

Semester	6
Programme	CHEMISTRY
Course	MAJOR (ORGANIC CHEMISTRY 6)
Paper Code	C3CH230641T
Credits	4 (THEORY: 4)
Hours/week	4 (THEORY: 4)
Category: Core/MDC/SEC/VEC	CORE
Theory/Practical/Composite	THEORY
Number of Modules	4
Syllabus	Module I: Heterocyclic Chemistry (12 Lectures) <i>Heterocyclic compounds:</i> 5- and 6-membered rings with one heteroatom; reactivity, orientation and important reactions (with mechanism) of furan, pyrrole, thiophene and pyridine; synthesis (including retrosynthetic approach and mechanistic details): pyrrole: Knorr synthesis, Paal-Knorr synthesis, Hantzsch; furan: Paal-Knorr synthesis, Feist- Benary synthesis and its variation; thiophenes: Paal-Knorr synthesis, Hinsberg synthesis; pyridine: Hantzsch synthesis; benzo-fused 5- and 6-membered rings with one heteroatom: reactivity, orientation and important reactions (with mechanistic details) of indole, quinoline and isoquinoline; synthesis (including retrosynthetic approach and mechanistic details): indole: Fischer, Madelung and Reissert; quinoline: Skraup, Doebner- Miller, Friedlander; isoquinoline: BischlerNapieralski synthesis. Module II: Organic Spectroscopy II (12 Lectures) <i>NMR Spectroscopy:</i> introduction; nuclear spin; NMR active molecules; basic principles of Proton Magnetic Resonance; equivalent and non-equivalent protons; chemical shift and factors influencing it; ring current effect; significance of the terms: up-/downfield, shielded and deshielded protons; spin coupling and coupling constant (1st order spectra); relative intensities of <i>first-order</i> multiplets; chemical and magnetic

equivalence in NMR ; elementary idea about *non-first-order* splitting; anisotropic effects in alkene, alkyne, carbonyls and aromatics; NMR peak area, integration; relative peak positions with coupling patterns of common organic compounds (both aliphatic and benzenoid-aromatic) and functional groups like alkene, alkyne, alcohol, ether, amines, carbonyls, acids and its derivatives, aromatic compounds; rapid proton exchange; interpretation of NMR spectra of simple organic compounds.

Mass spectrometry: Principles, instrumentation and applications of mass spectrometry. Methods of generation of ions in EI, CI, FD and FAB and other techniques.

Detection of ions, ion analysis, ion abundance, molecular ion peak, metastable peak, isotopes, ion-molecule interaction and analysis of fragmentation patterns.

Applications of mass spectroscopy to simple structural and mechanistic problems.

Module III: Carbohydrates (12 Lectures)

Monosaccharides: Aldoses up to 6 carbons; structure of D-glucose & D-fructose (configuration & conformation); ring structure of monosaccharides (furanose and pyranose forms). Ring size determination of D-glucose. Haworth representations and non-planar conformations; anomeric effect (including stereoelectronic explanation); mutarotation; epimerization; reactions (mechanisms in relevant cases): Fischer glycosidation, osazone formation, bromine-water oxidation, HNO₃ oxidation, selective oxidation of terminal –CH₂OH of aldoses, reduction to alditols, Lobry de Bruyn-van Ekenstein rearrangement; stepping-up (Kiliani-Fischer method) and stepping-down

	(Ruff's & Wohl's methods) of aldoses; endgroup- interchange of aldoses; acetonide (isopropylidene) and benzylidene protections; & related conversions. <i>Disaccharides</i>: Glycosidic linkages, concept of glycosidic bond formation by glycosyl donor-acceptor; structure of sucrose, inversion of cane sugar. Module IV: Bio-Organic Chemistry (12 Lectures) <i>Amino acids</i>: synthesis with mechanistic details: Strecker, Gabriel, acetamido malonic ester, Erlenmeyer azlactone, Bücherer hydantoin synthesis, synthesis involving diketopiperazine; isoelectric point, zwitterions; electrophoresis, reaction (with mechanism): ninhydrin reaction, Dakin-West reaction; resolution of racemic amino acids. <i>Peptides</i>: peptide linkage and its geometry; syntheses (with mechanistic details) of peptides using Nprotection & C-protection, solid-phase (Merrifield) synthesis; peptide sequence: C-terminal and Nterminal unit determination (Edman, Sanger & 'dansyl' methods); partial hydrolysis; specific cleavage of peptides: use of CNBr. <i>Nucleic acids</i>: Definition and classification of nucleic acids. Structure of nucleosides and nucleotides, primary and secondary structure of DNA, Watson-Crick model, Types of RNA and their functions.
Course Overview	Theory: Students will have <i>knowledge about</i> i) Study of Heterocyclic compounds ii) ¹H NMR spectroscopy and mass spectrometry of organic molecules iii) Chemistry of Carbohydrates iv) Study of Biomolecules (Amino acids, peptides and nucleic acids)

