Identify the absorption frequencies of common functional groups and explain the effects of electronic and steric factors, as well as hydrogen bonding, on vibrational spectra.
4. Compare and contrast the principles and applications of atomic spectroscopy, UV-Visible spectroscopy, and emission spectroscopy, and demonstrate proficiency in analyzing spectra of various compounds.
5. Understand the principles, instrumentation, and techniques used in NMR spectroscopy, including chemical shifts, spin-spin interactions, and nuclear coupling constants.
6. Apply NMR spectroscopy to classify and interpret spectra of different coupling types, such as AB, ABC, AMX, and A2B2, and demonstrate knowledge of lanthanides shift reagents and spin relaxation processes.
7. Comprehend the basic principles and applications of Electron Spin Resonance (ESR) spectroscopy, including the effects of hyperfine splittings, g-values, anisotropic effects, and the EPR of triplet states.
8. Analyze optical rotatory dispersion, circular dichroism, and their applications in determining the absolute configuration of complexes and identifying isomerism due to non-planarity of chelate rings.
9. Understand the basic principles and conditions of Mössbauer spectroscopy, interpret spectral parameters, and analyze temperature-dependent effects and their structural implications for iron and tin complexes.

10. Integrate theoretical knowledge with practical applications by performing spectroscopic analyses, interpreting spectral data, and effectively communicating results.

Course Description: This course provides a detailed understanding of various spectroscopic techniques used in chemical analysis and characterization. The course is divided into four units, each focusing on different aspects of spectroscopy and its applications.

Course Outline:

Unit 1

Rotational and Vibrational Spectroscopy: (i) Microwave Spectroscopy: Rigid diatomic molecule, intensities of spectral lines, isotopic substitution, non-rigid rotor, polyatomic molecules. (ii) Infrared Spectroscopy: Simple harmonic oscillator, anharmonic oscillator,

diatomic vibrating rotator, polyatomic molecules, vibration modes. Absorption frequency of common functional groups, electronic and steric effects, effects of Hydrogen bonding. Interpretation of IR spectra. iii) Raman Spectroscopy: Principles of Raman Spectroscopy and its comparison with IR spectroscopy. Applications of vibrational spectroscopy: Symmetry and shapes of AB 2 , AB 3 , AB 4 , modes of bonding in ambidentate ligands.

Unit 2

Atomic, UV-Vis and Emission Spectroscopy: (i) Atomic spectroscopy: Principles and Application (ii) UV-Visible Spectroscopy: Principles and Applications: dienes, polyenes, carbonyl compounds and α, β-unsaturated carbonyl compounds. Woodward Hoffman rule and its application in aromatic compounds. (iii) Emission Spectroscopy: Principle and application of Fluorescence, phosphorescence, chemi-luminescence

Unit 3

Spin Resonance spectroscopy (i) NMR Spectroscopy: Principle, instrumentation and different techniques (continuous wave and Fourier transformed) of NMR spectroscopy, factors influencing chemical shifts of the spectra, anisotropy, spin-spin interactions, coupling constant (J), spin-decoupling, Nuclear Overhauser Effect (NOE), classification of AB, ABC, AMX and A 2 B 2 type couplings, First order spectra, lanthanides shift reagent, spin-spin and spin lattice

relaxation processes. Applications. (ii) Electron Spin Resonance Spectroscopy: Basic principle, Hyperfine splittings (isotropic systems); the g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer’s degeneracy); Anisotropic effects (the g-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes.

Unit 4

(i) Optical Rotatory Dispersion and Circular Dichroism: Linearly and circularly polarized lights; optical rotatory power and circular birefringence, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects; Assignment of electronic transitions; applications of ORD and CD for the determination of absolute configuration of complexes and isomerism due to non-planarity of chelate rings. (ii) Mössbauer Spectroscopy: Basic principle, conditions for Mössbauer spectroscopy, Spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature-dependent effects, structural deductions for iron and tin complexes, miscellaneous applications.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Demonstrate a comprehensive understanding of the principles and concepts underlying rotational and vibrational spectroscopy, including microwave spectroscopy, infrared spectroscopy, and Raman spectroscopy.	[PO1][PO2]
CLO2	Apply their knowledge to analyze and interpret spectra of rigid diatomic molecules, non-rigid rotors, and polyatomic molecules using rotational and vibrational spectroscopy techniques.	[PO1][PO2][PO3]
CLO3	Identify the absorption frequencies of common functional groups and explain the effects of electronic and steric factors, as well as hydrogen bonding, on vibrational spectra.	[PO2][PO3]
CLO4	Compare and contrast the principles and applications of atomic spectroscopy, UV-Visible spectroscopy, and emission spectroscopy, and demonstrate proficiency in analyzing spectra of various compounds.	[PO2][PO3]
CLO5	Understand the principles, instrumentation, and techniques used in NMR spectroscopy, including chemical shifts, spin-spin interactions, and nuclear coupling constants.	[PO1]
CLO6	Apply NMR spectroscopy to classify and interpret spectra of different coupling types, such as AB, ABC, AMX, and A2B2, and demonstrate knowledge of lanthanides shift reagents and spin relaxation processes.	[PO2][PO3]
CLO7	Comprehend the basic principles and applications of Electron Spin Resonance (ESR) spectroscopy, including the effects of hyperfine splittings, g-values, anisotropic effects, and the EPR of triplet states.	[PO1]
CLO8	Analyze optical rotatory dispersion, circular dichroism, and their applications in determining the absolute configuration of complexes and identifying isomerism due to non-planarity of chelate rings.	[PO1][PO2]
CLO9	Understand the basic principles and conditions of Mössbauer spectroscopy, interpret spectral parameters, and analyze temperature-dependent effects and their structural implications for iron and tin complexes.	[PO1][PO2]
CLO10	Integrate theoretical knowledge with practical applications by	[PO3]

	performing spectroscopic analyses, interpreting spectral data, and effectively communicating results.	

Performance Indicators (PIs):

1. Demonstrate proficiency in analyzing and interpreting spectra from rotational and vibrational spectroscopy techniques.
2. Apply knowledge of functional group absorption frequencies and their effects on vibrational spectra to identify and characterize compounds.
3. Successfully analyze and interpret atomic, UV-Visible, and emission spectra of different compounds.
4. Apply principles and techniques of NMR spectroscopy to interpret chemical shifts, spin-spin interactions, and coupling constants in spectra.
5. Classify and interpret NMR spectra of different coupling types, such as AB, ABC, AMX, and A2B2.
6. Demonstrate understanding of the principles and applications of ESR spectroscopy, including the effects of hyperfine splittings and anisotropic interactions.
7. Apply optical rotatory dispersion and circular dichroism techniques to determine absolute configuration and identify isomerism in chelate rings.
8. Interpret and analyze Mössbauer spectra, including spectral parameters and temperature-dependent effects.
9. Effectively perform spectroscopic analyses, interpret data accurately, and communicate results clearly.
10. Demonstrate a comprehensive understanding of the theoretical principles and practical applications of the spectroscopic techniques covered in the course.

Suggested Readings:

Text Books

1. R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.

2. J.R.Dyer, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall, New Delhi (1978).

3. A. B. P. Lever, Inorganic Electronic Spectroscopy Elsevier, 1984, 2nd Ed.

4. D.L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy Harcourt College Publisher, NY, 2001

5. R.M. Silverstein and F.X. Webster, Spectroscopic Identification of Organic Compounds, 6 th Edition (2003) John Wiley, New York.

6. W. Kemp, Organic Spectroscopy, 3rd Edn. (1991), Macmillan, London.

7. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry – An Introduction, 7 th Edition (2000), Saunders College Publishing, Philadelphia, London.

8. J. M. Hollas, Modern Spectroscopy, 4th edition (2004) John Wiley & Sons, Ltd.,Chichester.

9. C. N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4^{th} edition (1994),Tata McGraw Hill, New Delhi.

10. R.J. Abraham and J.Fishe and P. Loftus, Introduction to NMR Spectroscopy John Wiley & Sons. 1994

11. J. A. Weil, J.R. Balton & J.E. Wertz, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications. John Wiley and Sons:NY, 1994.

Reference Books

1. D.H. Williams and I.F. Fleming, Spectroscopic Methods in Organic Chemistry, 4 th Edition (1988), Tata-McGraw Hill, New Delhi.

2. P.Y Bruice, Organic Chemistry, 2nd Edition (1998) Prentice – Hall, New Delhi.

3. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.

4. G. Aruldhas, Molecular Structure and spectroscopy, Prentice Hall of India Pvt. Ltd., New Delhi (2001).

5. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.

6. G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.

7. J. H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.

8. A Carrington and A. D. Mc Lachlan, Introduction to Magnetic Resonance, Chapman and Hall, London (1979).

9. R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, Addison Wesley, Longman Ltd, London (1986).

10. G. Hertzburg, Infrared and Raman Spectra (1945), Spectra of Diatomic Molecules (1950), Von Nostrand, New York.

11. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill

12. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 4th Edn. (1986), John Wiley & Sons, New York.

SEMESTER II

Course Name: Cyber Security **Code:** CHE-V-505

Semester: I **Course Level:** 500 **Total Marks:** 50

L+T+P: 1+1+0 =2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Open Course

Course Learning Outcomes:

1. Understand the concepts and principles of cyber security and the challenges it presents in today's digital world.
2. Identify different types of cyber crimes and their impact on individuals, organizations, and society.
3. Analyze the modus operandi of cybercriminals and develop strategies to report and address cyber-crimes effectively.
4. Apply remedial and mitigation measures to protect against cyber threats and ensure data security.
5. Evaluate the legal framework governing cyber security, including the IT Act 2000 and its amendments.
6. Assess the security aspects of e-commerce and digital payment systems, including common frauds and preventive measures.
7. Understand the guidelines and provisions related to digital payments, customer protection, and unauthorized banking transactions set by regulatory authorities like RBI.
8. Gain insights into the National Cyber Security Policy and Strategy and its implications for safeguarding digital infrastructure.
9. Analyze and interpret case studies to understand real-world cyber security challenges and develop effective solutions.
10. Develop a comprehensive understanding of ethical and professional practices in the field of cyber security.

Course Description: This course provides a comprehensive understanding of cyber security, including the challenges and issues associated with it. Students will learn about cyber crimes, cyber laws, and the modus operandi of cybercriminals. The course covers remedial and mitigation measures, as well as the legal perspective of cybercrime, including the IT Act 2000 and its amendments. Case studies will be used to illustrate real-world examples.

Course Outline:

Unit 1: Introduction to cyber security. Issues and challenges of cyber security. Cybercrimes and cyber laws. Cybercriminals modus-operandi, Reporting of cyber-crimes, Remedial and mitigation measures, Legal perspective of cybercrime, IT Act 2000 and its amendments. Case Studies.

Unit 2: e-commerce and Digital Payments. E-Commerce security. Banking Cards, Unified Payment Interface (UPI), e-Wallets, Unstructured Supplementary Service Data (USSD), Aadhar enabled payments, Digital payments related common frauds and preventive measures. RBI guidelines on digital payments and customer protection in unauthorised banking transactions. Relevant provisions of Payment Settlement Act,2007. National cyber security policy and strategy

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Understand the concepts and principles of cyber security and the challenges it presents in today's digital world.	PO1
CLO2	Identify different types of cyber crimes and their impact on individuals, organizations, and society.	PO2
CLO3	Analyze the modus operandi of cybercriminals and develop strategies to report and address cyber-crimes effectively	[PO] [PO2] [PO3]
CLO4	Apply remedial and mitigation measures to protect against cyber threats and ensure data security.	[PO1][PO3]
CLO5	Evaluate the legal framework governing cyber security, including the IT Act 2000 and its amendments.	PO1
CLO6	Assess the security aspects of e-commerce and digital payment systems, including common frauds and preventive measures.	PO3
CLO7	Understand the guidelines and provisions related to digital payments, customer protection, and unauthorized banking transactions set by regulatory authorities like RBI.	PO3
CLO8	Gain insights into the National Cyber Security Policy and Strategy and its implications for safeguarding digital infrastructure.	PO1
CLO9	Analyze and interpret case studies to understand real-world cyber security challenges and develop effective solutions.	PO2
CLO10	Develop a comprehensive understanding of ethical and professional practices in the field of cyber security.	PO3

Performance Indicators (Ps):

1. Demonstrate knowledge and understanding of key concepts and principles of cyber security.
2. Analyze and evaluate different types of cybercrimes and their impact on individuals, organizations, and society.
3. Effectively report and document cybercrimes, including providing accurate and detailed information.
4. Implement appropriate remedial and mitigation measures to protect against cyber threats and ensure data security.
5. Apply relevant provisions of cyber laws, including the IT Act 2000 and its amendments, in practical scenarios.

6. Evaluate the security aspects of e-commerce and digital payment systems, identifying vulnerabilities and proposing effective preventive measures.
7. Interpret and apply guidelines and regulations related to digital payments, customer protection, and unauthorized banking transactions issued by regulatory authorities.
8. Analyze the National Cyber Security Policy and Strategy and its implications for safeguarding digital infrastructure.
9. Analyze and propose solutions to real-world cyber security challenges based on case studies and industry best practices.
10. Demonstrate ethical and professional conduct in all aspects of cyber security, including respecting confidentiality, privacy, and legal requirements.

Suggested Readings:

1. Cyber Security Understanding Cyber Crimes, Computer Forensics and Legal Perspectives by Sumit Belapure and Nina Godbole, Wiley India Pvt. Ltd.
2. Information Warfare and Security by Dorothy F. Denning, Addison Wesley.
3. Security in the Digital Age: Social Media Security Threats and Vulnerabilities by Henry A. Oliver, Create Space Independent Publishing Platform.
4. Data Privacy Principles and Practice by Natraj Venkataramanan and Ashwin Shriram, CRC Press.
5. Information Security Governance, Guidance for Information Security Managers by W. KragBrothy, 1st Edition, Wiley Publication.
6. Auditing IT Infrastructures for Compliance By Martin Weiss, Michael G. Solomon, 2nd Edition, Jones Bartlett Learning.

SEMESTER II

Course Name: Chemistry Practical II **Code:** CHE-P-556

Semester: II **Course Level:** 500 **Total Marks:** 100

L+T+P: 0+0+4 = 4 Credits (Lecture = 0 hrs; Tutorial = 0 hrs; Practical = 60 hrs)

Type: Core Practical

Course Learning Outcomes (CLOs): By the end of this course, students will be able to:

1. Analyze and select appropriate methods for estimating metal ions or compounds.
2. Calculate the quantitative estimation of constituents in a mixture.
3. Exhibit expertise in employing column chromatography and thin-layer chromatography (TLC) to effectively separate desired compounds from natural products.
4. Successfully isolate and characterize specific compounds of interest, such as caffeine, casein, nicotine dipicrate, cinchonine, piperine, lycopene, β-carotene, oleic acid, eugenol, and limonene, utilizing appropriate techniques and instrumental analysis.
5. Conduct spectro-photometric (UV/VIS) estimations of various compounds with precision and accuracy.
6. Demonstrate proficiency in the proficient handling and utilization of laboratory equipment, techniques, and strict adherence to safety protocols throughout the experimental procedures.
7. Document and communicate experimental procedures, observations, and results with precision and clarity in well-structured written reports and comprehensive laboratory notebooks.

Course Description:

The Chemistry Practical II course provides hands-on experience in various techniques and procedures used in the estimation, extraction and analysis. Through a combination of laboratory experiments and data analysis, students will develop practical skills and gain a deeper understanding of priciples of chemistry.

Course Outline:

1. Ore, Alloy and Commercial Product Analysis (Any two)

a) Determination of Copper and iron from chalcopyrite.
b) Determination of iron from hematite by complexometric titration.
c) Determination of tin & lead from solder.
d) Determination of iron & chromium from mild steel.
e) Determination of copper and nickel from cupronickel.
f) Determination of iron from hematite using UV-Vis spectrophotometer.
g) Determination of phosphoric acid in soft drinks
h) Analysis of Cement

i) Determination of fluoride in toothpaste
j) Determination of Silica and Manganese in pyrolusite

2. Extraction of Organic Compounds from Natural Source (Any three)

a) Isolation of caffeine, an alkaloid, from tea leaves.
b) Isolation of casein from milk (the students are required to try some typical colour reactions of proteins)
c) Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported.)
d) Isolation of nicotine dipicrate from tobacco.
e) Isolation of cinchonine from cinchona bark.
f) Isolation of piperine from black pepper.
g) Isolation of lycopene from tomatoes.
h) Isolation of β-carotene from carrots.
i) Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid.
j) Isolation of eugenol from cloves.
k) Isolation of limonine from citrus rinds.
l) Extraction and identification of DNA from green peas and onions

3. Spectro-photometric (UV/VIS) Estimations (Any two)

a) Amino acids
b) Proteins
c) Carbohydrates
d) Cholesterol
e) Ascorbic acid
f) Aspirin
g) Caffeine

4. Physical and Analytical methods: Experiments based on (Any five**)**

a) UV - Visible spectroscopy with application
b)Fluorescence Spectroscopy with application
c)Infrared Spectroscopy
d) Determination of g-value by ESR method
e)NMR Spectroscopy
f)Solvents effects in spectra
g)Differential Scanning Calorimetry
h)High Pressure Liquid Chromatography
i)Cyclic voltametry
j)Enzymetic reaction
k)Polymer
l)Magnetic nanoparticles
m)Ionic liquids
n)Liquid crystals
o)Optical materials
p)Carbon based nanomaterials
q)Paper and column chromatography of plant pigments
r)Acetylation of ferrocene and its purification by column chromatography
s)Ternary phase diagram

t)Determination of surface tension by differential capillary method.
u)Determination of molecular weight of a macromolecule by viscometry.
v)Determination of molecular weight by Victor Meyer's method.
w)Cryoscopy and determination of degree of dissociation.
x)Analysis of a UV spectrum, Raman spectrum, IR spectrum, NMR spectrum and EPR spectrum. Calculation of oscillator strength and transition moment.
y) Potentiometric titrations using the pH meter and determination of pI
z) Conductometric titrations and determination of dissociation constant

Suggested Teaching-Learning Approaches:

1. Engaging Lectures: Employing interactive lectures coupled with live discussions and vivid demonstrations of laboratory skills and techniques.
2. Experiential Learning: Encouraging hands-on practice to actively engage students in real-life applications, fostering a deeper understanding of the subject matter.
3. Collaborative Learning: Facilitating group discussions, promoting active participation, and encouraging the exchange of ideas among students, leading to enhanced critical thinking and problem-solving skills.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Assignment	Oral Test, Viva-Voce, Presentation	Presentation
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Exhibit expertise in employing column chromatography and thin-layer chromatography (TLC) to effectively separate desired compounds from natural products.	[PO1][PO2]
CLO2	Isolate and characterize specific compounds of interest, such as caffeine, casein, nicotine dipicrate, cinchonine, piperine, lycopene, β-carotene, oleic acid, eugenol, and limonene, using appropriate techniques and instrumental analysis.	[PO2]
CLO3	Conduct spectro-photometric (UV/VIS) estimations of various organic	[PO3]

	compounds with precision and accuracy.	
CLO4	Execute targeted synthesis experiments, including the Diels-Alder reaction of anthracene and maleic anhydride, aspirin synthesis, Sandmeyer's reaction, Cannizzaro reaction, preparation of tribromobenzene, and acetoacetic ester condensation.	[PO1][PO2][PO3]
CLO5	Predict the identity and purity of synthesized compounds by employing melting point determination and employing diverse spectroscopic methods.	[PO1][PO2][PO3]
CLO6	Demonstrate proficiency in the proficient handling and utilization of laboratory equipment, techniques, and strict adherence to safety protocols throughout the experimental procedures.	[PO3]
CLO7	Document and communicate experimental procedures, observations, and results with precision and clarity in well-structured written reports and comprehensive laboratory notebooks.	[PO7]

Performance Indicators (PI)

1. Extract and isolate organic compounds from natural sources, achieving satisfactory yields and purities.
2. Execute chromatographic techniques, including column chromatography and TLC to separate and purify compounds effectively.
3. Perform spectro-photometric (UV/VIS) estimations of organic compounds accurately and obtain reliable concentration data.
4. Demonstrate proficiency in the synthesis of organic compounds by following synthetic procedures, monitoring reactions, and achieving desired products and their purification through recrystallization.
5. Characterize synthesized compounds using the spectroscopic data obtained from various instrumental techniques, including IR, UV-Vis, PL, NMR, and mass spectral analysis.
6. Follow safety protocols and handle laboratory equipment and chemicals responsibly to ensure personal safety and prevent accidents.
7. Communicate experimental procedures, observations, and results through well-organized and concise written reports and laboratory notebooks.

