Semester	**7**
Programme	**CHEMISTRY**
Course	**MAJOR (ORGANIC CHEMISTRY 7)**
Paper Code	**C4CH230712T / C4CH230712P**
Credits	**4 (THEORY: 3; PRACTICAL: 1)**
Hours/week	**6 (THEORY: 3; PRACTICAL: 3)**
Category: Core/MDC/SEC/VEC	**CORE**
Theory/Practical/Composite	**COMPOSITE**
Number of Modules	**4**
Syllabus	**Theory:** **Module I: Pericyclic reactions 12L** Pericyclic reactions: Mechanism, stereochemistry, regioselectivity in case of Electrocyclic reactions: FMO approach involving 4π- and 6π-electrons (thermal and photochemical) and corresponding cycloreversion reactions. Cycloaddition reactions: FMO approach, Diels-Alder reaction, photochemical [2+2] cycloadditions. Sigmatropic reactions: FMO approach, sigmatropic shifts and their order; [1,3]- and [1,5]-H shifts and [3,3]-shifts with reference to Claisen and Cope rearrangements. Analysis of electrocyclic reactions with symmetry property according to Woodward and Hofmann's correlation diagram. Construction of correlation diagrams. Mechanistic explanation of electrocyclic reactions with PMO method, selection rules. Application of PMO method in the [1, j]-sigmatropic rearrangement. Cheletropic reactions and mechanistic explanation of cheletropic reactions with FMO approach. Mechanistic explanation of 'Ene' and 'Group-transfer' reactions with FMO approach. Pericyclic reactions under polar conditions **Module II: Reagent chemistry- I 12L** Oxidizing and reducing reagents in organic synthesis Oxidation and oxidizing agents: Epoxidation reactions, Sharpless epoxidation, oxidation with OsO_4, $KMnO_4$, $Pb(OAc)_4$, HIO_4, Oxidation with Mn(VII), Mn(IV) and Cr(VI) reagents (Jones reagent, Collin's reagent, Corey's reagent), Oxidation with non-metal-based reagents: Activated DMSO - Swern

	oxidation, SeO_2, CAN, IBX and Dess-Martin Periodinane oxidation. Reduction and reducing agents: Reduction involving dissolving metals in ketones (conjugated and non-conjugated), hydride transfer reducing agents, reductions using aluminium alkoxide. Wilkinson's catalyst. **Module III: Reagent chemistry- II and Introduction to Asymmetric Synthesis 12L** Organosulphur, and organo-transition metal reagents in organic synthesis Organosulphur- Chemistry of organosulphur compounds, Sulphur- stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylides, chiral sulphoxides. Chemistry of organo-transition metal compounds: Brief idea on Pauson Khand reaction, Heck, Suzuki, Sonogashira, Negishi, Stille, Buchwald-hartwig, olefin metathesis. Principles and methods of asymmetric synthesis: chiral auxiliaries, chiral reagents, asymmetric catalysis, asymmetric aldol reaction, enantio- and diastereoselective synthesis, cyclopropanation, electrophile induced cyclisation, iodolactonisation. **Practical:** Group A • Study on the excited state acidity constants of some molecules. • Protein – drug binding interactions – experimental and theoretical studies. • Using FTIR to illustrate isomer concepts - special reference to xylem. Group B • Synthesis and purification (column chromatography) of redox non-innocent ligands possessing conjugated azo skeleton. • Synthesis and purification (column chromatography) of ligands possessing imino-quinone function in conjugation with other groups. • Designed synthesis and purification (column chromatography) of redox non-innocent ligands possessing pyridyl/ benzothiazole skeleton in conjunction with other functions. Group C • Synthesis of diisopropylidene D- glucose. • Selective 5,6- deprotections by AcOH. • Synthesis of corresponding aldehyde with NaIO4. Group D

