Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHO-500 **Title of the course:** Fundamentals of Organic Chemistry

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
Course Objective:	1. To study the various concepts based on molecular orbital theory. 2. To understand the concepts of topicity, prostereoisomerism and chemo-, regio- and stereoselectivity in organic reactions. 3. To understand the mechanistic aspects of various type of reactions in organic synthesis.	
Content	**1.Molecular orbitals and delocalized chemical bonding** a. Qualitative description of molecular orbitals of simple acyclic and monocyclic systems, frontier molecular orbitals. b.Conjugation, cross conjugation, resonance, hyperconjugation and tautomerism (types and examples). c. Aromaticity: Origin of Huckel's rule, examples of aromatic, non-aromatic and antiaromatic compounds; concept of Mobius aromaticity.	No of hours 08
	2.Structure & Reactivity a. Acidity, basicity and pKa of organic compounds; Acid and base strengths; HSAB concept & Factors affecting it, effect of structure & medium on acid and base strength. b. Concept of superacids and superbases. c. Electrophilicity&nucleophilicity, examples of ambident nucleophiles & electrophiles. (Including revision of aromatic electrophilic and nucleophilic substitution)	08
	3.Stereochemistry a. Brief revision of configurational nomenclature: R & S; D & L; E & Z; cis & trans and *syn* & *anti* nomenclature. Chirality in molecules with two and more chiral centres. b. Conformational analysis of open chain compounds (Butane, 2, 3-butane diol, 2,3-dibromobutane etc.). *Erythro*and *threo*nomenclature. c. Topicity and Prostereoisomerism: Topicity of ligands and faces-homotopic, enantiotopic and Cram's rule /diastereotopic ligands and faces. d. Introduction to chemoselective, regioselective and stereoselective reactions.	14

	e. Stereochemistry of *cis*- and *trans*-decalins, conformation and reactivity of cyclohexane and substituted cyclohexanes, cyclohexene / cyclohexanone. conformational isomerism and analysis in acyclic and simple cyclic systems –substituted ethanes, cyclopentane, cyclohexane cycloheptane, cyclooctane and decalins, f. optical isomerism - optical activity - molecular dissymmetry and chirality - elements of symmetry. optical isomerism in biphenyls, allenes and spirans - optical isomerism of nitrogenous compounds racemisation and resolution.	
	4.Reaction Mechanism a. Brief revision of carbocations, carbanions, free radicals, carbenes, Arynes and nitrenes with reference to generation, structure, stability and reactivity; b. Types of mechanisms, types of reactions, thermodynamic and kinetic control. c. The Hammond postulate and principle of microscopic reversibility, d. Methods of determining reaction mechanisms like- i. Identification of products, ii. Determination of the presence of intermediates (isolation, detection, trappingandaddition of suspected intermediate, iii. Isotopic labelling, iv. Stereochemical evidence, v. Kinetic evidence and vi. Isotope effect (at least two reactions to exemplify each method be studied)	08
	5.Aliphatic Nucleophilic substitution a. Brief revision of nucleophilic substitutions with respect to Mechanism, various factors affecting such reactions; b. The Neighbouring Group Participation (NGP)/ Anchimeric assistance: General approach to various NGP processes; NGP by unshared/lone pair of electrons; NGP by π-electrons; NGP by aromatic rings (formation of phenonium ion intermediate); NGP by sigma bonds with special reference to bornyl and nor-bornyl system (formation of nonclassical carbocation)	08
	6.Elimination reactions a. The E2, E1 and E1cB mechanisms. Orientation of the double bond, Saytzeff and Hofmann rule. b. Effects of changes in the substrate, base, leaving group and medium on i. Overall reactivity, ii. E1 vs. E2 vs. E1cB	08

	iii. Elimination vs substitution, Mechanism and orientation in pyrolytic *syn* elimination (various examples involving cyclic and acyclic substrates to be studied).	
	7. Selective reagents for Organic transformation a. Oxidation of organic compounds, PCC, PDC and MnO_2, ozonolysis, peracids. b. Reduction of organic compounds: $NaBH_4$, LAH, DIBAL reduction and reduction with borane and dialkylboranes. Clemmensen reduction, Birch reduction and Wolff-Kishner reduction	06
Pedagogy	Mainly lectures and tutorials. Seminars/term papers/assignments/presentations/ self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
References / Readings	1. W. Caruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 4th Ed., 2016. 2. M. B. Smith, Organic Synthesis, McGraw–HILL, New York, International Edition, 1994. 3. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2nd Ed., 2012. 4. R. Bruckner, Advanced Organic Chemistry – Reaction Mechanisms, San Diego, CA: Harcourt /Academic Press, San Diego, 2002. 5. J. Fuhrhop, G. Penxlin, Organic Synthesis – Concepts, Methods, Starting Materials, VCH Publishers Inc., New York, 1994. 6. H. O. House, Modern Synthetic Reactions, W. A. Benjamin, 2ndEd.,1965 7. M. Nogradi, Stereoselective Synthesis, VCH Publishers, Inc., Revised and Enlarged Edition, 1994. 8. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry, Springer India Private Limited, 5thEd, 2007. 9. T. Laue, A. Plagens, Named Organic Reactions, John Wiley and Sons, Inc., 2005.	
Course outcomes:	1. Students will be in a position to evaluate the effect of delocalization of electrons & presence or absence of aromaticity in organic compounds. 2. Students will be able to apply various concepts in stereochemistry to understand stereochemical outcome in a reaction. 3. Students shall be in a position to understand/propose plausible mechanism of organic reactions. 4. Students will understand and apply various reagents for desired organic transformations.	