Course Outcomes	Upon successful completion of this course, students will be able to: CO1: Explain the reactivity, orientation rules, and electronic characteristics of 5- and 6-membered heterocyclic rings (furan, pyrrole, thiophene, pyridine) and their benzo-fused derivatives (indole, quinoline, isoquinoline). CO2: Design forward synthetic schemes and outline mechanistic pathways for simple and benzo-fused heterocycles using classical methods (e.g., Knorr, Paal-Knorr, Feist-Benary, Fischer-Indole, Skraup, Bischler-Napieralski) along with a retrosynthetic approach. CO3: Apply the principles of nuclear spin, chemical shift, magnetic/chemical equivalence, anisotropic effects, and first-order spin-spin coupling to predict the expected ¹H-NMR spectrum of aliphatic and aromatic organic compounds. CO4: Interpret ionization modes (EI, CI, FD, FAB) and fragmentation patterns in mass spectrometry to identify key molecular structure characteristics, including molecular ion, isotopic, and metastable peaks. CO5: Deduce the complete chemical structures of unknown organic compounds by performing a joint analysis of complementary ¹H - NMR and mass spectral data matrices. CO6: Analyze the configurations, non-planar conformations, ring size assignments, and stereoelectronic behaviors (such as the anomeric effect and mutarotation) of monosaccharides and disaccharides (sucrose). CO7: Plan structural alterations of carbohydrates, including chain stepping-up (Kiliani-Fischer), stepping-down (Ruff/Wohl), end group interchanges, protection-deprotection actions (acetonides, benzylidenes), and glycosidic bond couplings. CO8: Formulate pathways for amino acid synthesis (Strecker, Gabriel, Malonic Ester, Erlenmeyer) and model the strategies for selective peptide assembly (solution phase, Merrifield solid-phase synthesis) and sequence determination (Edman, Sanger, CNBr cleavage). CO9: Characterize the chemical properties, isoelectric behaviors, and zwitterionic structures of amino acids, as well as the structural architectures of nucleosides, nucleotides, DNA (Watson-Crick model), and RNA variants. CO10: Evaluate risks and interpret safety profiles when working with biomolecules or spectroscopic instruments, and communicate complex structural problems clearly using technical data.
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.
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Module	Course Outcome (CO)	Cognitive Domain (Bloom's K-Values)	Mapped Program Outcomes (POs)
Module I: Heterocyclic Chemistry	CO1: Explain the reactivity, orientation rules, and electronic characteristics of 5- and 6-membered heterocyclic rings (furan, pyrrole, thiophene, pyridine) and their benzo-fused derivatives (indole, quinoline, isoquinoline).	K2 (Understanding)	PO1: Fundamental Knowledge
	CO2: Design forward synthetic schemes and outline mechanistic pathways for simple and benzo-fused heterocycles using classical methods (e.g., Knorr, Paal-Knorr, Feist-Benary, Fischer-Indole, Skraup, Bischler-Napieralski) along with a retrosynthetic approach.	K4 (Analyzing) K6 (Creating)	PO1: Fundamental Knowledge PO3: Problem Solving
Module II: Organic Spectroscopy II	CO3: Apply the principles of nuclear spin, chemical shift, magnetic/chemical	K3 (Applying)	PO1: Fundamental Knowledge