Suggested Readings:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.

2. Addison Ault Techniques and Experiments for Organic Chemistry 6th Ed. University Science Books (1998).

3. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry 4th Ed. Orient Longmans (1990).

4. Vogel, A. I. Vogel's Textbook of Practical Organic Chemistry 5th Ed. (revised by A.R. Tatchell et al.) Wiley (1989) ISBN 0582-46236-3

Distribution of marks:

Evaluation Methods	Marks
Experiment (Analysis/synthesis)	50
Home assignment/Internal Assessment	20
Laboratory Record	05
Attendance	05
Viva-voce	20

SEMESTER III

Course Name: Instrumental Techniques II **Code:** CHE-C-601

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Core Theory

Course Learning Outcomes (CLOs):

On completion of the course, students will be able to:

1. Demonstrate a solid understanding of chemical instrumentation and its components.
2. Apply electrochemical methods for qualitative and quantitative analysis.
3. Utilize advanced NMR techniques for molecular analysis.
4. Interpret spectroscopy and microscopy data using various techniques.
5. Analyze and interpret mass spectrometry data for compound identification.
6. Apply thermal analysis techniques for material characterization.

Course Description:

Instrumentation Techniques II is an advanced course that builds upon the foundational knowledge gained in Instrumentation Techniques I.

Course Outline:

Unit 1

A. Chemical Instrumentation: Elementary Electronics, Simple integrated circuit, Semiconductor, Power supply, transformer, operational amplifier, Lock-in amplifiers, Detectors (Oscilloscope and recorders), transducers, Rectifiers, Signal to noise ratio, Electronic components (Resistors, capacitors, inductors, transistors), Measuring instruments for pressure, temperature, pH, speed, flow, current and voltage.

B. Electrochemical Methods:

i)Polarography: Origin of polargraphy, Current-voltage relationship, Theory of polarographic waves, Instrumentation, Ilkovič equation, Qualitative and quantitative applications.

ii)Corrosion: Definition, causes and types of corrosion, electrochemical theories of corrosion, kinetics of corrosion (corrosion current and corrosion potential). Corrosion measurements, units of corrosion rate, passivity and its breakdown. Prevention of Corrosion.

iii) Cyclic Voltammetry: Cell design, instrumentation, current-potential relation for linear sweep voltammetry (LSV), cyclic voltammetry, interpretation of voltammograms.

Unit 2

Advanced NMR methods:Introduction to ^{13}C NMR, principles of decoupling, Application of DEPT. ^{1}H-^{1}H CLOSY, HETCOR, NOESY, ROESY. Basic introduction to ^{19}F and ^{31}P NMR and heteronuclear coupling. Solid-state NMR: Basic principles and applications.

Unit 3

Spectroscopy and Microscopy:

i) Electron Spectroscopy: Theory, Instrumentation and applications of Electron spectroscopy (ESCA and Auger)

ii) UV and X-ray photoelectron spectroscopy.

iii) Microscopy: Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning tunnelling microscopy (STM) and Atomic force microscopy (AFM).

iv) Plasma Emission Spectroscopy: Theory, Instrumentation and Analytical applications of inductively coupled plasma emission spectroscopy (ICPE).

Unit 4

A. Mass Spectrometry: Introduction, ion production, fragmentation, factors influencing ion abundance, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak; Ionization techniques (EI and FAB).

B. Thermal Analysis: Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Learning Outcomes (CLOs) with Program Outcomes (POs)

CLO1	Demonstrate a solid understanding of chemical instrumentation and its components.	[PO1]
CLO2	Apply electrochemical methods for qualitative and quantitative analysis.	[PO2] [PO3]
CLO3	Utilize advanced NMR techniques for molecular analysis.	[PO2] [PO3]
CLO4	Interpret spectroscopy and microscopy data using various techniques.	[PO2]
CLO5	Analyze and interpret mass spectrometry data for compound identification.	[PO2] [PO3]
CLO6	Apply thermal analysis techniques for material characterization.	[PO3]

Performance Indicators:

1.Students can demonstrate their understanding of chemical instrumentation by correctly identifying and explaining the function of various electronic components, measuring instruments, and detectors.

2.Students can apply electrochemical methods by performing polarographic measurements, interpreting current-voltage relationships, and accurately analyzing corrosion kinetics.

3.Students can utilize advanced NMR techniques by interpreting NMR spectra, identifying functional groups, and applying heteronuclear coupling concepts.

4.Students can analyze and interpret spectroscopy and microscopy data by accurately interpreting electron spectroscopy results, UV and X-ray photoelectron spectroscopy data, and microscopy images.

5.Students can analyze and interpret mass spectrometry data by identifying molecular ion peaks, analyzing fragmentation patterns, and recognizing isotopic effects.

6.Students can apply thermal analysis techniques by accurately interpreting thermogravimetric analysis (TGA), differential thermal analysis (DTA), and differential scanning calorimetry (DSC) data for material characterization.

Suggested Readings:

Text Books

1. R. S. Drago, Physical Methods in Chemistry, International Edition (1992), Affiliated East-West Press, New Delhi.
2. J.R.Dyer, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall, New Delhi (1978).
3. A. B. P. Lever, Inorganic Electronic Spectroscopy Elsevier, 1984, 2nd Ed.
4. D.L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy Harcourt College Publisher, NY, 2001
5. R.M. Silverstein and F.X. Webster, Spectroscopic Identification of Organic Compounds, 6 th Edition (2003) John Wiley, New York.
6. W. Kemp, Organic Spectroscopy, 3rd Edn. (1991), Macmillan, London.
7. D. A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Analytical Chemistry – An Introduction, 7 th Edition (2000), Saunders College Publishing, Philadelphia, London.
8. J. M. Hollas, Modern Spectroscopy, 4th edition (2004) John Wiley & Sons, Ltd.,Chichester.
9. C. N. Banwell and E.M. Mc Cash, Fundamentals of Molecular Spectroscopy, 4^{th} edition (1994),Tata McGraw Hill, New Delhi.
10. R.J. Abraham and J.Fishe and P. Loftus, Introduction to NMR Spectroscopy John Wiley & Sons. 1994
11. J. A. Weil, J.R. Balton & J.E. Wertz, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications. John Wiley and Sons:NY, 1994.

Reference Books

1. D.H. Williams and I.F. Fleming, Spectroscopic Methods in Organic Chemistry, 4 th Edition (1988), Tata-McGraw Hill, New Delhi.
2. P.Y Bruice, Organic Chemistry, 2nd Edition (1998) Prentice – Hall, New Delhi.
3. E. A. V. Ebsworth, D. W. H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, 1st Edn.(1987), Blackwell Scientific Publications, Oxford, London.

4. G. Aruldhas, Molecular Structure and spectroscopy, Prentice Hall of India Pvt. Ltd., New Delhi (2001).
5. R. L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, Modern Methods of Chemical Analysis, 2nd Edition (1976), John Wiley, New York.
6. G. D. Christian, Analytical Chemistry, 5th Edition (1994), John Wiley & Sons, New York.
7. J. H. Kennedy, Analytical Chemistry: Principles, 2nd Edition (1990), Saunders Holt, London.
8. A Carrington and A. D. Mc Lachlan, Introduction to Magnetic Resonance, Chapman and Hall, London (1979).
9. R. K. Harris, Nuclear Magnetic Resonance Spectroscopy, Addison Wesley, Longman Ltd, London (1986).
10. G. Hertzburg, Infrared and Raman Spectra (1945), Spectra of Diatomic Molecules (1950), Von Nostrand, New York.
11. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill
12. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, 4th Edn. (1986), John Wiley & Sons, New York.

SEMESTER III

Course Name: Organometallic Chemistry **Code:** CHE-E-602

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs):

On completion of course, students will be able to:

1. Analyze and differentiate the bonding and structure of σ- and π-bonded organometallic complexes.
2. Illustrate the structure and explain the reactivity of metal carbonyls.
3. Identify the factors contributing to the formation and stability of metal carbonyls and their clusters.
4. Recognize and explain the key reaction mechanisms involved in organometallic chemistry.
5. Compare and classify the applications of organometallic chemistry in homogeneous and heterogeneous catalysis

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Course Description: Organometallic Chemistry is an advanced course that explores the principles, synthesis, structure, bonding, and reactivity of organometallic compounds. The course covers a wide range of topics, including complexes of σ-donor π-acceptor ligands, metal carbonyls and metal clusters, organometallic reaction mechanisms, and the applications of organometallics in homogeneous and heterogeneous catalysis.

Course Outline:

Unit 1

Complexes of *σ*- donor *π*-acceptor ligands: (a) *σ* –bonded systems: metal-alkyls, -aryls and -hydrides, stability, preparation and reactivity, metal-carbonyls, metal-phosphines, metal-nitrosyls, metal-isocyanides: structures, reactivity and bonding, Metal-carbenes, metal-carbynes, Fischer carbenes, Schrock carbenes, complexes with N-heterocyclic carbenes, olefin metathesis.

(b) *π*-Complexes of Unsaturated Molecules: Structure, bonding and reactivity of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis, haptacity, 18 electron rule,

Unit 2

Metal Carbonyls and Metal Clusters. Metal carbonyls: Synthesis, structure and reactivity; bonding in metal carbonyls, variants of CO bridging, vibrational spectra of metal carbonyls, principal reaction types of metal carbonyls. Low nuclearity (M3-M4) and high nuclearity (M5-M10) carbonyl clusters. Metal-metal bonding(MO), skeletal electron counting. Wade-Mingos Lauher rule, isolobal analogy.

Unit 3

Organometallic reaction mechanism: Ligand exchange, Associative mechanism: Brookhart Polymerization Catalysts, 16 electron rule, Dissociative meachanism: Oxidative addition;, Reductive elimination; transmetallation: Suzuki-Miyaura, Migratory Insertion / De-insertion, Agostic interaction, β-Hydride Elimination: Wacker Oxidation, Heck Arylation.

Unit 4

Homogeneous & Heterogeneous Catalysis .Applications of organometallics in organic synthesis: C-C bond coupling reactions (Heck, Sonogashira, Suzuki), reduction using transition metal hydrides, asymmetric hydrogenation. Alkene isomerization; Hydrogenation; Hydroformylation; Monsanto acetic acid process; Alkene polymerization; Cross coupling reactions; Metathesis; C-H activation and functionalization; Buchwald-Hartwig Reaction and Metathesis reaction, Oxidation of olefins;

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Learning Outcomes (CLOs) with Program Outcomes (POs):

CLO1	Analyze and differentiate the bonding and structure of σ- and π-bonded organometallic complexes.	**[PO1] [PO2]**
CLO2	Illustrate the structure and explain the reactivity of metal carbonyls.	**[PO1] [PO2]**
CLO3	Identify the factors contributing to the formation and stability of metal carbonyls and their clusters.	[PO1][PO2]
CLO4	Recognize and explain the key reaction mechanisms involved in organometallic chemistry.	[PO1][PO2]
CLO5	Compare and classify the applications of organometallic chemistry in homogeneous and heterogeneous catalysis.	[PO1][PO3][PO2][PO4]

Performance Indicators (PIs):

1. Demonstrates a thorough understanding of the principles and concepts related to σ-donor π-acceptor ligands in organometallic complexes.
2. Analyzes the synthesis, structure, bonding, and reactivity of metal carbonyls and metal clusters.

3. Applies knowledge of organometallic reaction mechanisms to explain and predict the outcomes of key reactions.

4. Evaluates the role of organometallic compounds in homogeneous and heterogeneous catalysis, including their applications in organic synthesis.

5. Demonstrates proficiency in the interpretation of spectroscopic data and molecular structures of organometallic compounds.

6. Applies critical thinking and problem-solving skills in analyzing and proposing mechanisms.

Suggested Readings:

1.Huheey, J. 1993 E. Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York.

2.Cotton F. A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John-Wiley & Sons, New York.

3.Crabtree, R.H. 1988 The Organometallic Chemistry of the Transition Metals, 1st Edn., John-Wiley & Sons, New York.

4.Shriver , D. F. and Atkins, P. W. 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.

5.Greenhood, 1976 Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.

6.Cleydon, J. , Greeves, N. , Warren, S. and Wolthers, P. , 2001 Organic Chemistry: Oxford

7.Collman, J. P. , Hegedus, L. S. , Norton J. R and Finke, Richard G. 1987 Principles and Applications of Organotransition Metal Chemistry, 1st Edn., University Science Books, Mill Valley, California.

8.Elschenbroich, Ch. and. Salzer, A, 1991 Organometallics: A CLOsize Introduction, 2nd Edn.,VCH

9.Mehrotra, R. C. and Singh, A., 2004 Organometallic Chemistry: A Unified Approach, New age international limited, 2nd Edn.

SEMESTER III

Course Name: Advanced Topics in Organic Chemistry **Code:** CHE-E-603

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs):

1. Classify different types of stereochemistry in organic compounds, including the determination of special chiralities, absolute configurations, and the concept of pseudo chirality.
2. Predict the shape and stability of various conformations in molecules with different ring sizes and functional groups, with a focus on cyclohexanes and decalin systems.
3. Apply different methods of stereoselective synthesis to introduce chirality or generate new chiral centers in molecules, utilizing chiral substrates, auxiliaries, reagents, and catalysts.
4. Evaluate the advantages and disadvantages of various techniques employed in asymmetric synthesis and demonstrate their applications in the synthesis of natural products.
5. Explain the synthesis and applications of organic materials, such as fullerenes, carbon nanotubes, graphenes, conducting polymers, organic superconductors, and liquid crystals.
6. Describe the principles of green chemistry and their practical implementation in organic synthesis, including the utilization of green synthetic methods, catalysis, organic reactions in aqueous media, ionic liquids, supercritical fluids, microwave radiation, and solid-phase synthesis.
7. Apply theoretical concepts and principles to solve intricate problems related to organic synthesis, stereochemistry, and the practical use of organic materials.

Course Description:

This course includes advanced stereochemistry concepts, stereoselective synthesis techniques, the synthesis and application of organic materials, and the principles of green chemistry.

Course Outline:

Unit 1

Special topics in stereochemistry:

General consideration of molecular asymmetry and dissymmetry, Determination of Special chiralities- axial, planner and helical chiralities, determination of their absolute configurations. Topicities and relations, pseudo chirality, prochiral faces of carbonyl and alkenes. Meaning absolute and relative stereo chemistry of a molecule. chemical transformation, Shape and stability of various conformations of molecules of different ring sizes and containing different functional groups, conformation and reactivity in cyclohexanes and decalin systems. quasiracemates, dynamic stereochemistry , atropisomerism of biphenyls.

Unit 2

Stereoselective synthesis:

Different methods to introduce chirality or generate new chiral centres in a molecule. Asymmetric synthesis using chiral substrate, chiral auxiliaries, chiral reagents and chiral catalysts with various examples. Advantages and disadvantages of each of these techniques., Application of each of these techniques in synthesis of various natural products.

Unit 3

Synthesis and application of organic materials: Organic Materials: Synthesis of Fullerenes, Carbon nanotubes, graphenes and various conducting polymers. Conducting organics - Conducting polymers. Organic superconductors. Liquid crystals: mesomorphic behaviour, optical properties of liquid crystals, display devices. Organic light emitting diodes.

Unit 4

Green Chemistry and solid phase reactions. Green Chemistry: Overview. Set of principles of green chemistry, green synthetic methods, catalysis, organics reactions in aqueous media, ionic liquids, supercritical fluids and under microwave radiations. Solvent from organics reactions, solid phase organics reaction and catalysis.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Learning Outcomes (CLOs) with Program Outcomes (POs):

CLO1	Classify different types stereochemistry in organic compounds, including the determination of special chiralities, absolute configurations, and the concept of pseudo chirality.	[PO1]
CLO2	Predict the shape and stability of different conformations of a molecules with various ring sizes and functional groups, particularly focusing on cyclohexanes and decalin systems.	[PO2]
CLO3	Utilize different methods of stereoselective synthesis to introduce chirality or generate new chiral centers in molecules, including the use of chiral substrates, auxiliaries, reagents, and catalysts.	[PO2][PO3]
CLO4	Recognize the advantages and disadvantages of various techniques used in asymmetric synthesis and their applications in the synthesis of natural products.	[PO2]
CLO5	Describe synthesis and applications of organic materials, including fullerenes, carbon nanotubes, graphenes, conducting polymers, organic superconductors, and liquid crystals.	[PO1]
CLO6	Describe the principles of green chemistry and its application in organic synthesis, including the use of green synthetic methods, catalysis, organics reactions in aqueous media, ionic liquids, supercritical fluids, microwave radiation and solid phase synthesis.	[PO1]

CLO7	Utilize theoretical concepts and principles to solve complex problems related to organic synthesis, stereochemistry and the application of organic materials.	[PO3]

Performance Indicators (PIs)

1. Determine the absolute configurations of molecules with specific chiralities, using appropriate methods and techniques.
2. Predict the shape and stability of different conformations in complex molecules, considering ring sizes and functional groups. Interpret the principles of dynamic stereochemistry and the phenomenon of atropisomerism in biphenyls.
3. Utilize stereoselective synthesis techniques to introduce chirality or generate new chiral centers in molecules. Demonstrate effective use of chiral substrates, auxiliaries, reagents, and catalysts.
4. Compare the advantages and limitations of various asymmetric synthesis methods and apply them to the synthesis of natural products.
5. Discuss the synthesis and applications of organic materials, such as fullerenes, carbon nanotubes, graphenes, conducting polymers, and liquid crystals, based on scientific principles.
6. Interpret the optical properties of liquid crystals and their relevance to display devices and OLED technology.
7. Apply the principles of green chemistry to design and perform environmentally friendly organic synthesis, employing appropriate methods, solvents, and reaction conditions.
8. Critically analyze scientific literature pertaining to advanced topics in organic chemistry, showcasing a thorough comprehension of the subject matter.

SuggestedReadings:

1. Stereochemistry of Organic Compounds,.Eliel E.L. and Wilen, S.H., Wiley Interscience, NewYork,1994
2. Stereochemistry of Organic Compounds. Principles and Applications. D. Nasipuri. John Wiley & Sons, Chichester, 1991.
3. Classics in Stereoselective Synthesis, Wiley, Erick M. Carreira, Lisbet Kvaerno 2008
4. Stereoselective Synthesis in Organic Chemistry, Atta-ur-Rahman, Zahir Shah; Springer-VerlagNewYork,1993
5. Stereoselective Synthesis: A Practical Approach, 2nd, Revised and Updated Edition; Mihály Nógrádi, Wiley;1994

6. Antibiotics: Targets, Mechanisms and Resistance; Claudio O. Gualerzi, Letizia Brandi, Attilio Fabbretti, CynthiaL.Pon; Wiley-VCH; 2013

7. Antibiotics: Challenges, Mechanisms, Opportunities; Christopher J. Walsh, T. Wencewicz; 2016 ASM Press; 2016

8. Carbon Nanotubes and Related Structures: Synthesis, Characterization, Functionalization, and Applications Dirk M. Guldi, Nazario Martín ; WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim;AcademicPress;2010

9. Flat Panel Displays, Advanced Organic Materials; S.M. Kelly; RSC Materials Monographs; The Royal Society of Chemistry 2000

10. Conducting Polymers, Fundamentals and Applications: A Practical Approach; Prasanna Chandrasekhar; Springer Science & Business, 2013

11. Green Chemistry: An Introductory Text:, Lancaster, M. Royal Society of Chemistry; 2002

SEMESTER III

Course Name: Advanced. Statistical Thermodynamics **Code:** CHE-6-E-604

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs):

On completion of the course, students will be able to:

1. Demonstrate a comprehensive understanding of statistical mechanical ensembles, including the Grand Canonical ensemble, and their applications to various systems.
2. Apply statistical mechanics to analyze and describe ideal classical and quantum systems, such as ideal Bose and Fermi systems, ideal gases (monoatomic and diatomic), and systems in chemical equilibrium.
3. Analyze and calculate the statistical mechanics of interacting gases, both classically and quantum mechanically, including the derivation of partition functions and equations of state.
4. Examine and interpret the statistical thermodynamics of solids and liquids, including theories such as Einstein's theory, Debye theory, superconductivity in metals, lattice dynamics, hard sphere fluid, and liquid crystal systems.
5. Apply perturbation theory and Flory-Huggins polymer solution theory to analyze and describe liquids.