	• Determination of cmc of detergents in aqueous solution. • Determination of Gibbs surface excess concentration for different detergents in water. • Determination of aggregation number of surfactants in micelle in aqueous solution. Group E • Setup of Linux environment (Bash), Fortran/Python compilers, and initialization of a project repository on GitHub. • Implementation of numerical differentiation and integration schemes. • Development of matrix operations and diagonalization routines for solving simple eigenvalue problems. Group F • Synthesis of quinoline based fluorescent probes. - i) Isolation and purification of the product • Synthesis of quinoline based fluorescent probes - ii) Characterisation of the product • Synthesis of quinoline based fluorescent probes - Iii) Photo physical (UV- VIS and Luminescence studies) Group G • Synthesis of organic linkers required for the construction of metallacycles, metal–organic frameworks, and coordination polymers. • Purification and characterization of synthesized linkers using standard laboratory and spectroscopic techniques. • Preparation of metallacycles using appropriate metal ions and pre-designed organic linkers. Group H • Synthesis and purification (column chromatography/distillation/crystallization) of macrocylic amine based ligands • Synthesis and purification (column chromatography/distillation/crystallization) of redox active ligands having Sulfur/Nitrogen/Phosphorous/Oxygen donor sites • Targeted synthesis of Mixed-metal oxide compounds and other molecular materials.
Course Overview	**Theory:**
Course Outcomes	Upon successful completion of this course, students will be able to: CO1: Explain the fundamental mechanisms, stereochemical pathways, and regioselectivity of electrocyclic, cycloaddition, and sigmatropic reactions using the Frontier Molecular Orbital (FMO) approach.

	CO2: Construct Woodward-Hofmann correlation diagrams using molecular orbital symmetry properties to establish and analyze selection rules for thermal and photochemical pericyclic pathways. CO3: Apply the Perturbative Molecular Orbital (PMO) method to provide mechanistic explanations and derive selection rules for electrocyclic and [1, j]-sigmatropic rearrangements. CO4: Categorize and compare the structural pathways of cheletropic, 'Ene', and 'Group-transfer' reactions, including pericyclic processes operating under polar conditions. CO5: Select, predict, and justify the stereochemical outcomes of selective organic oxidations using metal-based (OsO_4, Sharpless, Cr/Mn) and non-metal-based (Swern, IBX, Dess-Martin) oxidizing agents. CO6: Analyze reduction mechanisms involving dissolving metals, selective hydride transfers, aluminum alkoxides, and homogeneous catalyst systems like Wilkinson's catalyst. CO7: Illustrate the synthetic utility, reaction conditions, and catalytic cycles of organosulfur reagents (ylides, chiral sulfoxides) and modern organo-transition metal cross-coupling reactions (Heck, Suzuki, Sonogashira, Metathesis). CO8: Design multi-step synthetic routes for asymmetric target molecules using chiral auxiliaries, asymmetric catalysis, stereoselective aldol reactions, and electrophile-induced cyclizations. CO9: Evaluate the chemical hazards, safety protocols, and environmental sustainability metrics (such as atom economy and green chemistry principles) associated with the specified reagents and catalytic cycles.
Program Outcomes	**PO1**. Fundamental Knowledge: Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. **PO2**. Laboratory Skills: Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. **PO3**. Problem Solving: Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design

	experiments and interpret data. **PO4**. Research Competency: Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. **PO5**. Interdisciplinary Applications: Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. **PO6**. Communication Skills: Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. **PO7**. Ethics and Sustainability: Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

Module	**Course Outcome (CO)**	**Cognitive Domain (Bloom's K-Values)**	**Mapped Program Outcomes (POs)**
Module I: Pericyclic Reactions	**CO1:** Explain the fundamental mechanisms, stereochemical pathways, and regioselectivity of electrocyclic, cycloaddition, and sigmatropic reactions using the Frontier Molecular Orbital (FMO) approach.	**K2** (Understanding) **K4** (Analyzing)	PO1: Fundamental Knowledge PO3: Problem Solving
	CO2: Construct Woodward-Hofmann correlation diagrams using molecular orbital symmetry properties to establish and analyze selection rules for thermal and	**K3** (Applying) **K4** (Analyzing)	PO1: Fundamental Knowledge PO3: Problem Solving