	equivalence, anisotropic effects, and first-order spin-spin coupling to predict the expected ^1H -NMR spectrum of aliphatic and aromatic organic compounds.	K4 (Analyzing)	PO3: Problem Solving
	CO4: Interpret ionization modes (EI, CI, FD, FAB) and fragmentation patterns in mass spectrometry to identify key molecular structure characteristics, including molecular ion, isotopic, and metastable peaks.	K4 (Analyzing)	PO1: Fundamental Knowledge PO3: Problem Solving
	CO5: Deduce the complete chemical structures of unknown organic compounds by performing a joint analysis of complementary ^1H - NMR and mass spectral data matrices.	K4 (Analyzing)	PO3: Problem Solving PO5: Modern Tool Usage
Module III: Carbohydrates	CO6: Analyze the configurations, non-planar conformations, ring size assignments, and stereoelectronic behaviors (such as the anomeric effect and mutarotation) of monosaccharides and disaccharides (sucrose).	K4 (Analyzing)	PO1: Fundamental Knowledge
	CO7: Plan structural alterations of carbohydrates, including chain stepping-up (Kiliani-Fischer), stepping-down (Ruff/Wohl), end group interchanges, protection-deprotection actions (acetonides, benzylidenes), and glycosidic bond couplings.	K3 (Applying) K6 (Creating)	PO1: Fundamental Knowledge PO3: Problem Solving

Module IV: Bio-Organic Chemistry	CO8: Formulate pathways for amino acid synthesis (Strecker, Gabriel, Malonic Ester, Erlenmeyer) and model the strategies for selective peptide assembly (solution phase, Merrifield solid-phase synthesis) and sequence determination (Edman, Sanger, CNBr cleavage).	K3 (Applying) K6 (Creating)	PO1: Fundamental Knowledge PO3: Problem Solving PO4: Research Competency
	CO9: Characterize the chemical properties, isoelectric behaviors, and zwitterionic structures of amino acids, as well as the structural architectures of nucleosides, nucleotides, DNA (Watson-Crick model), and RNA variants.	K2 (Understanding)	PO1: Fundamental Knowledge PO5: Interdisciplinary Applications
Cross-Cutting / All Modules	CO10: Evaluate risks and interpret safety profiles when working with biomolecules or spectroscopic instruments, and communicate complex structural problems clearly using technical data.	K5 (Evaluating)	PO2: Laboratory Skills PO6: Communication Skills PO7: Ethics & Sustainability
Reading/Reference Lists	Theory: 1. Clayden, J., Greeves, N., Warren, S. <i>Organic Chemistry</i> , Second edition, Oxford University Press 2012. 2. Sykes, P. <i>A guidebook to Mechanism in Organic Chemistry</i> , Pearson Education, 2003. 3. Smith, J. G. <i>Organic Chemistry</i> , Tata McGraw-Hill Publishing Company Limited. 4. Loudon, G. M. <i>Organic Chemistry</i> , Fourth edition, Oxford University Press, 2008. 5. Morrison, R. N. & Boyd, R. N. <i>Organic Chemistry</i> ,		

	Dorling Kindersley (India) Pvt. Ltd. (Pearson Education). 6. Finar, I. L. <i>Organic Chemistry (Volume 1 & Volume 2)</i> Pearson Education. 7. Graham Solomons, T.W., Fryhle, C. B. <i>Organic Chemistry</i>, John Wiley & Sons, Inc. 8. Gilchrist, T. L. <i>Heterocyclic Chemistry</i>, Pearson, 2005. 9. Pavia, D. L. <i>Introduction to Spectroscopy</i>, Cengage India Private Limited, 2015. 10. Joule, J. A., Mills, K. <i>Heterocyclic Chemistry</i>, Wiley, 2010. 11. Kalsi, P. S. <i>Spectroscopy of Organic Compounds</i>, New Age International (P) Limited, 2005. 12. Kemp, W. <i>Organic Spectroscopy</i>, Palgrave Macmillan, 1991. 13. Gross, J. H., <i>Mass Spectrometry</i>, Springer, 2011. Voet, D. & Voet, J. G. <i>Biochemistry</i>, Wiley, 2010.
Evaluation	Theory: 100 Internal: 30 (CIA:20, Other mode of Assesment:5, Attendance: 5) Semester Exam:70
Paper Structure for Theory Semester Exam	Answer SEVEN out of NINE questions, of 10 marks each.