6. Evaluate the statistical mechanical theories of ionic solutions and their implications for the behavior of electrolytes.
7. Analyze phase transitions using models such as the Ising model, lattice gas, mean field theory, Kaanoff transformation, and renormalization group theory.
8. Apply theoretical concepts and principles from statistical thermodynamics to solve complex problems and conduct advanced calculations.
9. Critically evaluate and synthesize scientific literature related to statistical thermodynamics and identify current research trends in the field.
10. Demonstrate effective communication skills by presenting and explaining complex statistical thermodynamics concepts and theories to both technical and non-technical audiences.

Course Description:

This course provides an in-depth exploration of advanced concepts and theories in statistical thermodynamics. Students will develop a comprehensive understanding of the statistical mechanical ensembles and their applications to various systems, including ideal classical and quantum systems, interacting gases, solids, liquids, and phase transitions.

Course Outline:

Unit 1

Statistical Mechanical ensembles: Grand Canonical and other ensembles. Statistics of ideal classical and quantum systems: Ideal Bose system (Photons gas, Phonon gas, Helium Gas), superfluidity, Ideal Fermi system, Ideal Gas (Monoatomic, Diatomic gases), Chemical Equilibria in gases, Electrons in metals

Unit 2

Statistical Mechanics of Interacting Gases:Classical and Quantum Calculation of partition function for low densities, Alternative derivation of van der Waals equations, Cluster expansion for classical systems, Equation of state. Cluster expansion for quantum systems Virial expansion of equation of state, Imperfect Bose Gas

Unit 3

Statistical Thermodynamics of Solids and Liquids: Einstein's theory, Debye theory, Superconductivity in metals, Ginzberg-Landau theory of Superconductivity. Lattice Dynamics, Hard sphere fluid, Born Green equation, Integral equation. liquid crystal, Perturbation Theory of Liquids, Florry-Higgins polymer solution theory. Statistical Mechanical Theories of Ionic Solutions.

Unit 4

Phase Transitions: Ising model., Lattice gas, Mean field theory, Kaanoff transformation, Renormalization group theory.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Learning Outcomes (CLOs) with Program Outcomes (POs):

CLO1	Demonstrate a comprehensive understanding of statistical mechanical ensembles, including the Grand Canonical ensemble, and their applications to various systems.	[PO1]
CLO2	Apply statistical mechanics to analyze and describe ideal classical and quantum systems, such as ideal Bose and Fermi systems, ideal gases (monoatomic and diatomic), and systems in chemical equilibrium.	[PO2]
CLO3	Analyze and calculate the statistical mechanics of interacting gases, both classically and quantum mechanically, including the derivation of partition functions and equations of state.	[PO2][PO3]

CLO4	Examine and interpret the statistical thermodynamics of solids and liquids, including theories such as Einstein's theory, Debye theory, superconductivity in metals, lattice dynamics, hard sphere fluid, and liquid crystal systems.	[PO1][PO2]
CLO5	Apply perturbation theory and Flory-Huggins polymer solution theory to analyze and describe liquids.	[PO1][PO2]
CLO6	Evaluate the statistical mechanical theories of ionic solutions and their implications for the behavior of electrolytes.	[PO1][PO2]
CLO7	Analyze phase transitions using models such as the Ising model, lattice gas, mean field theory, Kaanoff transformation, and renormalization group theory.	[PO1][PO2]
CLO8	Apply theoretical concepts and principles from statistical thermodynamics to solve complex problems and conduct advanced calculations.	[PO3]
CLO9	Critically evaluate and synthesize scientific literature related to statistical thermodynamics and identify current research trends in the field.	[PO3]
CLO10	Demonstrate effective communication skills by presenting and explaining complex statistical thermodynamics concepts and theories to both technical and non-technical audiences.	[PO7]

Performance Indicators (PIs):

1. Demonstrate the ability to apply statistical mechanical ensembles to analyze and describe different systems, as evidenced by accurate and appropriate use of ensemble methods in problem-solving.
2. Successfully analyze and interpret the statistical mechanics of ideal classical and quantum systems, including the ability to calculate relevant properties and explain their significance.
3. Calculate and interpret equations of state for interacting gases, showcasing an understanding of the underlying concepts and their application in describing real-world systems.
4. Show an understanding of the thermodynamics of solids, liquids, and phase transitions, as demonstrated by the ability to explain relevant theories and phenomena associated with these systems.
5. Apply theoretical concepts to analyze superconductivity, lattice dynamics, and polymer solutions, showcasing an understanding of their principles and implications.

6. Evaluate the statistical mechanics of ionic solutions and electrolytes, including the ability to analyze their behavior and make connections to experimental observations.
7. Successfully apply models and theories to analyze and explain phase transitions, demonstrating an understanding of their mechanisms and properties.
8. Solve complex problems using statistical thermodynamics principles, showcasing the ability to apply appropriate mathematical techniques and logical reasoning to arrive at accurate solutions.
9. Critically evaluate scientific literature related to statistical thermodynamics, including the ability to identify key findings, assess the validity of methodologies, and recognize gaps or areas for further research.
10. Communicate statistical thermodynamics concepts effectively through written reports, presentations, and discussions, showcasing clear and concise explanations that are accessible to both technical and non-technical audiences.

Suggested Readings

1.Hill T. L., An Introduction to Statistical Thermodynamics: Dover Publications, New York
2.Chandler D. Introduction To Modern Statistcal Mechanics: Oxford University, Press, New York
3.Reif F., Fundamentals of Statistical and Thermal Physics, Levant Books, Kolkata
4. Mc Quarrie Donald, Statistical Mechanics, Harper and Row Publishers
5. Sinha S. K., Introduction to Statistical Mechanics, Narosa Publisher

SEMESTER III

Course Name: Chemistry of Inorganic Materials **Code:**CHE-E-605

Semester: III **Course Level:** 600 **Total Marks:**100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Outcomes (CLOs):

By the end of this course, students will be able to:

1. Apply knowledge of solid-state chemistry principles to analyze and identify the nature of bonding in solid state compounds.
2. Classify compounds based on their crystal systems and distinguish the differences in ion packing structures.
3. Compare and differentiate the nature of non-covalent interactions in supramolecular systems.
4. Recognize mesophases and evaluate their birefringence properties.
5. Classify different types of inorganic polymers and assess their applications.

Course Description:

Chemistry of Inorganic Materials provides an in-depth exploration of the chemistry of inorganic materials, with a focus on solid-state chemistry, structure of solids, supramolecular chemistry, and metallomesogens & inorganic polymers. Students will gain a comprehensive understanding of the principles and applications of inorganic materials, including their synthesis, characterization, and properties.

Course Outline:

Unit- I: Solid State Chemistry:

Bonding in solids and Crystal energetic. Crystal classifications, Madelung constant and Lattice energy. Electronic properties and Band theory of solids. Free electron model, Refinement to simple band theory- k-space and Brillouin Zones, Band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, Doped semiconductors, p-n junctions.

Unit- II: **Structure of Solids:** Crystal systems; Designation of crystal faces, lattice structures and unit cell; Bragg's law; X-ray diffraction by crystals; Close packing, radius ratio rules, calculation of some limiting radius ratio values; Structures of NaCl, KCl, ZnS, CsCl and CaF_2; Stoichiometric and nonstoichiometric defects, impurity defects, semi-conductors.Packing in solids, Crystal structures of representative systems, Pervoskites, Silicates and Zeolites, Cements, Glasses, Quasicrystals, Nanostructures.

Unit III: Supramolecular Chemistry

Origin of supramolecular chemistry-"Chemistry beyond the molecules". Concepts and terminology of supramolecular chemistry. Natural types of supramolecular interactions (Hydrogen bonding, van der Waal‟s interaction, π-stacking, CH---π interaction. supramolecular chemistry in inorganic perspective. Inorganic crystal engineering and design principle of metal organic framework (MOF) and inorganic-organic hybrid material. Application of MOFs in material science

Unit IV: Metallomesogens & Inorganic Polymers

Basic concepts, types of meso-phases, synthetic strategies, characterization and applications.

Inorganic Polymers: Classification, Types of Inorganic Polymerization, Comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulfur-nitrogen, sulfur-nitrogen-fluorine compounds, chalcogenide clusters – binary and multi-component systems, homolytic inorganic systems.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Outcome (CLOs) with Program Outcome (POs):

CLO1	Apply knowledge of solid-state chemistry principles to analyze and identify the nature of bonding in solid state compounds	[PO1[PO2]
CLO2	Classify compounds based on their crystal systems and distinguish the differences in ion packing structures.	[PO1[PO2]
CLO3	Compare and differentiate the nature of non-covalent interactions in supramolecular systems	[PO1][PO2]
CLO4	Recognize mesophases and evaluate their birefringence properties	[PO1][PO2][PO4]
CLO5	Classify different types of inorganic polymers and assess their applications	[PO3]

Performance Indicators (PIs):

1. Demonstrates a strong understanding of solid-state chemistry, including the bonding in solids, crystal energetics, and electronic properties of materials.
2. Applies the principles of crystallography and X-ray diffraction to determine crystal structures and analyze the packing in solids.
3. Utilizes knowledge of supramolecular chemistry to explain and predict the behavior of inorganic materials beyond individual molecules.
4. Applies the principles of inorganic polymerization to classify and compare inorganic polymers with organic polymers.
5. Demonstrates an understanding of the synthesis, characterization, and applications of metallomesogens and inorganic polymers.
6. Applies the principles of metal-organic frameworks (MOFs) in the design and application of materials in material science.
7. Analyzes and evaluates the structure-property relationships of inorganic materials, including their electronic, optical, and mechanical properties.
8. Demonstrates proficiency in laboratory techniques for synthesizing and characterizing inorganic materials, including X-ray diffraction, spectroscopy, and microscopy.
9. Demonstrates effective problem-solving skills in the analysis of complex inorganic materials systems.
10. Communicates scientific ideas and findings effectively through written reports and oral presentations.

Suggested Readings:

1. Greenwood N. N. and. Earnshaw, A. 1997 Chemistry of the Elements, 2nd Edn., Butterworth Heinemann, London.
2. Lehn J. M., 1995 Supramolecular Chemistry, VCH, Weinheim.
3. Kahn O., 1993 Molecular Magnetism, VCH, Weinheim.Cotton, F. A., Wilkinson, G., Murillo C. A. and Bochmann, M., 2003, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons (Asia), Singapore.
4. Mark, J. E., Allcock, H. R. and West, |R. 2004 Inorganic Polymers, 2nd Edn., Oxford University Press.
5. Huheey, J. 1993 Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York
6. Miessler G. L. and Tarr, D. A. 1999 Inorganic Chemistry, 2nd Edn., Prentice Hall International Inc., London.
7. Serrano, J. L. 1996 Metallomesogens, VCH, Weinheim.

SEMESTER III

Course Name: Instrumental Techniques for Organic Chemistry **Code:** CHE-E-606

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs)

1. Explain the advanced concepts of ^{1}H NMR spectroscopy and ^{13}C NMR spectroscopy, including the interpretation of chemical shifts, spin-spin coupling, complex spin-spin interactions, factors influencing coupling constants, and the classification of spin systems.
2. Apply advanced concepts in ^{1}H NMR spectroscopy, such as chemical exchange, spin decoupling, contact shift reagents, solvent effects, nuclear Overhauser effect (NOE), and the resonance of other nuclei such as ^{31}P and ^{19}F.
3. Define the principles and applications of 2D NMR techniques, including CLOSY, TOCSY, HMQC, HMBC, NOESY, and 2D-INADEQUATE experiments, and utilize these techniques for structure elucidation.
4. Discuss the principles and instrumentation of mass spectrometry, including ionization methods, detectors, fragmentation rules, the nitrogen rule, and the interpretation of mass spectra.

5. Employ a combination of UV, IR, PMR, CMR, 2D NMR, and mass spectrometry to determine molecular structures and elucidate reaction sequences.
6. Explain the principles of molecular dissymmetry and chiroptical properties, including circular birefringence, circular dichroism, ORD and CD curves, Cotton effects, Faraday and Kerr effects, and their applications in structural and stereochemical analysis.
7. Describe the principles, theory, instrumentation, and applications of separation techniques such as gas-liquid chromatography, HPLC, size exclusion chromatography, GC-MS, LC-MS, UPLC, HPTLC, ion pair and ion exchange chromatography, and supercritical fluid chromatography.

Course Description:

This course provides an in-depth exploration of advanced spectroscopic techniques and structure elucidation methods used in organic chemistry. Students will develop a comprehensive understanding of the principles, instrumentation, and applications of various spectroscopic and separation techniques.

CourseOutline:

Unit 1

^{1}H NMR Spectroscopy and ^{13}C NMR spectroscopy :

^{1}H NMR Spectroscopy: Chemical exchange, effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant “J”, classification of spin system like AB, AX, AX_2, ABX, AMX, ABC, A_2B_2. Spin decoupling, Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic 4 double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear overhauser effect (NOE), resonance of other nuclei like ^{31}P, ^{19}F. ^{13}C NMR spectroscopy: FT NMR, Types of ^{13}C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, Homonuclear (^{13}C-^{13}C) and Hetero nuclear (^{13}C-^{1}H)coupling constants.

Unit 2

2D NMR Techniques: General idea about two-dimensional NMR spectroscopy, Correlation spectroscopy (CLOSY)- Homo CLOSY (1H-1H), TOCSY, Hetero CLOSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Mass Spectrometry: Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupoule mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors influencing ion abundance, single and multiple bond cleavage, rearrangements, Nitrogen rule and interpretation of mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak;

Unit 3

Structure elucidation through the application of UV, IR, PMR, CMR, 2D NMR and Mass spectrometry. (Including reaction sequences)

Unit 4

Molecular dyssemetry and chiroptical properties Linear and circularly polarized lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effects, Faraday and Kerr effects. The axial halo-ketone rule, Octent diagrams, Helicity and Lowe's Rule. Application of ORD and CD to structural and stereochemical problems.

Separation techniques: Fundamental principles, theory, instrumentation and application of Gas-liquid chromatography, HPLC, Size Exclusion chromatography, GC-MS, LC-MS, UPLC, HPTLC, Ion Pair & Ion Exchange Chromatography and Supercritical Fluid Chromatography.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs

CLO1	Explain the advanced concepts of ^{1}H NMR spectroscopy and ^{13}C NMR spectroscopy, including the interpretation of chemical shifts, spin-spin coupling, complex spin-spin interactions, factors influencing coupling constants, and the classification of spin systems.	PO1
CLO2	Apply advanced concepts in ^{1}H NMR spectroscopy, such as chemical exchange, spin decoupling, contact shift reagents, solvent effects, nuclear Overhauser effect (NOE), and the resonance of other nuclei such as ^{31}P and ^{19}F.	PO2
CLO3	Define the principles and applications of 2D NMR techniques, including CLOSY, TOCSY, HMQC, HMBC, NOESY, and 2D-INADEQUATE experiments, and utilize these techniques for structure elucidation.	PO1
CLO4	Discuss the principles and instrumentation of mass spectrometry, including ionization methods, detectors, fragmentation rules, the nitrogen rule, and the interpretation of mass spectra.	PO1
CLO5	Employ a combination of UV, IR, PMR, CMR, 2D NMR, and mass spectrometry to determine molecular structures and elucidate reaction sequences.	[PO1] [PO2]
CLO6	Explain the principles of molecular dissymmetry and chiroptical properties, including circular birefringence, circular dichroism, ORD and CD curves, Cotton effects, Faraday and Kerr effects, and their applications in structural and stereochemical analysis.	PO1
CLO7	Describe the principles, theory, instrumentation, and applications of separation techniques such as gas-liquid chromatography, HPLC, size exclusion chromatography, GC-MS, LC-MS, UPLC, HPTLC, ion pair and ion exchange chromatography, and supercritical fluid chromatography.	[PO1] [PO2][PO3]

Performance Indicators (PIs)

1. Accurately interpret 1H NMR and 13C NMR spectra, correctly identifying chemical shifts, spin-spin coupling patterns, and complex spin-spin interactions in various types of spin systems.

2. Apply advanced concepts of proton and carbon NMR spectroscopy, such as chemical exchange, spin decoupling, and the nuclear Overhauser effect (NOE), to analyze and interpret complex spectra, extracting valuable structural information.

3. Interpret 2D NMR spectra, including CLOSY, TOCSY, HMQC, HMBC, NOESY, and 2D-INADEQUATE, to establish signal correlations and gain insights into the structural and stereochemical properties of complex molecules.

4. Identify fragmentation patterns in mass spectra, recognize molecular ion peaks, and understand the impact of isotopes on mass spectra.

5. Determine molecular structures and elucidate reaction sequences accurately by integrating UV, IR, PMR, CMR, 2D NMR, and mass spectrometric data.

6. Analyze chiroptical properties such as circular dichroism (CD) and optical rotatory dispersion (ORD) curves, Cotton effects, Faraday, and Kerr effects, to gain insights into the structural and stereochemical characteristics of molecules.

7. Critically evaluate the advantages and disadvantages of different chromatographic techniques, including gas-liquid chromatography, HPLC, size exclusion chromatography, GC-MS, LC-MS, UPLC, HPTLC, ion pair and ion exchange chromatography, and supercritical fluid chromatography, for the separation, purification, and analysis of organic compounds.

SuggestedReadings:

1.Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 4th Ed. Cengage Learning, 20082. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, David Kiemle, David L. Bryce; 8th Ed. John Wiley and Sons. 2014

2.A Complete Introduction to Modern NMR Spectroscopy, Roger S. Macomber, Wiley, 1997

3.High-Resolution NMR Techniques in Organic Chemistry 3rd Edition Timothy D.W. ClaridgeElsevierScience,2016

4.Modern NMR Spectroscopy: A Guide for Chemists; Second Edition; Jeremy K. M. Sanders,BrianK.Hunter;Wiley,1993

5.Solving Problems with NMR Spectroscopy, 2nd Edition; Atta-ur-Rahman Muhammad ChoudharyAtia-tul-Wahab;AcademicPress,2015

6.Eberhard Breitmaier. Structure elucidation by NMR in organic chemistry. A practical guide. Wiley,Chichester,2002

7.Guide to Fluorine NMR for Organic Chemists, 2nd Edition, William R. Dolbier, Jr.,Wiley,2016

8.Organic Structures from Spectra, Fifth Edition, L D Field, S Sternhell, J R Kalman John Wiley

andSonsLtd.2015
9.Organic Structures from 2D NMR Spectra, L. D. Field, H. L. Li, A. M. Magill
11.Phosphorus-31 NMR Spectroscopy A Concise Introduction for the Synthetic Organic and OrganometallicChemist,OlafKühl,Springer
12. Organic Structure Determination Using 2-D NMR Spectroscopy, A Problem-Based ApproachJeffreyH.Simpson,AcademicPress,2008
13. Introduction to Modern Liquid Chromatography, Third Edition; Lloyd R. Snyder, Joshep J.Kirkland, John W. Dolan, A John Wiley & Sons, Inc., Publication, 2010
14.Chiral Chromatography, Thomas E. Beesley, Raymond P.W. Scott, Wiley,
15.Mass Spectrometry, Principles and Applications, Third Edition, Edmond de Hoffmann
16.Mass Spectrometry in Medicinal Chemistry; Klaus T. Wanner, Georg Ho¨fner, Wiley, 2007
17. ManMohan Srivastava, High-Performance Thin Layer Chromatography (HPTLC) SpringerHeidelbergDordrechtLondonNewYork,2011
18. LC/MS Applications in Drug Development, Mike S. Lee, Dominic M. Desiderio, Nico M.Nibbering,WileyInterscience,2002
19.Ord and Cd in Chemistry and Biochemistry, 1st Edition, Pierre Crabbe, Academic Press, 1972
20.Basic Gas Chromatography, 2nd Edition, Harold M. McNair, James M. Miller, Wiley, 2009
21.Practical Gas Chromatography, A Comprehensive Reference Dettmer-Wilde, Katja, Engewald,WernerSpringer2014
22. Gas Chromatography and Mass Spectrometry: A Practical Guide, 2nd Edition, O. David Sparkman Zelda Penton Fulton Kitson, Academic Press, 2011

SEMESTER III

Course Name: Nanochemistry **Code:** CHE-E-607

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Description:

This course provides a comprehensive understanding of nanochemistry, focusing on key concepts such as length scale, quantum confinement, and crystallography. Students will analyze synthesis methods and characterization techniques used in nanomaterials and gain insights into their optical, magnetic, and structural properties. The course explores nucleation and growth processes in nanoscale systems and covers surface functionalization and core/shell synthesis techniques. Students will learn to interpret characterization techniques like XRD, TEM, and AFM. The properties and applications of quantum dots, magnetic nanoparticles, metal nanoparticles, and carbon-based materials in various fields will be evaluated.