	photochemical pericyclic pathways.		
	CO3: Apply the Perturbative Molecular Orbital (PMO) method to provide mechanistic explanations and derive selection rules for electrocyclic and [1, j]-sigmatropic rearrangements.	**K3** (Applying)	PO1: Fundamental Knowledge PO3: Problem Solving
	CO4: Categorize and compare the structural pathways of cheletropic, 'Ene', and 'Group-transfer' reactions, including pericyclic processes operating under polar conditions.	**K2** (Understanding) **K4** (Analyzing)	PO1: Fundamental Knowledge PO3: Problem Solving
Module II: Reagent Chemistry - I	**CO5:** Select, predict, and justify the stereochemical outcomes of selective organic oxidations using metal-based (OsO_4, Sharpless, Cr/Mn) and non-metal-based (Swern, IBX, Dess-Martin) oxidizing agents.	**K3** (Applying) **K5** (Evaluating)	PO1: Fundamental Knowledge PO3: Problem Solving

	CO6: Analyze reduction mechanisms involving dissolving metals, selective hydride transfers, aluminum alkoxides, and homogeneous catalyst systems like Wilkinson's catalyst.	**K4** (Analyzing)	PO1: Fundamental Knowledge PO2: Laboratory Skills
Module III: Reagent Chemistry - II & Asymmetric Synthesis	**CO7:** Illustrate the synthetic utility, reaction conditions, and catalytic cycles of organosulfur reagents (ylides, chiral sulfoxides) and modern organo-transition metal cross-coupling reactions (Heck, Suzuki, Sonogashira, Metathesis).	**K2** (Understanding) **K3** (Applying)	PO1: Fundamental Knowledge PO5: Interdisciplinary Applications
	CO8: Design multi-step synthetic routes for asymmetric target molecules using chiral auxiliaries, asymmetric catalysis, stereoselective aldol reactions, and electrophile-induced cyclizations.	**K4** (Analyzing) **K6** (Creating)	PO1: Fundamental Knowledge PO3: Problem Solving PO4: Research Competency

Cross-Cutting / All Modules	**CO9:** Evaluate the chemical hazards, safety protocols, and environmental sustainability metrics (such as atom economy and green chemistry principles) associated with the specified reagents and catalytic cycles.	**K2** (Understanding) **K5** (Evaluating)	PO2: Laboratory Skills PO6: Communication Skills PO7: Ethics and Sustainability

Reading/Reference Lists	1. Clayden, J., Greeves, N. & Warren, S. Organic Chemistry, Second edition, Oxford University Press, 2012. 2. Keeler, J., Wothers, P. Chemical Structure and Reactivity – An Integrated approach, Oxford University Press. 3. Sykes, P. A guidebook to Mechanism in Organic Chemistry, Pearson Education, 2003. 4. Smith, J. G. Organic Chemistry, Tata McGraw-Hill Publishing Company Limited. 5. Carey, F. A., Guiliano, R. M. Organic Chemistry, Eighth edition, McGraw Hill Education, 2012. 6. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994. 7. Nasipuri, D. Stereochemistry of Organic Compounds, Wiley Eastern Limited. 8. Morrison, R. N. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education). 9. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education) 10. Fleming, I. Molecular Orbitals and Organic Chemical Reactions, Reference/Student Edition, Wiley, 2009. 11. James, J., Peach, J. M. Stereochemistry at a Glance, Blackwell Publishing, 2003. 12. Robinson, M. J. T., Stereochemistry, Oxford Chemistry Primer, Oxford University Press, 2005. 13. Collman, J. P., Hegedus, L. S., Norton, J. R. Principles and Applications of Organotransition Metal Chemistry, University Science Books,U.S., 1987.

	14. Zweifel, G. S., Nantz, M. H., Somfai, P. Modern Organic Synthesis: An Introduction, Wiley, 2017. 15. Carruthers, W., Coldham, I. Modern Methods of Organic Synthesis, Cambridge University Press, 2015.	
Evaluation	Theory: 60 Internal: 15 (CIA: 10; Other form of Assessment: 2; Attendance: 3) Semester Exam: 45	Practical: 40 CA: 38; Attendance:2
Paper Structure for Theory Semester Exam	Answer THREE out of FOUR questions, of 15 marks each.	