Course Learning Outcomes (CLOs)

On completion of the course, students will be able to:

1. Understand the concepts of length scale, quantum confinement, and crystallography in nanochemistry.
2. Analyze synthesis methods and characterization techniques used in nanomaterials.
3. Describe the optical, magnetic, and structural properties of nanomaterials and their applications.
4. Explain nucleation and growth processes in nanoscale systems.
5. Apply surface functionalization and core/shell synthesis techniques in nanomaterials.
6. Interpret characterization techniques for nanomaterials, including XRD, TEM, and AFM.
7. Evaluate the properties and applications of quantum dots, magnetic nanoparticles, metal nanoparticles, and carbon-based materials in various fields.

Course Outline:

Unit 1

Concept of length scale, de Broglie wavelength in a semiconductor, Exciton Bohr Radius, Quantum confinement, Density of states, The Fermi Energy, Fermi Velocity and Kubo gap, The Drude- Lorentz Model, Electron mean free path in metals. Super paramagnetic limit in magnetic nanoparticles. Wave particle duality in C_{60}. Basic crystallography, unit cell, Bravais lattice, Miller indices, planes, crystallographic directions, Single element crystals (SC, FCC, BCC), diamond structure, Zinc blende, Rock salt, Wurtzite, Spinel, Rutile, Perovskite, surface to volume ratio, calculation of density using unit cell approach. Debye Scherrer equation. Concept of concentration, Determination of molar extinction coefficient. Surface defects, Surface oxidation. Chemistry of small surfaces: Curvature and neighbouring-charge effects on chemical reactivity and equilibria (pKa's, redox potentials), Effect on melting temperature.

Unit 2

Nucleation and growth: Classical Theory, Monodispersity, Lamer Plot, Ostwald ripening, Digestive Ripening Homogeneous vs. heterogeneous nucleation and applications of nanomaterials, Anisotropic growth and shape control, catalyzed (seeded) growth, Nanocrystal doping, solid solutions and Vegard's rule. Non-classical growth. Effect of precursor reactivity and stability on size. Unusual precursor kinetics in III-V semiconductor nanocrystal formation.

Unit 3

Synthesis and characterization: Basics of CVD, sol-gel, microemulsion, template and hydrothermal methods. Hot injection (Bawendi and Murray method), heating up, Ion-exchange, Doping, Influence of Precursor reactivity. Reaction kinetics and influence of reaction parameters on the synthesis of CdSe, InP, PbS, Au, magnetite, perovskite nanocrystals. Synthesis and functionlaisation of Carbon nanotubes, Fullerenes and Graphenes. Core/shell synthesis, SILAR. Purification techniques. Phase transfer: solid phase, solution phase. Surface functionalisation with small molecules, drugs, antibody, cell penetrating peptide, contrast agents. Role of Linkers. Optical characterization: Absorption and photoluminescence (PL & PLE) spectroscopes, steady-state vs. fast spectroscopy, dynamic light scattering. Structural characterization: XRD, TEM, AFM, Deviations between bulk and near-surface crystal structures

Unit 4:

Properties and application: Quantum dots: Colloidal quantum dots, Optical properties of II-VI (CdSe, CdTe, ZnS), III-V (InP and InAs) and IV-VI (PbS and PbSe) colloidal quantum dots, lead halide Perovskite nanocrystals. Photostability of QDs in solution, thin film. Surface passivation, Core/shell nanocrystals. Determination of band gap. Application in solar cell, LED and bioimaging. Magnetic nanoparticles: Single domain. Multiple domains. Superparamagnetic. Finite size effects in magnetic nanoparticles, superparamagnetic limit, Neel-Brown expression, Blocking temperature. Properties of magnetite nanoparticles. Application in biology and magnetic recording.

Metal nanoparticles: Surface Plasmon resonance in Au nanoparticles. Surface Plasmon resonance, Mie theory of metal nanoparticles, Application in biology. Crystal structure of Co nanoparticles. Carbon based materials: Properties of C60, carbon nanotubes, fluorescence in carbon dots and fullerene. FRET.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of (CLOs) with Program Outcomes (POs):

CLO1	Understand the concepts of length scale, quantum confinement, and crystallography in nanochemistry.	[PO1]
CLO2	Analyze synthesis methods and characterization techniques used in nanomaterials.	[PO2]
CLO3	Describe the optical, magnetic, and structural properties of nanomaterials and their applications.	[PO1] [PO2]
CLO4	Explain nucleation and growth processes in nanoscale systems.	[PO1][PO2]
CLO5	Apply surface functionalization and core/shell synthesis techniques in nanomaterials.	[PO1] [PO2][PO3]
CLO6	Interpret characterization techniques for nanomaterials, including XRD, TEM, and AFM.	[PO2]
CLO7	Evaluate the properties and applications of quantum dots, magnetic nanoparticles, metal nanoparticles, and carbon-based materials in various fields.	[PO1][PO2] [PO3]

Performance Indicators

Unit 1: Concept of length scale, de Broglie wavelength, and Quantum confinement

1. Students can explain the concept of length scale and its significance in nanomaterials.
2. Students can calculate the de Broglie wavelength of electrons in a semiconductor.
3. Students can describe the concept of quantum confinement and its effect on electronic properties.
4. Students can analyze the density of states and its relationship to the electronic band structure.
5. Students can explain the Fermi energy, Fermi velocity, and Kubo gap in semiconductors.
6. Students can apply the Drude-Lorentz model to understand the electrical conductivity of metals.
7. Students can calculate the electron mean free path in metals.
8. Students can analyze the superparamagnetic limit in magnetic nanoparticles.
9. Students can discuss the wave-particle duality of C60.
10. Students can identify and describe different crystal structures and their properties.

Unit 2: Nucleation and growth of nanomaterials

1. Students can explain the classical theory of nucleation and growth.
2. Students can analyze the Lamer plot and understand its implications in nanomaterial synthesis.
3. Students can describe the phenomenon of Ostwald ripening and its effect on nanoparticle size distribution.
4. Students can compare and contrast homogeneous and heterogeneous nucleation processes.
5. Students can discuss the applications of nanomaterials based on their nucleation and growth mechanisms.
6. Students can explain anisotropic growth and shape control in nanomaterial synthesis.
7. Students can describe catalyzed (seeded) growth and its importance in achieving desired nanoparticle properties.
8. Students can discuss doping and solid solutions in nanocrystal synthesis.
9. Students can explain Vegard's rule and its application in determining the lattice constant of solid solutions.
10. Students can analyze non-classical growth phenomena in nanomaterials.

Unit 3: Synthesis and characterization of nanomaterials

1. Students can describe various synthesis methods such as CVD, sol-gel, microemulsion, template, and hydrothermal methods.
2. Students can explain the principles and applications of hot injection methods in nanomaterial synthesis.

3. Students can discuss the influence of precursor reactivity and stability on nanoparticle size and properties.
4. Students can analyze the reaction kinetics and the effect of reaction parameters on the synthesis of specific nanocrystals.
5. Students can describe the synthesis and functionalization of carbon nanotubes, fullerenes, and graphenes.
6. Students can explain core/shell synthesis and the principles of SILAR.
7. Students can discuss purification techniques for nanomaterials.
8. Students can explain phase transfer techniques for nanomaterials.
9. Students can describe surface functionalization methods and their applications.
10. Students can demonstrate knowledge of optical and structural characterization techniques for nanomaterials.

Unit 4: Properties and applications of nanomaterials

1. Students can explain the optical properties of different types of quantum dots (e.g., II-VI, III-V, IV-VI, and lead halide Perovskite nanocrystals).
2. Students can discuss the photostability of quantum dots and the importance of surface passivation.
3. Students can determine the band gap of quantum dots and relate it to their optical properties.
4. Students can describe the applications of quantum dots in solar cells, LEDs, and bioimaging.
5. Students can explain the properties and applications of magnetic nanoparticles, including single domain and superparamagnetic particles.
6. Students can discuss the finite size effects

Suggested Readings:

1. Kuno, M. Introductory Nanoscience, 2011, Taylor & Francis Group.
2. Rigach, A. L. (Editor), Semiconductor nanocrystal quantum dots: synthesis, assembly and applications.
3. Klimov, V. I. Semiconductor and Metal Nanocrystals: Synthesis and Electronic and Optical Properties (Optical Science and Engineering).
4. Thanh, N.T. K. and Sayed, M. A. 2012 Magnetic Nanoparticles: From Fabrication to Clinical Applications.
5. Huck, W. T. and Huck, Wilhelm T. S. (Editor) Nanoscale Assembly: Chemical Techniques.
6. Dresselhaus, M. S, Dresselhaus, G. and Avouris, P. Springer-Verlag. Carbon Nanotubes: Synthesis, Structure, Properties, and Applications.
7. Acklin, B. and Lautens, E. Magnetic Nanoparticles: Properties, Synthesis, and Applications.

8. Taurozzi, J. S. (2011) Nanoparticle-polymer composite membranes: Synthesis, characterization, and environmental applications.

9. Karn, B., Colvin, V., and Alivasatos, P. (2004) Nanotechnology and the Environment.

10. Zhou, B., Hermans, S., Somorjai, G. A. (Editors) Nanotechnology in Catalysis Volumes 1 and 2.

SEMESTER III

Course Name: Chemicals in Industry **Code:** CHE-E-608

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcome:

On completion of the course, students will be able to:

1. Demonstrate a comprehensive understanding of the role of chemicals in various industries, including dairy, leather, dyes, pigments, oils, soaps, detergents, food, drugs, and agrochemicals.
2. Identify and analyze the chemical processes involved in industrial applications and their impact on product quality, safety, and environmental considerations.
3. Apply theoretical knowledge to practical scenarios related to chemical processes and their utilization in industrial settings.
4. Evaluate the chemical composition, properties, and manufacturing processes of different chemicals used in industrial sectors.
5. Understand the significance of soil chemistry, including soil formation, classification, reactions, and their impact on agricultural productivity and fertility.
6. Assess the nutritional value, properties, and preservation techniques of common foodstuffs, as well as the effects of different processing methods on food quality.
7. Describe the properties, production, and applications of drugs and agrochemicals, with a particular focus on organophosphorus pesticides.
8. Demonstrate effective communication skills in presenting chemical concepts, experimental findings, and research outcomes related to industrial chemistry

Course Outline:

Unit 1

Dairy Chemistry: milk, milk proteins, enzymes, Leather chemistry: contituents of animal skin, processes used in leather preparation, Use of phosphorous and sulphur and nitrogen in various industries.

Unit 2

Dyes and Pigments: Classification of Dyes, Methods of preparation of commercial dyes of different classes with suitable examples. Typical manufacturing processes of few dyes, Fluorescent brightening agents, Photosensitive dyes, dyes as food additives, natural dyes. Oils, Soaps and Detergents: Refining of edible oils, Manufacturing of soaps, Detergents, Liquid Soaps. Manufacturing of fatty Acids and glycerol, greases from fatty acids, turkey –red oil. Soil Chemistry: Introduction, formation, classification and reactions of soil, soil acidity, alkalinity, productivity and fertility, chemical fertilizers and their effect, organic manures, micronutrients, bio-fertilizers.

Unit 3

Food Chemistry: Classification, chemical composition and nutritional value of common food stuffs, properties of foods, food preservation and processing, food deterioration, methods of preservation and processing by heat, cold, chill storage, deep freezing, drying, concentration, fermentation, and radiation, .

Unit 4 Drugs and Agrochemicals: Organophosphorus pesticides: Malathion, Monocrotophos, dimethoate, chloropyriphos, Dichlorpyriphos, Dichlororous, phenthoate.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Demonstrate a comprehensive understanding of the role of chemicals in various industries, including dairy, leather, dyes, pigments, oils, soaps, detergents, food, drugs, and agrochemicals.	[PO1]
CLO2	Identify and analyze the chemical processes involved in industrial applications and their impact on product quality, safety, and environmental considerations.	[PO1][PO2]
CLO3	Apply theoretical knowledge to practical scenarios related to chemical processes and their utilization in industrial settings.	[PO2]
CLO4	Evaluate the chemical composition, properties, and manufacturing processes of different chemicals used in industrial sectors.	[PO1][PO2]
CLO5	Understand the significance of soil chemistry, including soil formation, classification, reactions, and their impact on agricultural productivity and fertility.	[PO2]
CLO6	Assess the nutritional value, properties, and preservation techniques of common foodstuffs, as well as the effects of different processing methods on food quality.	[PO2]
CLO7	Describe the properties, production, and applications of drugs and agrochemicals, with a particular focus on organophosphorus pesticides.	[PO1]
CLO8	Demonstrate effective communication skills in presenting chemical concepts, experimental findings, and research outcomes related to industrial chemistry.	[PO7]

Performance Indicators

Unit 1

1. Knowledge of milk composition and processing techniques.
2. Understanding of milk proteins and their role in dairy product manufacturing.
3. Familiarity with leather constituents and preparation techniques.
4. Awareness of the use of phosphorus, sulfur, and nitrogen in various industries.

Unit 2

1. Classification of dyes and knowledge of their manufacturing processes.
2. Understanding of fluorescent brightening agents, photosensitive dyes, and natural dyes.
3. Proficiency in refining edible oils, manufacturing soaps and detergents.
4. Knowledge of soil formation, classification, and soil acidity/alkalinity.
5. Awareness of chemical fertilizers, organic manures, micronutrients, and bio-fertilizers.

Unit 3

6. Classification and composition of common food stuffs.
7. Understanding of food properties and preservation techniques.
8. Knowledge of food deterioration and various preservation methods.

Unit 4

1. Familiarity with specific organophosphorus pesticides and their applications in agriculture.

Suggested Readings:

1.N. N. Melnikow: Chemistry of Pesticides, Springer

2.M. B. Green, G. S. Hartley West: Chemicals for Crop Protection and Pest Management, Pergamon.

3.R. Cremlyn: Pesticides

4.K.H. Buchel: Chemistry of Pesticides.

5.H.B. Scher: Advances in pesticides formulation Technology (ACS)

6.K. Venkatraman: The Chemistry of Synthetic Dyes Vol. 1-7 (A.P)

7.Abranart: Dyes and Their intermediates (Pergaman).

8.Beech: Fiber reactive Dyes (Logos Press).

9.Frig and David – Dyes intermediate.

10.Allan: Color Chemistry

SEMESTER III

Course Name: Mathematical Methods for Chemistry **Code:** CHE-S-609

Semester: III **Course Level:** 600 **Total Marks:** 50

L+T+P: 1+1+0 =2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Skill Enhancement

Course Learning Outcomes (CLOs):

On completion of course, students will be able to:

1. Apply differential and integral calculus techniques to solve problems and analyze chemical phenomena.
2. Solve differential equations using separation of variables, homogeneous, exact, and linear equation methods.
3. Analyze and apply Fourier series and Laplace transformation in the analysis of chemical systems.
4. Utilize probability distributions to model and analyze chemical data.
5. Perform vector operations and apply matrices and determinants in chemistry-related contexts.
6. Apply complex numbers in chemical calculations and understand their role in physical chemistry.

Course Description: This course provides a comprehensive introduction to mathematical methods relevant to the field of chemistry. Students will explore various functions, calculus techniques, differential equations, Fourier analysis, probability distributions, vectors, matrices, determinants, and complex variables. Emphasis will be placed on understanding the physical significance and applications of these mathematical concepts in chemistry.

Course Outline:

Unit I:Functions, Calculus, and Differential Equations

Functions: Linear, Quadratic, Cubic, Logarithmic, Exponential, Trigonometric, and Hyperbolic functions. Properties, graphical representation, and practical applications of these functions in chemistry. Differential Calculus: Limits, derivative, and physical significance of derivatives. Basic rules of differentiation, including chain rule and product rule. Maximum and minimum points, optimization, and curve sketching. Applications of differentiation in chemical contexts. Integral Calculus: Indefinite and definite integrals. Rules of integration, including substitution and integration by parts. Exact and inexact differentials. Partial differentiation and its applications. Taylor and McLaurin series and their applications. Differential Equations: Separation of variables, homogeneous, exact, and linear equations. Equations of second order and series solution method. Introduction to Fourier series and Fourier analysis. Laplace transformation and its applications.

Unit II: Probability Distributions, Vectors, Matrices, and Complex Variables

Probability Distributions: Permutations, combinations, and their applications. Theory and applications of binomial, Gaussian, and Poisson distributions in chemistry. Vectors, Matrices, and Determinants: Introduction to vectors and their properties. Dot product, cross product, and triple product of vectors. Introduction to matrix algebra, addition, and multiplication of matrices. Inverse, adjoint, and transpose of matrices. Unit and diagonal matrices. Complex Variables: Introduction to complex numbers and their representation. Basic operations on complex numbers. Applications of complex variables in chemistry

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Mapping of CLOs and POs:

	Course Outcome (CLOs)	(POs)
CLO1	Apply differential and integral calculus techniques to solve problems and analyze chemical phenomena.	[PO2]

CLO2	Solve differential equations using separation of variables, homogeneous, exact, and linear equation methods.	[PO2]
CLO3	Analyze and apply Fourier series and Laplace transformation in the analysis of chemical systems.	[PO2]
CLO4	Utilize probability distributions to model and analyze chemical data.	[PO2][PO3]
CLO5	Perform vector operations and apply matrices and determinants in chemistry-related contexts.	[PO6]
CLO6	Apply complex numbers in chemical calculations and understand their role in physical chemistry.	[PO1] [PO2][PO3]

Performance Indicators:

1. Understand and apply various functions, calculus, and differential equations in chemistry.
2. Apply differentiation and integration techniques to solve problems and analyze chemical phenomena.
3. Solve differential equations using separation of variables and series solution methods.
4. Analyze and apply Fourier series and Laplace transformation in chemical systems.
5. Utilize probability distributions in modeling and analyzing chemical data.
6. Perform operations on vectors, matrices, and determinants in chemistry-related contexts.
7. Apply complex numbers in chemical calculations and understand their role in complex variables

Suggested Readings:

1. Margenau, H. and Murphy, G. M. (1956). The Mathematics of Chemistry and Physics - van Nostrand, Princeton, NJ.
2. Daniels, F. (1972). Mathematical Preparation for Physical Chemistry. McGraw Hill.
3. Steiner, E. (1996). The Chemical Maths Book. Oxford University Press.
4. Press, W. H., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P. (1996). Numerical Recipes in FORTRAN/C. Cambridge University Press, 2nd Ed.
5. Xavier, C. (2002). Fortran 77 and Numerical Methods. New Age International.
6. Boas, M. L. (Wiley, 2nd edition). Mathematical Methods in the Physical Sciences.
7. Mortimer, R. G. (Elsevier). Mathematics for Physical Chemistry.
8. Norris, A. C. (Computational Chemistry). John Wiley.

SEMESTER III

Course Name: Scientific Writing and Communication **Code:** CHE-S-610

Semester: III **Course Level:** 600 **Total Marks:** 50

L+T+P: 1+1+0 =2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Skill Enhancement

Course Learning Outcome (CLOs)

On completion of the course, students will be able to:

1. Understand the principles and conventions of scientific writing and communication.
2. Develop skills for organizing and structuring scientific information effectively.
3. Write clear and concise scientific research papers and reports.
4. Conduct literature reviews and integrate relevant sources into scientific writing.
5. Use proper citation styles and understand ethical considerations in scientific communication.
6. Deliver effective scientific presentations, including oral and visual communication techniques.
7. Apply critical thinking and analytical skills to evaluate and improve scientific writing and communication.

Course Description:

This course provides an introduction to scientific writing and communication. Students will learn the importance of scientific writing, the structure of scientific papers, and how to write clear and concise sections. They will also explore effective use of visuals, literature review and citations, editing techniques, peer review processes, and ethical guidelines. In addition, students will develop skills in designing and delivering scientific presentations, adapting communication for different audiences, and using various media platforms. The course aims to enhance students' abilities to effectively communicate scientific information.

Course Outline:

Unit 1: Introduction to Scientific Writing and Communication. Importance and characteristics of scientific writing. Differences between scientific and other forms of writing. Structure and organization of scientific papers. Writing clear and concise abstracts, introductions, methods, results, and discussions. Effective use of visuals (tables, figures) and captions. Literature Review and Citations. Editing and proofreading techniques. Peer review processes. Collaborative writing and feedback. Plagiarism, authorship, acknowledgement and intellectual property. Ethical guidelines in scientific writing and publishing.

Unit 2: Principles of effective oral communication. Designing and delivering scientific presentations. Visual aids and slide design techniques. Scientific Communication for Different Audiences. Case Study: Conference Lecture by a Renowned Scientist. Adapting scientific communication to various stakeholders. Communicating science to the general public (popular lecture). Communicating science through different media (websites, social media). Case study: popular lecture by a renowned Scientist.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Understand the principles and conventions of scientific writing and communication.	PO1
CLO2	Develop skills for organizing and structuring scientific information effectively.	PO2
CLO3	Write clear and concise scientific research papers and reports	PO3
CLO4	Conduct literature reviews and integrate relevant sources into scientific writing.	PO3

CLO5	Use proper citation styles and understand ethical considerations in scientific communication.	[PO1] [PO5]
CLO6	Deliver effective scientific presentations, including oral and visual communication techniques.	[PO1] [PO7]
CLO7	Apply critical thinking and analytical skills to evaluate and improve scientific writing and communication.	[PO1][PO2 [PO3] [PO7]

Performance Indicators (PIs)

Unit 1: Introduction to Scientific Writing and Communication

1. Students can explain the importance of scientific writing and its characteristics.
2. Students can distinguish between scientific writing and other forms of writing.
3. Students can demonstrate understanding of the structure and organization of scientific papers.
4. Students can write clear and concise abstracts, introductions, methods, results, and discussions.
5. Students can effectively use visuals (tables, figures) and write appropriate captions.
6. Students can conduct literature reviews and properly cite references.
7. Students can apply editing and proofreading techniques to improve the clarity and readability of their writing.
8. Students can explain the peer review process and its role in scientific publishing.
9. Students can engage in collaborative writing and provide constructive feedback to their peers.
10. Students can discuss the ethical considerations, such as plagiarism, authorship, acknowledgement, and intellectual property, in scientific writing and publishing.

Unit 2: Principles of effective oral communication

1. Students can design and deliver effective scientific presentations.
2. Students can create visually appealing slides and use appropriate slide design techniques.
3. Students can adapt their scientific communication style to different audiences and stakeholders.
4. Students can analyze and critique a conference lecture given by a renowned scientist.
5. Students can effectively communicate scientific concepts to the general public through a popular lecture.
6. Students can utilize different media platforms, such as websites and social media, to communicate science effectively.
7. Students can evaluate and discuss the impact of a popular lecture given by a renowned scientist.
8. Students can deliver scientific presentations with clarity, confidence, and appropriate body language.
9. Students can respond to questions and engage in discussions during scientific presentations.

10. Students can apply effective storytelling techniques to engage and captivate their audience during scientific presentations.

Suggested Readings:

1. Laura Bowater, Kay Yeoman (2012) Science Communication: A Practical Guide for Scientists
2. R.R. Jordan (1999) Academic writing Course New Edition

SEMESTER III

Course Name: Scientific Writing and Communication **Code:** CHE-S-611

Semester: III **Course Level:** 600 **Total Marks:** 50

L+T+P: 1+1+0 =2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Open Theory

Course Learning Outcome (CLOs)

On completion of the course, students will be able to:

1. Describe and differentiate different types of carbohydrates and their roles in controlling various metabolic processes
2. Explain/describe the importance of recognition in regulation various biological processes.
3. Explain/describe the roles of nucleic acids and proteins in controlling various aspects of biological systems
4. Explain/describe the roles of lipids and membranes and the importance various structural units in controlling the divers functions of lipids and membranes
5. Differentiate types of energetics involved in diversecatabolic and anabolic processes.
6. Explain/describe the roles of enzymes in modulating the metabolic processes in myriad ways.
7. Explain/describe the roles of metal ions in modulating the activity of various bio-molecules.

Course Description:

The course will provide fundamental understanding of the role of carbohydrates, nucleic acids, amino acids, proteins, lipids and membranes in context of both structure and functionality. The course will also cover different types of metabolism and energetics active in the biological system. The role of different metal ions in biology and their applications will be covered.

Course Outline:

Unit I: Carbohydrates: Glycosides, Oligosaccharides and polysaccharides. Role of sugar In molecular recognition. Nucleic Acids: RNA, DNA, base-pairing, double helical structure of DNA, Gene regulatory protein- Zinc finger protein.

Aminoacids and Proteins: Aminoacids, peptide links and oligopeptides. Proteins: primary, secondary, tertiary, and quaternary structure of proteins. Structure, purification and denaturation of proteins.

Lipids and membranes: Lipids, fatty acids, Classification of lipids, self-association of lipids micelles, reverse micelles and membranes, transport of cations through membranes.

Unit II: Metabolism and Energetics

Catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation. Photosystems (PSI & PSII).

Enzyme Enzyme kinetics and applications of enzymes in organic synthesis. Enzyme inhibitors and co enzymes in organics reactions. Drugs based on enzyme inhibition.

Metal ions in biological systems and their role in ion transport across the membranes (molecular mechanism) Oxygen-uptake proteins, cytochromes and ferredoxins. Oxygen uptake proteins: Hemoglobin, Myoglobin, hemerythrin and hemocyanin. Metal complexes in medicine. Chemotherapy.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (25 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (25 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Performance Indicators:

1. Distinguish carbohydrates in terms of structure and functionality.
2. Identify the critical aspects of functionality of the carobhydrates
3. Identify different type of nucleic acids and explain their importance in building macrstructures
4. Ability to explain the structural and functional aspects of RNA and DNA
5. Identify different type of amino acids and explain their chemistry and importance.
6. Describe the importance of various structures of protein and their stability
7. Describe and differentiate catabolic and anabolic process and their role in modulating biological activity.
8. Explain/describe the role of enzymes in modulating different types of metabolic processes.
9. Explain the role of inhibitors and coenzymes
10. Describe the role of metal ions present in different biological molecules in modulating their activity.
11. Describe/explain the working of various proteins involved in uptake and transport of oxygen

Suggested Readings:

1. Stryer L., 2002 Biochemistry, 5th edition, Freeman & Co., New York.
2. Nelson D. L. and Cox M.M., 2002 Lehninger Principles of Biochemistry, 3rd edition McMillanNorth Publication.
3. Hughes M. N. , 1981 Inorganic Chemistry of Biological Processes, John Wiley.
4. Smith M.B., 1995 Organic Synthesis, McGraw Hill Inc., New York.
5. Ariga K. and Kunitake T. 2006 Supramolecular Chemistry – Fundamentals and Applications, Springer
6. Crabtree R. H., Organometallics in Organic synthesis Vol-II – Organometallics of Transition Metals in Organic Synthesis
7. Voet D., Voet J.G and Pratt C. W., 1999 Fundamentals of Biochemistry, John Wiley & Sons, New York

SEMESTER III

Course Name: Inorganic Elective Practical **Code:** CHE-P-612

Semester: III **Course Level:** 600 **Total Marks:** 100

L+T+P: 0+0+4 = 4 Credits (Lecture = 0 hrs; Tutorial = 0 hrs; Practical = 60 hrs)

Type: Core Practical

Course Learning Outcomes (CLOs): Upon completion of the practical course, students will be able to:

1. Apply critical thinking and scientific inquiry to perform, design, interpret, and document laboratory experiments effectively.
2. Evaluate and select appropriate methods for synthesis and characterization of inorganic compounds.
3. Assess the progress of chemical reactions through monitoring and analysis.
4. Collaborate effectively within a team setting to achieve common laboratory goals.
5. Compile comprehensive laboratory reports and manuals, demonstrating proficiency in laboratory reporting methods.
6. Identify and evaluate potential laboratory hazards and implement appropriate safety precautions.
7. Critically review scientific literature and effectively communicate scientific findings through written and oral means.

Course Description:

This practical course in inorganic chemistry is designed to provide hands-on experience in synthesis, characterization, and analysis of various inorganic compounds. The course consists of three components: synthesis and characterization of selected compounds, analysis of known compounds, and development of chemistry communication skills.

Course Outline:

1. Synthesis and characterization of the following (any five synthesis)

a. Pervoskite (bulk and nanoparticles)

b. Prussian blue

c. HKUST-1, $Cu_3(BTC)_2$ metal organic framework

d. Metallic nanoparticles (Ni, Co and Cu)

e. Polyoxometallate (V, Mo and W)

f. Layered materials (In_2O_3 and Fe_2O_3)

g. Synthesis of metalloporphyrins

Characterization techniques to be used for each experiments (wherever applicable) are XRD, UV-vis, FT-IR, TGA/DTA, Surface Area analysis (BET), Magnetic susceptibility measurements, Cyclic Voltammetry, ICP-MS and AAS.

2. Analysis of known compounds (any two)

a. Cyclic voltammetry, ^{1}H and ^{13}C NMR of Ferrocene

b. ^{13}C-NMR and FT-IR of iron carbonyls

c. TGA measurement of $CuSO_4$. $5H_2O$ /

d. Surface ligand analysis by TGA and FTIR of nanoparticles

e. Magnetic susceptibility measurements of $Fe(acac)_3$ (Evans method)

f. Assignement of absolute configuration using circular dichroism(CD).

3. Chemistry Communication Skills:

a. How to draw chemical structures- Use of CHEMDRAW. How to write and draw equations (both chemical and mathematical).

b. How to find compound related data in the literature?

c. Use and management of mined data- End note.

d. Use of spectral databases and how to report compound data and procedures. Use of other specialized databases- CCDC, PDB, other nuclei NMR databases.

e. Data integrity and recording experiments in the lab notebook.

f. How to write new and views (reviews)? How to make presentation slides and present reviews to an audience?

Suggested-teaching learning strategy

1. Engaging Lectures: Employing interactive lectures coupled with live discussions and vivid demonstrations of laboratory skills and techniques.

2. Experiential Learning: Encouraging hands-on practice to actively engage students in real-life applications, fostering a deeper understanding of the subject matter.

3. Collaborative Learning: Facilitating group discussions, promoting active participation, and encouraging the exchange of ideasamong students, leading to enhanced critical thinking and problem-solving skills.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Assignment	Oral Test, Viva-Voce, Presentation	Presentation
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Apply critical thinking and scientific inquiry to perform, design, interpret, and document laboratory experiments effectively.	[PO1][PO9]
CLO2	Evaluate and select appropriate methods for synthesis and characterization of inorganic compounds.	[PO1][PO2][PO3]
CLO3	Assess the progress of chemical reactions through monitoring and analysis.	[PO1][PO2][PO3]
CLO4	Collaborate effectively within a team setting to achieve common laboratory goals.	[PO1][PO2][PO3]
CLO5	Compile comprehensive laboratory reports and manuals, demonstrating proficiency in laboratory reporting methods.	[PO1][PO5][PO7]
CLO6	Identify and evaluate potential laboratory hazards and implement appropriate safety precautions.	[PO1][PO5][PO7]
CLO7	Critically review scientific literature and effectively communicate scientific findings through written and oral means.	[PO1][PO5][P06]

Performance Indicators (PIs)

1. Estimate technical skills to work in a laboratory
2. Identify the use of appropriate synthetic, separation and characterization methods
3. Ability to monitor the progress of the reaction and to mark the end point of the reaction
4. Ability to efficiently distribute work within team members
5. Documentation of the laboratory note book and the accounts of the progress of the experiments.
6. Classify and identify laboratory hazards, toxicity and its precaution

7. Ability to write a summary of a journal paper.

Suggested Readings:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. A text book of Quantitative Inorganic Analysis – A. I. Vogel
3. A Text Book of Quantitative Inorganic Analysis- A. I. Vogel
4. Experimental Inorganic Chemistry - W. G. Palmer
5. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.
6. Chemistry experiments for Instrumental Methods by Donald T. Sawyer, William R. Heineman & Jalice M. Beebe , John Wiley & Sons ,1984.
7. Experimental Physical Chemistry by G. Peter Matthews, Clarendon Press, 1985.
8. Handbook of Inorganic Synthesis: G. Brauer
9. Inorganic Synthesis: R. B. King
10. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, Gregory S. Girolami, Thomas B. Rauchfuss and Robert J. Angelici. University Science Books.

SEMESTER III

Course Name: Organic Elective Practical **Code:** CHE-P-613

Semester: III **Course Level**: 600 **Total Marks**: 100

L+T+P: 0+0+4 = 4 Credits (Lecture = 0 hrs; Tutorial = 0 hrs; Practical = 60 hrs)

Type: Core Practical

Course Learning Outcomes (CLOs):

Upon completion of the practical course, students will be able to:

1. Conduct organic reactions and optimize yields.
2. Purify organic compounds using various techniques.
3. Characterize compounds using spectroscopic methods.
4. Extract and purify natural products and biomolecules.
5. Practice safe laboratory procedures and analyze data.
6. Develop critical thinking and problem-solving skills.
7. Understand the applications of organic chemistry in different scientific disciplines.

Course Description:

This course, focuses on basic techniques for synthesizing organic compounds, purifying them through methods like re-crystallization and chromatography, and characterizing them using spectroscopic methods. The course also covers the extraction and purification of natural products and biomolecules. Through hands-on experiments, students will develop essential laboratory skills and gain a deeper understanding of the applications of organic chemistry in various scientific fields.

Course Outline:

A.Organic Special Practical

Preparation of organic compounds by typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PLC, determination of Rf value as required, m.p/b.p.].

B.Characterization of organic compounds by spectroscopic means

Multistep Organic Preparation. Extraction and Purification of Natural Products and Biomolecules.

Suggested-teaching learning strategy

1 .Engaging Lectures: Employing interactive lectures coupled with live discussions and vivid demonstrations of laboratory skills and techniques.

2 .Experiential Learning: Encouraging hands-on practice to actively engage students in real-life applications, fostering a deeper understanding of the subject matter.

3. Collaborative Learning: Facilitating group discussions, promoting active participation, and encouraging the exchange of ideas among students, leading to enhanced critical thinking and problem-solving skills.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Assignment	Oral Test, Viva-Voce, Presentation	Presentation
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOS with POs:

CLO1	Conduct organic reactions and optimize yields.	[PO1]
CLO2	Purify organic compounds using various techniques.	[PO1] [PO2]PO3]
CLO3	Characterize compounds using spectroscopic methods.	[PO1][PO2] [PO3]
CLO4	Collaborate effectively within a team setting to achieve common laboratory goals.	PO6
CLO5	Extract and purify natural products and biomolecules.	[PO1][PO3]
CLO6	Practice safe laboratory procedures and analyze data.	[PO4][PO9]
CLO7	Develop critical thinking and problem-solving skills.	[PO3][PO9]

Performance Indicators:

1. Successfully perform organic reactions and obtain desired products with high yields.
2. Demonstrate proficiency in purifying organic compounds through effective utilization of techniques such as re-crystallization, TLC, and PLC.
3. Accurately interpret spectroscopic data (IR, NMR, MS) to identify functional groups, determine molecular structures, and propose reaction mechanisms.
4. Apply extraction and purification techniques to isolate and obtain pure natural products and biomolecules.
5. Follow proper safety protocols in the laboratory, including handling hazardous materials, using protective equipment, and maintaining a clean work environment.
6. Analyze experimental data, draw appropriate conclusions, and effectively communicate findings through written reports.
7. Apply critical thinking skills to troubleshoot experimental issues, propose alternative approaches, and optimize synthetic procedures.
8. Demonstrate an understanding of the diverse applications of organic chemistry in areas such as pharmaceuticals, materials science, and biochemistry through class discussions and assignments.
9. Actively participate in group work and collaborative laboratory experiments, showing effective teamwork and communication skills.
10. Show an ongoing commitment to professional development, staying updated with current research and advancements in the field of organic chemistry.

Suggested Readings:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. Addison Ault Techniques and Experiments for Organic Chemistry 6th Ed. University Science Books (1998).
3.Mann, F. G. & Saunders, B. C. Practical Organic Chemistry 4th Ed. Orient Longmans (1990).
4.Vogel, A. I. Vogel's Textbook of Practical Organic Chemistry 5th Ed. (revised by A.R. Tatchell et al.) Wiley (1989) ISBN 0582-46236-3

SEMESTER III

Course Name: Physical Chemistry Elective Practical		**Code:** CHE-P-614
Semester: III	**Course Level:** 600	**Total Marks:** 100

L+T+P: 0+0+4 = 4 Credits (Lecture = 0 hrs; Tutorial = 0 hrs; Practical = 60 hrs)

Type: Core Practical

Course Learning Outcomes (CLOs): Upon completion of the Experimental Solid State and Nanomaterials practical course, students will be able to:

1. Conduct synthesis and characterization of nanoparticles.
2. Calculate and determine the molar extinction coefficient.
3. Isolate and characterize Fullerene C60.
4. Measure and determine the size of nanoparticles.
5. Calculate and determine the quantum yield of quantum dots.
6. Perform solution and solid-state ligand exchange in nanoparticles.
7. Develop and execute computational codes.
8. Utilize quantum mechanical software for simulations and analysis.
9. Implement minimization algorithms and numerical methods in coding.
10. Analyze data and interpret results clearly.
11. Effectively communicate research findings.
12. Recognize the importance of teamwork and adhere to ethical laboratory practices

Course Description:

The Elective Physical Chemistry Practical course is designed to provide students with hands-on experience in the synthesis, characterization, and analysis of nanomaterials and their properties. The course focuses on the experimental techniques used in the field of solid-state chemistry and nanoscience, with an emphasis on the synthesis and characterization of nanoparticles, determination of their physical properties. The second section of the course focusses on the Computational Physical Chemistry which is designed to introduce students to the fundamental concepts and techniques used in computational chemistry. This course focuses on the application of computational methods to simulate and analyze physical and chemical phenomena. Students will learn how to write and execute computational codes, use quantum mechanical software, implement minimization algorithms, and apply numerical methods to solve mathematical problems encountered in physical chemistry

Course Outline:

Elective Physical Chemistry Practical 4 credits

A. Experimental Solid state and Nanomaterials

1. Synthesis and Characterisation of Nanoparticles (Metal, Spinel, Rutile, Zinc blende, Wurtzite Pervoskite)
2. Determination of Molar extinction coefficient of Nanoparticles.
3. Isolation and physical characterization of Fullerene C60 from natural sources.
4. Determination of size of nanoparticles using UV-Vis spectrophotometer and X-Ray Diffraction
5. Determination of quantum yield of quantum dots.
6. Solution and solid-state ligand exchange in nanoparticles.

B. Computational Chemistry

1.Writing and executing computational codes for the following –Radioactive Decay, Other First-Order Reactions etc.

2.Use of quantum mechanical software – Gaussian, MPQC – calculation of energies of molecules.

3.Coding Minimization Algorithms: LBFGS etc.

4.Numerical Methods Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion.

5.Numerical integration.

6.Statistical treatment of data, variance and correlations, Least square curve fitting

Suggested-teaching learning strategy

1.. Engaging Lectures: Employing interactive lectures coupled with live discussions and vivid demonstrations of laboratory skills and techniques.

2. Experiential Learning: Encouraging hands-on practice to actively engage students in real-life applications, fostering a deeper understanding of the subject matter.
3. Collaborative Learning: Facilitating group discussions, promoting active participation, and encouraging the exchange of ideas among students, leading to enhanced critical thinking and problem-solving skills.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Assignment	Oral Test, Viva-Voce, Presentation	Presentation
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Conduct synthesis and characterization of nanoparticles.	PO1
CLO2	Calculate and determine the molar extinction coefficient.	[PO1][PO2]
CLO3	Isolate and characterize Fullerene C60.	[PO1][PO2]
CLO4	Measure and determine the size of nanoparticles.	[PO1] [PO2]
CLO5	Calculate and determine the quantum yield of quantum dots.	[PO1][PO2]
CLO6	Perform solution and solid-state ligand exchange in nanoparticles.	[PO1
CLO7	Develop and execute computational codes.	[PO1] [PO2] [PO3]
CLO8	Utilize quantum mechanical software for simulations and analysis.	[PO1][PO2]
CLO9	Implement minimization algorithms and numerical methods in coding.	[PO1] [PO2]
CLO10	Analyze data and interpret results clearly.	PO2
CLO11	Effectively communicate research findings.	PO7
CLO12	Recognize the importance of teamwork and adhere to ethical laboratory practices.	[PO5] [PO6]

Performance Indicators (PIs)

A. Experimental Solid state and Nanomaterials

1. Synthesis and Characterisation of Nanoparticles

i) Students can successfully synthesize nanoparticles of various materials (metal, spinel, rutile, zinc blende, wurtzite perovskite).

ii) Students can characterize the synthesized nanoparticles using appropriate techniques (e.g., TEM, SEM, XRD).

2. Determination of Molar extinction coefficient of Nanoparticles

i) Students can accurately determine the molar extinction coefficient of nanoparticles using spectrophotometric methods.

3. Isolation and physical characterization of Fullerene C60 from natural sources

i) Students can isolate Fullerene C60 from natural sources and perform its physical characterization (e.g., melting point determination, spectroscopic analysis).

4. Determination of size of nanoparticles using UV-Vis spectrophotometer and X-Ray Diffraction

i) Students can measure the size of nanoparticles using UV-Vis spectrophotometry and analyze the data obtained.

ii) Students can analyze X-Ray Diffraction patterns to determine the size of nanoparticles.

5. Determination of quantum yield of quantum dots

i) Students can accurately determine the quantum yield of quantum dots using appropriate spectroscopic techniques.

6. Solution and solid-state ligand exchange in nanoparticles

i) Students can successfully perform solution and solid-state ligand exchange in nanoparticles and analyze the resulting changes in their properties.

B. Computational Chemistry

1. Writing and executing computational codes for various reactions

i) Students can write and execute computational codes for radioactive decay, first-order reactions, and other relevant chemical processes.

2. Use of quantum mechanical software

i) Students can utilize quantum mechanical software (e.g., Gaussian, MPQC) to perform calculations and determine the energies of molecules accurately.

3. Coding Minimization Algorithms

i) Students can code and implement minimization algorithms (e.g., LBFGS) for optimizing molecular structures and energy calculations.

4. Numerical Methods

i) Students can apply numerical methods to solve problems such as finding roots of polynomials, solving linear simultaneous equations, performing matrix multiplication and inversion, and numerical integration.

5. Statistical treatment of data and least square curve fitting

i) Students can apply statistical techniques to analyze data, determine variance and correlations, and perform least square curve fitting for experimental data.

SEMESTER IV

Course Name: Magnetochemistry **Code:** CHE-E-651

Semester: IV **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs):

Upon completion of the course, students will be able to:

1. Demonstrate a thorough understanding of the fundamental principles and theories of magnetochemistry.
2. Explain the different types of magnetism, including paramagnetism, diamagnetism, ferromagnetism, antiferromagnetism, and ferrimagnetism.
3. Utilize experimental techniques such as the Gouy balance method, Faraday method, NMR spectroscopy, and SQUID magnetometry to measure and determine magnetic susceptibility.
4. Correlate magnetic properties with structural characteristics in different materials.
5. Critically analyze and evaluate research literature in magnetochemistry, and discuss recent advancements in the field.
6. Utilize the knowledge gained in magnetochemistry to propose solutions for real-world problems and contribute to the development of magnetic materials with tailored properties.

Course Description:

This course delves into the principles and applications of magnetochemistry, providing students with a comprehensive understanding of the underlying theories and experimental techniques. Through a combination of theoretical lectures and hands-on laboratory sessions, students will develop the knowledge and skills necessary to analyze and interpret magnetic phenomena in a wide range of materials.

Course Outline:

Unit 1

Magnetic properties of substances, orbital and spin angular momentum of electrons, paramagnetic moment and magnetic susceptibility. Paramagnetic and diamagnetic materials, ferromagnetism, ferrimagnetism, antiferromagnetism, magnetic permeability, magnetic susceptibility, magnetization, classical theory of diamagnetism and paramagnetism, diamagnetism and Pascal"s constants, zero-field splitting, spin-orbit coupling. Determination of magnetic susceptibility by these methods: Gouy, Faraday, NMR method and SQUID.

Unit 2

Magnetic properties and temperature – The curie and Curie- Weiss law, derivation of Curie law. Microstates, hole formalism, multiplet, multiplet width, Lande interval rule, magnetic moments for different multiplet widths, crystal field diagram, quenching of orbital contribution, high spin/low spin equilibrium. Antiferromagnetic interactions in inorganic compounds: Mechanism like – direct interaction, superexchange interactions and elucidation with poly nuclear metal complexes as well as oxide and halide salts of transition metals.

Unit 3

Ferromagnetism and Magnetic domains, Hysteresis, Molecular field theory, magnetic sublattice, Ferrimagnetism, Canting and Weak ferromagnetism Heisenberg and Ising model, Correlation of magnetic and structural properties.

Unit 4

Magnetic materials, long range ordering, superparamagnetism, molecular magnets, metamagnetism, single chain magnet, magnetic ordering, magnetic behaviour of lanthanides and actinides, design of molecular magnets, physical investigations and applications.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOS with POs:

CLO1	Demonstrate a thorough understanding of the fundamental principles and theories of magnetochemistry.	PO1
CLO2	Explain the different types of magnetism, including paramagnetism, diamagnetism, ferromagnetism, antiferromagnetism, and ferrimagnetism.	PO1
CLO3	Utilize experimental techniques such as the Gouy balance method, Faraday method, NMR spectroscopy, and SQUID magnetometry to measure and determine magnetic susceptibility.	[PO1][PO2]
CLO4	Correlate magnetic properties with structural characteristics in different materials.	[PO1][PO2]
CLO5	Critically analyze and evaluate research literature in magnetochemistry, and discuss recent advancements in the field.	PO2
CLO6	Utilize the knowledge gained in magnetochemistry to propose solutions for real-world problems and contribute to the development of magnetic materials with tailored properties.	PO3

Performance Indicators:

Unit 1:

i).Demonstrate an understanding of the magnetic properties of substances, including orbital and spin angular momentum of electrons.

ii).Calculate and determine paramagnetic moment and magnetic susceptibility for different materials.

iii).Apply knowledge of ferromagnetism, ferrimagnetism, and antiferromagnetism to analyze magnetic behavior in various systems.

iv).Use appropriate methods such as Gouy, Faraday, NMR, and SQUID to determine magnetic susceptibility.

Unit 2:

i).Apply the Curie and Curie-Weiss laws to analyze the relationship between magnetic properties and temperature.

ii).Explain the concept of microstates, hole formalism, multiplet, and multiplet width in relation to magnetic moments.

iii).Construct crystal field diagrams and interpret the quenching of orbital contributions in high spin/low spin equilibrium.

iv).Analyze the mechanisms of antiferromagnetic interactions in inorganic compounds, including direct interaction and superexchange interactions.

Unit 3:

i). Explain the concept of magnetic domains and analyze their role in ferromagnetism.

ii).Apply molecular field theory to understand magnetic sublattices, ferrimagnetism, and weak ferromagnetism.

iii).Apply the Heisenberg and Ising models to correlate magnetic and structural properties.

Unit 4:

i). Analyze the magnetic behavior of different types of magnetic materials, such as long-range ordering, superparamagnetism, and molecular magnets.

ii).Discuss the concept of metamagnetism, single-chain magnetism, and magnetic ordering in materials.

iii).Understand the magnetic behavior of lanthanides and actinides and their applications.

iv). Discuss the design of molecular magnets and their physical investigations.

v).Analyze the practical applications of magnetic materials in various fields.

Suggested Readings:

1. Cotton, F.A. and Wilkinson, G. (1999). Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons, New York.

2. Huheey, J. E. (1993). Inorganic Chemistry, 4th Ed., Addison-Wesley Pub. Co., New York.

3. Drago, R. S. (1971). Physical Methods in Inorganic Chemistry, International Edn., Affiliated East-West Press, New Delhi.

4. Shriver, D. F. and Atkins, P. W. (1999). Inorganic Chemistry, 3rd Edn., ELBS, London.

5. Cotton, F. A., Wilkinson, G., and Gaus, P.L. Basic Inorganic Chemistry, 3rd Edition, John Wiley & Sons, New York.

6. Greenhood (1976). Spectroscopic Properties of Inorganic and Organometallic Compounds, Royal Society of Chemistry.

7. Lee, J. D. (1999). Concise Inorganic Chemistry, Blackwell Science.

8. Purcell K. F. and Kotz J. C. (1987). Inorganic Chemistry, W. B. Sauders Com., Hong Kong.

9. Cotton, F.A. (1990). Chemical Applications of Group Theory, 3rd Ed., Wiley-Blackwell.

SEMESTER IV

Course Name: Advances in Organic Synthesis		**Code:** CHE-E-652
Semester: IV	**Course Level:** 600	**Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs)

1. Critically analyze different synthetic approaches to drug discovery, including combinatorial synthesis, diversity-oriented synthesis, and total synthesis, along with their importance, utilities, advantages, and disadvantages.
2. Employ retrosynthetic analysis to plan organic synthesis by working backward from the target molecule, identifying disconnections, synthons, functional group interconversions, and selecting appropriate synthetic strategies.
3. Categorize and utilize important organic reactions as synthetic tools in organic synthesis, such as multi-component reactions (Ugi, Passerini, Biginelli, Mannich), click chemistry (Sharpless azide cycloadditions), coupling reactions (Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada, Hiyama, Negishi, Buchwald-Hartwig, Noyori), and metathesis (Grubbs catalyst, olefin cross-coupling, ring-closing, and ring-opening metathesis) for planning the synthesis of important complex organic structures.
4. Exploit various ring formation reactions, including Pausan-Khand, Bergman, Nazerov cyclization, and intramolecular cycloaddition reactions, to achieve structural and stereochemical complexity.
5. Describe important named reactions, such as Wittig, Horner-Wadsworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe, Peterson olefination, titanium-carbene mediated olefination, Baylis-Hillman, Eschenmoser-Tanabe fragmentation, and Mitsunobu reactions.

6. Effectively explain the current trends in organic synthesis, including organocatalysis, photoredox catalysis, and C-H activation, and apply them in synthetic strategies.

Course Description:

Advances in Organic Synthesisis an advanced course designed for students with a strong foundation in organic chemistry. This course focuses on various synthetic approaches to drug discovery, important reaction and synthetic tools in organic synthesis, other significant reactions, and retrosynthetic analysis. Through a combination of lectures, discussions, and practical examples, students will deepen their understanding of organic chemistry principles and develop skills necessary for designing and executing complex organic syntheses.

Course Outline:

Unit 1

Various synthetic approaches to drug discovery:

Combinatorial synthesis, Diversity oriented synthesis, Total synthesis, their importance, utilities, advantages and disadvantages.

Unit 2

Important reaction and synthetic tools in organic synthesis:

Multi-component reactions: Ugi, Passerini, Biginelli and Mannich reactions; Click chemistry: criterion for click reaction, Sharpless azides cycloadditions; Coupling reactions: Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada, Hiyama, Negishi, Buchwald-Hartwig, Noyori, Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, applications Ring formation reactions: Pausan-Khand, Bergman and Nazerov cyclization, Various intramolecular cycloaddition reactions (INC)

Unit 3

Other important reactions:

Important named reactions: Wittig, Horner-Wordworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions, Titanium-carbene mediated olefination: Tebbe, Petasis and Nysted reagent, Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction.

Current trends in organic synthesis: Organocatalysis, Photoredox catalysis. C-H activation.

Unit 4

Retrosynthetic analysis:

Synthesis backwards, disconnections, synthons, choosing disconnections, functional group interconversion, two group disconnections, C–C disconnections, donor-acceptor synthons, natural reactivity and umpolung. Synthesis: Illustrative synthesis of complex natural products with relevant examples.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs

CLO1	Critically analyse different synthetic approaches to drug discovery, including combinatorial synthesis, diversity-oriented synthesis, and total synthesis, along with their importance, utilities, advantages, and disadvantages.	PO2
CLO2	Employ retrosynthetic analysis to plan organic synthesis by working backward from the target molecule, identifying disconnections, synthons, functional group interconversions, and selecting appropriate synthetic strategies.	PO3
CLO3	Categorized and utilized important organic reaction as synthetic tools in organic synthesis, such as multi-component reactions (Ugi, Passerini, Biginelli, Mannich), click chemistry (Sharpless azide cycloadditions), coupling reactions (Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada, Hiyama, Negishi, Buchwald-Hartwig, Noyori), and metathesis (Grubbs catalyst, olefin cross coupling, ring closing,	PO1

	and ring opening metathesis) for planning synthesis of important complex organic structures.	
CLO4	Exploit various ring formation reactions, including Pausan-Khand, Bergman, Nazerov cyclization, and intramolecular cycloaddition reactions for achieving structural and stereochemical complexity.	[PO1][PO2][PO3]
CLO5	Describe about important named reactions, such as Wittig, Horner-Wordsworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe, Peterson olefination, titanium-carbene mediated olefination, Baylis-Hillman, Eschenmoser-Tanabe fragmentation, and Mitsunobu reactions.	PO1
CLO6	Effectively explain the current trends in organic synthesis, including organocatalysis, photoredox catalysis, and C-H activation, and apply them in synthetic strategies.	PO1

Performance Indicators (PI)

1. Effectively illustrate different synthetic approaches and evaluate their suitability for drug discovery, considering factors such as efficiency, diversity, and target specificity.
2. Demonstrate proficiency in performing retrosynthetic analysis, including identifying appropriate disconnections, synthons, and functional group interconversions.
3. Utilize retrosynthetic analysis to design plans for the synthesis of various complex organic molecules.
4. Apply multi-component reactions, click chemistry, coupling reactions, and metathesis in the synthesis of target molecules, showcasing the ability to select appropriate reactions and reactants.
5. Design intra/inter-molecular ring formation reactions, demonstrating the ability to efficiently form complex cyclic structures.
6. Utilize different named reactions, such as Wittig, Horner-Wadsworth-Emmons, and Mitsunobu reactions, to achieve desired synthetic transformations with suitable stereochemistry.
7. Demonstrate knowledge of current trends in organic synthesis, including organocatalysis, photoredox catalysis, and C-H activation, and effectively apply them in designing synthetic strategies.

SuggestedReadings:

1.Combinatorial Chemistry: From Theory to Application, Volume 26, Second Revised Edition; Willi Bannwarth, Berthold Hinzen; Wiley-VCH Verlag GmbH & Co. KGaA, 2006
2.Combinatorial Chemistry: Synthesis Analysis, Screening; Günther Jung; WILEY-VCH VerlagGmbH,1999
3.Diversity-Oriented Synthesis: Basics and Applications in Organic Synthesis, Drug Discovery,andChemicalBiologyAndreaTrabocchi,Wiley,2013
4.Diversity-oriented Synthesis of Alkaloids for Chemical Genetic Screening; Alexander MertonTaylorHarvardUniversity,2007
5.Organic chemistry; Clayden, J., Greeves, N. , Warren, S. and Wothers, P.; Oxford University Press, 2000
6.Multicomponent Reactions in Organic Synthesis; Jieping Zhu, Qian Wang, Mei-Xiang Wang;WileyVCHVerlagGmbH&Co.KGaA,2015
7.Multicomponent Reactions: Concepts and Applications for Design and Synthesis; Raquel P. Herrera,EugeniMarques-López;Wiley,2015
8.Advance Organic Chemistry; 5th Ed. Carey F. A. and Sundburg R. J.; Springer, 2007
9.Strategic Applications of Named Reactions in Organic Synthesis; Laszlo Kurti Barbara Czako;AcademicPress;2005
10. Name Reactions and Reagents in Organic Synthesis, Second Edition; Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro, Jr; John Wiley & Sons, Inc., 2013
11. C-H Bond Activation in Organic Synthesis; Jie Jack Li; CRC Press 2015
12. C-H Activation; Jin-Quan Yu, Zhangjie Shi; Springer; 2010
13. Photoredox Catalysis in Organic Chemistry, Megan H. Shaw, Jack Twilton, and David W. C. MacMillan J. Org. Chem., 2016, 81 (16), pp 6898–6926
14. Organic Photoredox Catalysis; Nathan A. Romero, David A. Nicewicz; Chem. Rev., 2016, 116 (17), pp 10075–10166

SEMESTER IV

Course Name: Advanced Quantum Chemistry **Code:** CHE-E-653

Semester: IV **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs)

1. Understand the principles and methods of quantum chemistry and electronic structure theory.
2. Apply ab initio and semi-empirical methods to analyze closed shell systems.
3. Interpret the physical significance of optimized orbitals and electron correlation energy.
4. Use density functional theory and time-dependent density functional theory for electronic structure calculations.
5. Describe the electronic structure and stability of linear and nonlinear molecules.
6. Analyze atom-radiation interactions and calculate line intensities, widths, and shapes.
7. Understand the principles and applications of quantum computation and information.

Course Description:

This course provides an in-depth exploration of quantum chemistry and electronic structure theory. It covers fundamental concepts and computational methods used to describe the behavior of closed shell systems, linear and nonlinear molecules, atom-radiation interactions, and the emerging field of quantum computation and information.

Course Outline:

Unit 1

Ab initio and Semi-empirical Methods for Closed Shell Systems:

Orbitals, Slater Determinants, The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation energy, Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations). Density functional theory, Time-

Dependent Density functional theory. Semiempirical Molecular Orbital Methods I - PI Electron Systems: The Huckel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method.Semiempirical Molecular Orbital Methods II

- All valence - Electron systems: The Extended HÃ¼ckel Method, The CNDO Method.

Unit 2

Electronic Structure of Linear and non linear Molecule

The Born-Oppenheimer Approximation, The MO - LCAO Approximation, The Hydrogen Molecule Ion, H+2 , The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, The stability of chemical bond, Hellmann-Feynman theorem, Molecular Perturbation Calculations. Electronic Structure of AH

nmolecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules. The Virial Theorem and Chemical Bonding, The Hellmann-Feynman Theorem, The ElectrostaticTheorem.

Unit 3

Atom-Radiation Interaction

Electromagnetic field and its interaction with one-electron atoms, Spontaneous emission, Electric dipole approximation, rotating-wave approximation (RWA), density matrix approach, Line intensities, widths and shapes, Rabi Oscillations, atomic coherence, Optical Bloch Equations, Photoionization, Scattering:

Partial wave analysis, Phase shifts, The Born Approximation.

Unit 4

Quantum Computation & Information

Bits, Quantum bits, The EPR Paradox, Bell's Theorem, Quantum algorithms,

Quantum information theory, Quantum computers: Physical realization, Entropy and information.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs

CLO1	Understand the principles and methods of quantum chemistry and electronic structure theory.	[PO1]
CLO2	Apply ab initio and semi-empirical methods to analyze closed shell systems.	[PO1][PO2]
CLO3	Interpret the physical significance of optimized orbitals and electron correlation energy.	[PO1]
CLO4	Use density functional theory and time-dependent density functional theory for electronic structure calculations.	[PO1][PO2][PO3]
CLO5	Describe the electronic structure and stability of linear and nonlinear molecules.	[PO1]
CLO6	Analyze atom-radiation interactions and calculate line intensities, widths, and shapes.	[PO2]
CLO7	Understand the principles and applications of quantum computation and information.	[PO1]

Performance Indicators (PIs)

1. Problem-solving proficiency in quantum chemistry using ab initio and semi-empirical methods.
2. Ability to generate and interpret optimized orbitals using the Hartree-Fock method.
3. Proficiency in using density functional theory for electronic structure calculations.
4. Understanding of electronic structure and stability of linear and nonlinear molecules.
5. Quantitative analysis of atom-radiation interactions, including line intensities and shapes.
6. Knowledge and evaluation of quantum computation and information applications.
7. Clear and coherent presentation of quantum chemistry concepts.
8. Proficiency in using computational tools for electronic structure calculations.
9. Critical evaluation of scientific literature in quantum chemistry.
10. Effective collaboration in group projects and discussions.
11. Application of problem-solving strategies and mathematical techniques in quantum chemistry.
12. Strong understanding of theoretical foundations in quantum chemistry.
13. Effective written and oral communication of scientific concepts in quantum chemistry.

Suggested Readings:

1. Levine, I.N. 2000 Quantum Chemistry, 5th edition, Pearson Educ., Inc. New Delhi.
2. Karplus M. and Porter, R. N., 1970 Atoms and Molecules, Benjamin, London.
3. Atkins P.W. and Friedman, R.S., 1997 Molecular Quantum Mechanics, 3rd edition, Oxford University Press. Oxford.
4. Pilar, Frank L. 1990 Elementary Quantum Chemistry 2nd Edition, McGraw – Hill Publishing Company.
5. Mc Quarrie D.A. and Simon, J.D. , 1998, Physical Chemistry: A Molecular Approach, Viva Books, New Delhi.
6. Murrell, J.N. ,. Kettle S.F.A and Tedder, J. M. , 1965, Valence Theory,2nd edition, John Viley,New York.
7. Chandra, A.K. , 1994 Introductory Quantum Chemistry, 4th edition, Tata McGraw Hill, NewDelhi.
8. Pualing L. and Wilson, E. B. , 1935 Introduction to Quantum Mechanics withApplications to Chemistry, McGraw Hill, New York.
9. B. H. Bransden and C. J. Joachain, 2003, Physics of atoms and molecules, 2nd edition, Pearson.
10. R. Loudon, 2000, The Quantum Theory of Light, 3rd edition, Oxford University Press.
11. Nielsen and Chuang, 2000, Quantum Computation and Quantum Information, Cambridge University Press.

SEMESTER IV

Course Name: Bio-inorganic chemistry **Code:** CHE-E-654

Semester: IV **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs):

1. Develop the ability to recognize and understand the role and action of metal ions in biological systems.
2. Illustrate the significance of metalloenzymes in various biological processes and their impact on biochemical reactions.
3. Identify and analyze key steps in life processes, gaining insight into the intricate nature of biochemical reactions.
4. Classify and compare different cancer therapeutic agents, enhancing the understanding of their mechanisms and applications.

Course Description:

This course provides an in-depth exploration of the vital role played by metal ions in biological systems.

Course Outline:

Unit 1

Role of alkali and alkaline earth metal ions in biological systems

A. Role of alkali metal ions: Na^+- K^+ Pump, ionophores and crown ethers. Transport of Na^+-K^+ through membranes

B. Catalysis of phosphate transfer by Mg^{2+} ion,

C. Regulatory role of Ca^{2+} - muscle contraction

Unit 2

Heme Proteins

Hemoglobin, myoglobin, hemerythrin, hemocyanin Oxygen activation: Cytochrome P450, Cytochrome c oxidase.

Non-heme proteins: Copper Proteins: Type I, II and III. Copper in cytochrome c oxidase and in respiratory chain, blue copper proteins

Unit 3

Proteins with reference to their oxygenation and oxidase activity

Anti-oxidative functions, Nitrate and nitrite reduction (NO3- and NO2- reductase), Synthetic models of iron-sulfur proteins, molybdo-enzymes – molybdenum cofactors (molybdenum-pterin complexes, nitrogen fixation through metal complexation, nitrogenase, Photosynthesis (PS-I and PS-II).

Unit 4

Metalloenzymes

Zinc enzymes- carboxypeptidase and carbonic anhydrase. Iron enzyme - catalases, peroxidase and cytochrome P-450. Copper enzyme-superoxide dismutase. Molybdenum oxo-transferase enzyme-xanthine oxidase. Urease and hydrogenase, and cyanocobalamine.

Metal ion storage and transport: Ferritin, transferritin, siderophores and metallothionein and hemosiderin.

Chemotherapeutic applications of metal complexes: Pt(II), Pt(IV) complexes and Ru(II), Ru(III) complexes as anticancer drugs, Au complexes as antiarthritis drugs

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of Course Learning Outcomes (CLOs) with POs:

CLO1	Develop the ability to recognize and understand the role and action of metal ions in biological systems.	[PO1] [PO2]
CLO2	Illustrate the significance of metalloenzymes in various biological processes and their impact on biochemical reactions.	[PO1] [PO2]
CLO3	Identify and analyze key steps in life processes, gaining insight into the intricate nature of biochemical reactions.	[PO1][PO2]
CLO4	Classify and compare different cancer therapeutic agents, enhancing the understanding of their mechanisms and applications.	[PO1][PO2][PO3]

Performance Indicators:

1. Demonstrate the ability to estimate the mode of transport, regulation, and activity of metal ions in biological systems.
2. Identify and explain the utilization of metal ions in enzymatic processes, highlighting their essential roles and contributions.
3. Develop the skill to correlate the mechanisms involved in different life processes, recognizing the interconnectedness and interplay of biochemical reactions.
4. Investigate and report on the mode of action of platinum-based cancer agents, comprehending their mechanisms and effects on cancer cells.

Suggested Readings

1. Hughes M. N., 1981 Inorganic Chemistry of Biological Processes, 2nd Ed., John-Wiley & Sons, New York.
2. Kaim W. and Schwederski B., 1995 Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York.
3. Lippard S. J. and Berg J. M., Principles of Bioinorganic Chemistry, University Science Books.
4.Bertini, I. , Grey H. B., Lippard S. J. and Valentine, J. S. , 1998 Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi.

SEMESTER IV

Course Name: Natural Products and Bio-Organic Chemistry **Code:** CHE-E-655

Semester: IV **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs)

Upon completion of the course, students will be able to:

1. Describe the biogenesis, biosynthesis, and structural features of natural products, including alkaloids, terpenoids, steroids, flavonoids, and prostaglandins.
2. Discuss the bonding, reaction mechanisms, and synthetic applications of organometallic compounds, including homogeneous hydrogenation, alkene complexes, carbonylation reactions, carbene complexes, and alkyne complexes.
3. Understand the classification, purification, and analysis of enzymes. Predict the mechanisms of action of specific enzymes and comprehend the chemistry of coenzymes.
4. Recognize the advantages of utilizing organo-transition metal chemistry and its applications in organic synthesis, including electron counting, bonding, and reaction mechanisms.
5. Discuss the synthesis and mechanisms of antibacterial agents, fluoroquinolones, anti-AIDS drugs, antihypertensive agents, calcium channel blockers, and gastric secretion inhibitors.
6. Integrate knowledge of natural product chemistry, organotransition metal chemistry, enzyme mechanisms, and medicinally important molecules to comprehend the synthesis, structure-activity relationship, and biological significance of bioactive compounds.

Course Description:

This course is designed to provide students with an in-depth understanding of natural products and bio-organic chemistry. It explores the structures, biosynthesis, and synthesis of various classes of natural products, including alkaloids, terpenoids, steroids, oxygen heterocycles, prostaglandins, and thromboxanes. Additionally, the course covers organotransition metal chemistry and its applications in organic synthesis, as well as the study of enzymes and their mechanisms of action. The chemistry of medicinally important molecules is also discussed, with a focus on antibacterial agents and their mechanisms, as well as the synthesis and mechanism of action of various drugs.

Course Outline:

Unit 1

Natural Products: Isoprene Rule, biogenesis and biosynthesis of representative examples.

Alkaloids: Structure, synthesis, and stereochemistry of Narcotine and Quinine; synthesis and stereochemistry of Morphine, Lysergic acid and Reserpine.

Terpenoids: Camphor, Longifolene, Abietic acid, and Taxol.

Steroids: Cholesterol, Aldosterone and Cortisone. Oxygen Hetrocycles: Flavonoids, isoflavonoids. Antioxidant properties of flavonoids.Prostaglandins and Thromboxanes: Introduction, nomenclature of prostaglandins andthromboxanes; approaches to prostaglandin synthesis-Woodward synthesis of PGF2a, Corey's synthesis of prostaglandins E and F

Unit 2

Organotransition Metal Chemistry: Applications to Organic Synthesis: Electron counting, bonding, organometallic reaction mechanism; Homogeneous hydrogenation; Organometallics as electrophiles; Synthetic applications of transition metal alkene complexes: Wacker oxidation. Synthetic applications of complexes containing metal – carbon σ bonds: Heck and related reactions, carbonylation reactions; Synthetic applications of transition metal carbene complexes: Fischer carbene, Schrock carbene, metathesis processes, Tebbe's reagent, Zieglar – Natta reaction; Synthetic applications of transition metal alkyne complexes: Pauson – Khand reaction, cyclooligomerisation;

Unit 3

Enzymes and Mechanism of Enzyme Action: Classification, isolation and purification. Methods of Enzyme analysis. Two substrate reactions;

Enzyme inhibition. Mechanism of action of chymotrypsin, aldolase, alcohol dehydrogenase, and lysozyme. Co-enzyme Chemistry: Cofactors as derived from vitamins; coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, NAD+, NADP+, FMN, FAD and vitamin B_{12}

Unit 4

Chemistry of Medicinally Important Molecules: antibacterial agents – mechanism with reference to β-lactam antibiotics; General method of synthesis of β-lactam ring: synthesis of penicillin, cephalosporin,

New generation antibiotics/ antibacterial agents: Synthesis and mechanism of action of

(i) fluoroquinolones – norfloxacin, ciprofloxacin, levofloxacin

(ii) anti AIDS drugs – AZT, lamivadine

(iii) antihypertensive agent –captopril

(iv) calcium channel blocker – amlodipine

(v) gastric secret Vitamins: inhibitor – omeprazole

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping Of CLOs with POs:

CLO1	Describe the biogenesis, biosynthesis, and structural features of natural products, including alkaloids, terpenoids, steroids, flavonoids, and prostaglandins.	PO1
CLO2	Discuss about the bonding, reaction mechanisms, and synthetic applications of organometallic compounds, including homogeneous hydrogenation, alkene complexes, carbonylation reactions, carbene complexes, and alkyne complexes.	[PO1][PO2]
CLO3	Aware about the classification, purification, and analysis of enzymes. They will be able to predict the mechanisms of action of specific enzymes and the chemistry of coenzymes.	PO1
CLO4	Describe the advantages of using organo-transition metal chemistry and its applications in organic synthesis, including electron counting, bonding, and reaction mechanisms.	PO1
CLO5	Discuss about synthesis and mechanisms of antibacterial agents,	[PO1][PO2]

	fluoroquinolones, anti-AIDS drugs, antihypertensive agents, calcium channel blockers, and gastric secretion inhibitors.	
CLO6	Integrate their knowledge of natural product chemistry, organotransition metal chemistry, enzyme mechanisms, and medicinally important molecules to understand the synthesis, structure-activity relationship, and biological significance of bioactive compounds.	PO3

Performance Indicators (PIs)

1. Demonstrate understanding of the biogenesis, biosynthesis, and structural features of natural products through written exams, quizzes, and assignments.
2. Propose synthetic routes for the selected natural products, considering stereochemistry and key reactions involved.
3. Discuss the nomenclature, synthesis approaches, and antioxidant properties of prostaglandins and thromboxanes.
4. Utilize the knowledge of organotransition metal chemistry to predict reaction mechanisms and propose synthetic applications for various transition metal complexes.
5. Predict the structures and biological functions of coenzymes derived from vitamins, and discuss their roles in enzymatic reactions.
6. Critically examine the synthesis methods and mechanisms of action of medicinally important molecules, such as β-lactam antibiotics, fluoroquinolones, anti-AIDS drugs, antihypertensive agents, calcium channel blockers, and gastric secret Vitamins inhibitors.

Suggested Readings

Text Books:

1. T.C. Bruice and S. Bentkovic, *Bioorganic Mechanisms*, Vol. I & II, W. A. Benjamin, New York (1966).
2. D. Voet, J.G. Voet & CW Pratt, *Fundamentals of Biochemistry*, John Wiley & Sons, New York (1999).
3. H. Dugas and C. Penney, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, Springer- Verlag, New York (1981).
4. J.W. Apsimon, *Total Synthesis of Natural Products*, Vol. 1-6, Wiley-Interscience Publications, New York.
5. J. Clayden, N. Greeves, S. Warren, and P. Wothers, *Organic Chemistry, Chapter 30,* Oxford University Press, Oxford (2001).

6. Burger's Medicinal Chemistry and Drug Discovery, 6th Edn. Donald J. Abraham (Editor), Wiley Interscience, 2003
7. Michael B. Smith, Jerry March, *March's Advanced Organic Chemistry. Reactions, Mechanisms, and Structure* 5th Edn, 2000 Wiley-Interscience

Reference Books:

1. I.L. Finar, *Organic Chemistry*, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd., New Delhi.
2. A.L. Lehninger, *Principles of Biochemistry,* CBS Publishers, Delhi (1992)
3. H.R. Mahler and E.H. Cordes, *Biological Chemistry*, 2nd Edition, Harper and Row Pub., New York (1971).
4. C. Walsh, *Enzymatic Reaction Mechanisms*, W.H. Freeman & Co., New York.
5. Nitya Anand, J.S. Bindra and S. Ranganathan, *Art in Organic Synthesis*, 2nd Edition (1970), Holden Day, San Francisco.
6. S.W. Pelletier, *Chemistry of the Alkaloids*, Van Nostrand Reinhold Co., New York (1970).
7. K.W. Bentley, *The Alkaloids*, Vol. I., Interscience Publishers, New York (1957).
8. J.S. Bindra and R. Bindra , *Creativity in Organic Synthesis*.
9. J.S. Bindra and R. Bindra, *Prostaglandins Synthesis*.
10. S. Waren, *Organic Synthesis:Disconnection Approach,* Wiley, New York (1982).
11. K. C. Nicolaou, *Classics in Total Synthesis of Natural Products,* Vol. I & II.
12. W.Kar, "*Medicinal Chemistry*", Wiley Eastern

Advanced Text Books:

1. The Science of Flavonoids: E. Grotewold, Springer
2. The Vitamin Book: H. M. Silverman, J. Romano, G. Elmer (1999)
3. Harper's Biochemistry: R. K. Murray, D. K. Granner, P. A. Mayes, V. W. Rodwell, 25th Ed. McGraw-Hill (2000)
4. An Introduction to Medicinal Chemistry: Graham L. Patrick (4th Ed). Oxford University Press (2009)
5. Medicinal Chemistry – Principle and Practice: F. D. King, 2nd ed. (2002); Springer
6. Heterocyclic Chemistry: J. A. Joule and K. Mills (4th Ed) Wiley-Blackwell.

SEMESTER IV

Course Name: Non-equilibrium Thermodynamics and Statistical Mechanics **Code:** CHE-E-656

Semester: IV **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs)

Upon completion of the course, students will be able to:

1. Demonstrate the ability to recognize irreversible processes
2. Apply the principles of kinetic theory to forecast irreversible processes
3. Predict the dynamics of quantum processes
4. Understand the non-linearity inherent in irreversible systems

Course Description:

Non-equilibrium Thermodynamics and Statistical Mechanics is an elective course offered in the fourth semester of the program. This course focusses on the fundamental principles and applications of non-equilibrium thermodynamics, with an emphasis on understanding the behavior of systems far from equilibrium. The course explores various theoretical frameworks and mathematical tools used to analyze and describe non-equilibrium phenomena in diverse systems, such as chemical reactions, transport processes, and quantum dynamics.

Course Outline:

Unit 1

Basics of non-equilibrium thermodynamics : Review of Irreversible Thermodynamics, Onsager relations, Flux-force concepts, Chemical reactions and relaxation phenomenon, heat conduction and diffusion,

electrical conduction,

Unit 2

Kinetic Theory amd Dynamics. Kinetic Theory of Gases, Collisons, Boltzmann Equation, Transport processes in dilute gases.

Brownian Motion and Langevin dynamics, time correlation functions, Fokker Planck Equations, Liouville equation, Master equations, Reaction rates, kinetic models, Navier-stokes equation.

Unit 3

Quantum Dynamics: Quantum Liouville Operator, Electron Transfer kinetics, Bloch Equations

Unit 4

Projection Operators and Non-linear Problems. Linear Response Theory, Langevin equations, Noise, Mode-Coupling theory

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Demonstrate the ability to recognize irreversible processes	[PO1]
CLO2	Apply the principles of kinetic theory to forecast irreversible processes	[PO1][PO2]
CLO3	Predict the dynamics of quantum processes	[PO1]
CLO4	Understand the non-linearity in irreversible systems	[PO1][PO2]

Performance Indicators (PIs)

1. Recognize irreversible processes in real systems
2. Acquire a fundamental understanding of kinetic theory to forecast irreversible processes
3. Forecast dynamics in quantum mechanical systems
4. Anticipate non-linearity in irreversible systems

Suggested Readings:

1. Zwanzig Robert, Non-equilibrium Statistical Mehanics, Oxford University Press
2. McQuarrie Donald, Statistical Mechanics, Harper and Row Publishers
3. Balescu Radu, Equilibrium and Non-equilibrium Statistical Mechanics, John Wiley and Sons
4. Chandler David, Introduction to Modern Statistical Mechanics,
5. Huang kerson, Statistical Mechanics, John Wiley and Sons
6. Shang Keng Ma, Statistical Mechanics, World Scientific

SEMESTER IV

Course Name: Solid-State Chemistry **Code:** CHE-E-657

Semester: IV **Course Level:** 600 **Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs):

Upon successful completion of the Solid-State Chemistry course, students will be able to:

1. Understand the principles and applications of solid-state reactions, including co-precipitation, kinetics, crystallization, and thin film preparation methods.
2. Analyze phase transitions in materials and differentiate between different types of phase transitions based on thermodynamics and kinetics.
3. Explain the electronic properties of solids using band theory, including the band structure of metals, insulators, and semiconductors.
4. Describe the magnetic properties of materials, including types of magnetism, determination of magnetic susceptibility, and the concept of magnetic domains.
5. Utilize structural characterization techniques such as X-ray diffraction, electron diffraction, neutron diffraction, and solid-state NMR to determine the crystal structure and properties of materials.
6. Analyze the structural features and properties of high-Tc oxide superconductors, including their normal state and superconducting state properties, as well as their applications.
7. Evaluate the properties and applications of non-linear materials, including molecular rectifiers, frequency doublers, photochromic materials, and their use in optical data storage and electronic devices.

Course Description:

Solid-State Chemistry is a comprehensive course that explores the principles, properties, and applications of solid-state materials. This course covers a wide range of topics, including solid-state reactions, phase transitions, electronic and magnetic properties, structural characterization techniques, and the study of high-Tc oxide superconductors. Through theoretical lectures, laboratory experiments, and hands-on activities, students will develop a deep understanding of the fundamental concepts and techniques in solid-state chemistry. This course is suitable for students pursuing master's degrees in chemistry, materials science, and related fields

Course Outline:

Unit 1

Solid State Reactions: General Principles, Experimental procedure, Co-precipitation a a precursor to solid-state reactions, Kinetics of solid-state reactions, Crystallization of solutions, melts, glasses and gels. Preparation of thin films (chemical, electrochemical and physicalmethods), Hydrothermal methods, Growth of single crystals: Czochralski method, Bridgman and Stockbarger methods. Zone Melting. Reactions at solid surfaces.

Unit 2

Phase transitions, electronic and magnetic properties. Phase Transitions: Thermodynamic and Burger's classification of phase transition, Kinetics of phase transition- nucleation and growth, T-T-T diagrams, Factors that influence kinetics of phase transition, Martensitic and order-disorder transitions.

Electronic Properties and Band Theory: Electronic structure of solids- band theory, Refinement to simple band theory- k-space and Brillouin Zones, Band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, Doped semiconductors, p- n junctions. Concepts of thin film devices. Field effect transistors, photovoltaics, Light emitting diodes.

Magnetic Properties: Classification of materials. Magnetism: Types, determination of magnetic susceptibility. Quantum theory of diamagnetism and paramagnetism. Cooperative phenomena. Magnetic domains. Hysteresis. Concepts of GMR, Solid State storage.

Unit 3

Structural characterisation techniques: X-ray Diffraction: Diffraction of X-rays by crystals: The Laue equations and Bragg's law, Definitions related to crystal structure. X-ray diffraction experiments: The powder method and the single crystal method. Reciprocal lattice. Structure factor. Structure factor and intensity. Electron density maps.

Electron diffraction: Scattering intensity versus scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cells.

Solid State NMR: Differences between solid and liquid state NMR, comparison with XRD, Magic Angle spinning, Chemical shielding, J-coupling, Dipolar coupling, Quadrupolar coupling.

Unit 4

High-Tc Oxide Superconductors: Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Normal state properties: anisotropy and temperature dependence of electrical resistance.Superconductingstate: heat capacity, coherence lengt h, relation between Tc and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high Tc-cuprates. Non-linear materials: Second and third order non-linear effects; molecular rectifiers and frequency doublers; unimolecular electronic devices. Photochromic materials; optical data storage, memory and switches.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	**Written**	**Oral**	**Integrated**
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of (CLOs) with Program Outcomes (POs):

CLO1	Understand the principles and applications of solid-state reactions, including co-precipitation, kinetics, crystallization, and thin film preparation methods.	PO1
CLO2	Analyze phase transitions in materials and differentiate between different types of phase transitions based on thermodynamics and kinetics.	[PO1] [PO2]
CLO3	Explain the electronic properties of solids using band theory, including the band structure of metals, insulators, and semiconductors.	[PO1][PO2]
CLO4	Describe the magnetic properties of materials, including types of magnetism, determination of magnetic susceptibility, and the concept of magnetic domains.	[PO1] [PO2]
CLO5	Utilize structural characterization techniques such as X-ray diffraction, electron diffraction, neutron diffraction, and solid-state NMR to determine the crystal structure and properties of materials.	[PO1] [PO]2 [PO3]
CLO6	Analyze the structural features and properties of high-Tc oxide superconductors, including their normal state and superconducting state properties, as well as their applications.	PO2
CLO7	Evaluate the properties and applications of non-linear materials, including molecular rectifiers, frequency doublers, photochromic materials, and their use in optical data storage and electronic devices.	PO3

Performance Indicators for Unit 1:

i) Demonstrate understanding of the general principles of solid-state reactions.

ii) Follow experimental procedures for solid-state reactions.

iii) Explain the concept of co-precipitation as a precursor to solid-state reactions.

iv) Analyze the kinetics of solid-state reactions.

v) Describe the crystallization processes of solutions, melts, glasses, and gels.

vi) Perform thin film preparation using chemical, electrochemical, and physical methods.

vii) Apply hydrothermal methods for the synthesis of materials.

Viii) Demonstrate knowledge of the growth methods of single crystals, such as the Czochralski method, Bridgman method, and Stockbarger method.

ix) Explain the principles of zone melting.

x)Understand and discuss reactions occurring at solid surfaces.

Performance Indicators for Unit 2:

i) Classify phase transitions according to thermodynamics and Burger's classification.

ii) Describe the kinetics of phase transitions, including nucleation and growth processes.

iii) Interpret T-T-T diagrams and explain factors influencing the kinetics of phase transition.

iv) Analyze martensitic and order-disorder transitions.

v) Explain band theory and its refinement, including k-space and Brillouin Zones.

vi) Compare and contrast the band structures of metals, insulators, and semiconductors.

vii) Understand intrinsic and extrinsic semiconductors, as well as doped semiconductors.

viii) Describe the operation and principles of p-n junctions and thin film devices.

ix) Explain the working principles and applications of field-effect transistors, photovoltaics, and light-emitting diodes.

x) Classify materials based on their magnetic properties.

xi) Determine magnetic susceptibility and explain the quantum theory of diamagnetism and paramagnetism.

xii) Describe cooperative phenomena, magnetic domains, and hysteresis.

xiii) Understand the concepts of Giant Magneto-Resistance (GMR) and solid-state storage.

Performance Indicators for Unit 3:

i) Explain the principles of X-ray diffraction, including the Laue equations and Bragg's law.

ii) Perform X-ray diffraction experiments using powder and single crystal methods.

iii) Understand reciprocal lattice and calculate structure factors.

iv) Analyze the relationship between structure factors and intensity in X-ray diffraction.

v) Describe electron diffraction, including the Wierl equation and measurement techniques.

vi) Interpret electron diffraction patterns to elucidate the structure of simple gas phase molecules.

vii) Understand low energy electron diffraction (LEED) and its application to surface structure determination.

viii) Explain the principles of neutron diffraction, including scattering by solids, liquids, and magnetic materials.

ix) Perform neutron diffraction measurements to determine the structure of magnetically ordered unit cells.

x) Compare solid-state NMR with liquid-state NMR and X-ray diffraction.

xi) Apply concepts of magic angle spinning, chemical shielding, J-coupling, and quadrupolar coupling in solid-state NMR.

Performance Indicators for Unit 4:

i) Identify the structural features of cuprate superconductors.

ii) Understand the structures of 1-2-3 and 2-1-4 cuprate superconductors.

iii) Explain the normal state properties of cuprate superconductors, including anisotropy and temperature dependence of electrical resistance.

iv) Analyze the superconducting state of cuprate superconductors, including heat capacity and coherence length.

v) Understand the relationship between Tc (critical temperature) and hole concentration in cuprate superconductors.

vi) Explain the mechanism of superconductivity in cuprate superconductors.

vii) Discuss the applications of high-Tc cuprate superconductors.

viii) Describe second and third-order

Suggested Readings:

1. C. Kittel, Introduction to Solid State Physics, John Wiley & Sons, Inc., New York, Chichester.

2. O. Madelung, Introduction to Solid State Theory

3. A. R. West, Solid State Chemistry and its Applications, (1984) John Wiley and Sons, Singapore.

4. L.V. Azaroff, Introduction to Solids, (1977) Tata McGraw-Hill, New Delhi.

5. A. J. Dekker, Solid State Physics, Prentice Hall

SEMESTER IV

Course Name: Analytical Chemistry		**Code:** CHE-E-658
Semester: IV	**Course Level:** 600	**Total Marks:** 100

L+T+P: 3+1+0 =4 Credits (Lecture = 45 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs):

1. Demonstrate the ability to recall and define fundamental concepts in analytical chemistry.
2. Explain the application of solvent extraction in separation techniques.
3. Compare, contrast, and describe the fundamental principles of gas and liquid chromatography.
4. Interpret the utilization of electrochemistry in electroanalytical techniques for separation, estimation, and catalytic applications.

Course Description:

Analytical Chemistry is a comprehensive course designed to provide students with a thorough understanding of the principles, techniques, and applications of analytical chemistry. This course covers a wide range of topics, including quantitative and qualitative analysis, instrumental methods, and data analysis.

Course Outline:

Unit-1: Fundamentals of Chemical Analysis

Recapitulation of the elementary concepts of Analytical Chemistry. Aim of analytical chemistry. Standardization and calibration. Quality assurance and quality control. Process control and validation. Classical methods of analysis: Gravimetry and titrimetry including neutralization, complexation and oxidation-reduction. Complex acid-base equilibrium. Separation of metal ions as their hydroxides, sulphides and chelates. Examples of gravimetric and complexometric analysis.

Unit-2: Solvent Extraction and Concept of Chromatography

Liquid-Liquid extraction – Cross and counter current process, multiple batch extraction, solvent extraction of metal ion, solid-phase extraction. Classification of chromatographic separation. Aqueous biphasic and supercritical fluid extraction. Band broadening and column efficiency, Theoretical plate model and the Rate theory of Chromatography.

Unit-3: Liquid Chromatography and Other Types of Chromatography:

Reverse and normal phase chromatography, gradient elution, solvent selection and classes, ion exchange and ion chromatography.

HPLC: Basic equipment, pumping and injection system, column stationary phase and structural types of column packing, Detector systems (UV, IR, Conductometric, Fluorescence), Sample preparation and applications.

Gas chromatography: gas-liquid and gas-solid chromatography, types of column and selection. Basic equipment, Injection systems, Detectors (FID, TCD, ECD, NPD) for GC, sample separation and applications.

Characteristics and applications of Size exclusion Chromatography, Affinity chromatography, Supercritical Fluid Chromatography, Capillary Electrophoresis.

Unit- 4: Electro-analytical techniques

Electrogravimetry: Theory of electrogravimetric analysis – electrolytic separation and determination of metal ions. Coulometry: Electrolytic cell-working electrodes – auxiliary electrode and reference electrode – Coulometric titrations. Voltammetry: Theory and application of polarography, Cyclic voltammetry – Stripping voltammetry – Chronopotentiometry, Amperometry: Amperometric titrations. Bioelectrochemistry; Electrocatalysis, Photoelectrochemistry.

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Demonstrate the ability to recall and define fundamental concepts in analytical chemistry.	[PO1][PO2]
CLO2	Explain the application of solvent extraction in separation techniques.	[PO1[PO2]
CLO3	Compare, contrast, and describe the fundamental principles of gas and liquid chromatography.	[PO1] [PO2]
CLO4	Interpret the utilization of electrochemistry in electroanalytical techniques for separation, estimation, and catalytic applications.	[PO1] [PO2]

Performance Indicators:

1. Apply classical analytical techniques to separate metal ions.
2. Recognize methods for separating solvents from a mixture.
3. Establish relationships between the factors that govern the functioning of gas and liquid chromatography.
4. Utilize electroanalytical techniques for electroplating, separating metal ions, estimating quantities, and directly applying them in electrocatalysis.

Suggested Readings:

1. Christian, G.D. Analytical Chemistry, 6th Ed. John Wiley & Sons, New York, 2004.
2. Mikes, O. & Chalmes, R.A. Laboratory Handbook of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
3. Ditts, R.V. Analytical Chemistry: Methods of separation. Van Nostrand, New York, 1974.
4. McMaster, M.C. HPLC: A Practical User's Guide, 2nd Ed John Wiley & Sons, New York, 2007.
5.Bard, Allen J., Faulkner, L. R. Electrochemical Methods: Fundamentals and Applications, 2nd Ed. John Wiley & Sons, New York, 2000.

SEMESTER IV

Course Name: Modern Synthetic Techniques **Code:** CHE-S-659

Semester: IV **Course Level:** 600 **Total Marks:** 100

L+T+P: 1+1+0 **=**2 Credits (Lecture = 15 hrs; Tutorial = 15 hrs; Practical = 0 hrs)

Type: Elective Theory

Course Learning Outcomes (CLOs)

1. Explain the principles and methodologies utilized in contemporary synthetic techniques within organic chemistry.
2. Acquire a comprehensive understanding of diverse synthetic strategies, encompassing total synthesis, formal synthesis, combinatorial synthesis, and diversity-oriented synthesis.
3. Comprehend the principles and practical applications of visible-light photocatalysis, electrocatalysis, mechanochemical synthesis, and microwave synthesis in the realm of organic synthesis.
4. Investigate the hydrothermal method and its utilization in synthesizing materials under conditions of high temperature and high pressure. CLO5: Obtain knowledge pertaining to the sol-gel method and its utilization in synthesizing materials possessing controlled porosity and composition.

Course Description:

This course introduces students to modern synthetic techniques in organic chemistry.

Course Outline:

Unit 1 Synthetic strategies

i) Total synthesis and formal synthesis

ii) Combinatorial synthesis

iii) Diversity oriented synthesis

Unit 2 Synthetic methods

i)Visible-light photocatalysis

ii)Electro catalysis

iii)Microwave synthesis

iv) Mechano chemistry

v)Hydrothermal method

vi) Sol Gel method

Suggested-teaching learning strategy

1. Lecture with interactive discussions and problem-solving activities.
2. Assignments and individual presentations.
3. Student-led classroom teaching.
4. Group discussions.

Assessment Framework

Modes	Written	Oral	Integrated
Formative (50 Marks)	Class Test, Open Book Test, Quiz, Online Test, Class Assignment, Home Assignment	Oral Test, Viva-Voce, Seminar	Presentation, Seminars
Summative (50 marks)	End-Semester Examination conducted by the University		

Note: The course teacher may select an appropriate mode of formative assessment based on the nature of the Course Learning Outcomes (CLOs) and its practicality.

Mapping of CLOs with POs:

CLO1	Describe the principles and strategies behind modern synthetic techniques in organic chemistry.	PO1
CLO2	Gain knowledge of different synthetic strategies, including total synthesis, formal synthesis, combinatorial synthesis, and diversity-oriented synthesis.	PO2
CLO3	Understand the principles and applications of visible-light	[PO1][PO2][PO3]

	photocatalysis, electrocatalysis, mechanochemical and microwave synthesis in organic synthesis.	
CLO4	Explore the hydrothermal method and its applications in synthesizing materials under high-temperature and high-pressure conditions.	[PO1][PO3]
CLO5	Gain knowledge of the sol-gel method and its applications in the synthesis of materials with controlled porosity and composition.	PO1

Performance Indicators (PIs)

1. Demonstrate understanding of the principles and strategies behind modern synthetic techniques through written exams and quizzes.
2. Discuss the concepts of total synthesis and formal synthesis, including the application of retrosynthetic analysis.
3. Illustrate the strategies for combinatorial synthesis and Diversity oriented synthesis considering the efficient generation of diverse compound libraries.
4. Discuss the principles and applications of visible-light photocatalysis in organic synthesis, considering its advantages and greener aspects.
5. Propose synthetic routes using electrocatalysis, considering its role in facilitating redox reactions and its advantages in terms of efficiency and sustainability.
6. Applications of microwave synthesis, in accelerating chemical reactions and its advantages in terms of efficiency and selectivity.
7. Discuss the applications of mechanochemistry in organic synthesis and its greener aspects.
8. Discuss the principles and applications of the hydrothermal method in synthesizing materials under high-temperature and high-pressure conditions.
9. Evaluate and propose synthetic routes using the sol-gel method, considering its applications in the synthesis of materials with controlled porosity and composition.
10. Communicate scientific concepts, experimental results, and applications of modern synthetic techniques through oral presentations, research papers, and group discussions.

Suggested Readings:

(1) Nicolaou, K. C. *Classics in Total Synthesis - Targets, Strategies, Methods*, 1st edition.; Wiley-VCH Verlag GmbH: Weinheim ; New York, 1996.

(2) Hanessian, S. *Total Synthesis of Natural Products: "Chiron" Approach*; Pergamon Press: Oxford Oxfordshire ; New York, 1983.

(3) Hanessian, S. *Total Synthesis of Natural Products : The "Chiron" Approach*; Pergamon, 1986.

(4) Front Matter. In *Total Synthesis of Bioactive Natural Products*; Brahmachari, G., Ed.; Elsevier, 2019; pp i–ii. https://doi.org/10.1016/B978-0-08-102822-3.09993-4.

(5) Wilson, S. R.; Czarnik, A. W. *COMBINATORIAL CHEMISTRY: SYNTHESIS AND APPLICATION*; Wiley India Pvt Ltd, 2013.

(6) Front Matter. In *Handbook of Combinatorial Chemistry*; John Wiley & Sons, Ltd, 2002; pp i–xxxi. https://doi.org/10.1002/3527603034.fmatter.

(7) Lenci, E.; Menchi, G.; Trabocchi, A. Carbohydrates in Diversity-Oriented Synthesis: Challenges and Opportunities. *Org. Biomol. Chem.***2016**, *14* (3), 808–825. https://doi.org/10.1039/C5OB02253C.

(8) Trabocchi, A.; Schreiber, S. L. *Diversity-Oriented Synthesis: Basics and Applications in Organic Synthesis, Drug Discovery, and Chemical Biology*, 1st edition.; Wiley, 2013.

(9) Stephenson, C. R. J.; Yoon, T. P.; MacMillan, D. W. C. *Visible Light Photocatalysis in Organic Chemistry*; John Wiley & Sons, 2018.

(10) *Theory and Experiment in Electrocatalysis | SpringerLink*. https://link.springer.com/book/10.1007/978-1-4419-5594-4 (accessed 2023-06-05).

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(12) Demetrios A. Kyriacou, D. K. ; J. *Electrocatalysis for Organic Synthesis*; Wiley: New York, 1986.

(13) *Practical Microwave Synthesis for Organic Chemists | Wiley Online Books*. https://onlinelibrary.wiley.com/doi/book/10.1002/9783527623907 (accessed 2023-06-05).

(14) Kappe, C. O.; Stadler, A.; Dallinger, D.; Mannhold, R.; Kubinyi, H.; Folkers, G. *Microwaves in Organic and Medicinal Chemistry: 52*, 2nd edition.; Wiley-VCH: Weinheim, 2012.

(15) Kappe, C. O.; Dallinger, D.; Murphree, S. S. *Practical Microwave Synthesis for Organic Chemists: Strategies, Instruments, and Protocols*; John Wiley & Sons, 2008.

(16) Mechanochemistry: A Practical Introduction from Soft to Hard Materials. In *Mechanochemistry*; De Gruyter, 2020. https://doi.org/10.1515/9783110608335.

(17) Front Matter. In *Mechanochemical Organic Synthesis*; Margetić, D., Štrukil, V., Eds.; Elsevier: Boston, 2016; p iii. https://doi.org/10.1016/B978-0-12-802184-2.01001-3.

(18) Schäf, O.; Ghobarkar, H.; Knauth, P. Hydrothermal Synthesis of Nanomaterials. In *Nanostructured Materials*; Knauth, P., Schoonman, J., Eds.; Electronic Materials: Science &

Technology; Kluwer Academic Publishers: Boston, 2004; Vol. 8, pp 23–41. https://doi.org/10.1007/0-306-47722-X_2.

(19) *Handbook of Hydrothermal Technology - 2nd Edition*. https://shop.elsevier.com/books/handbook-of-hydrothermal-technology/byrappa/978-0-12-375090-7 (accessed 2023-06-05).

(20) Aguilar, G. V. *Sol-Gel Method - Design and Synthesis of New Materials with Interesting Physical, Chemical and Biological Properties*; 2019. https://doi.org/10.5772/intechopen.76535.

(21) Front Matter. In *The Sol-Gel Handbook*; John Wiley & Sons, Ltd, 2015; p I–XLVI. https://doi.org/10.1002/9783527670819.fmatter.

(22) Schreiber, S. L. Target-Oriented and Diversity-Oriented Organic Synthesis in Drug Discovery. *Science***2000**, *287* (5460), 1964–1969. https://doi.org/10.1126/science.287.5460.1964.

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(24) Spring, D. R. Diversity-Oriented Synthesis; a Challenge for Synthetic Chemists. *Org. Biomol. Chem.***2003**, *1* (22), 3867–3870. https://doi.org/10.1039/B310752N.

(25) Xuan, J.; Xiao, W.-J. Visible-Light Photoredox Catalysis. *Angewandte Chemie International Edition***2012**, *51* (28), 6828–6838. https://doi.org/10.1002/anie.201200223.

(26) Pitre, S. P.; Overman, L. E. Strategic Use of Visible-Light Photoredox Catalysis in Natural Product Synthesis. *Chem. Rev.***2021**. https://doi.org/10.1021/acs.chemrev.1c00247.

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(28) Romero, N. A.; Nicewicz, D. A. Organic Photoredox Catalysis. *Chem. Rev.***2016**, *116* (17), 10075–10166. https://doi.org/10.1021/acs.chemrev.6b00057.