Programme: M. Sc. Part-I (Chemistry)
Course Code: OCC-401
Title of the Course: Structure, reactivity, stereochemistry and reaction mechanism
Number of Credits: 03 **Effective from AY: 2018-19**

Prerequisites for the course:	Should have studied the courses / topics in Organic Chemistry at F Y B Sc, S Y B Sc and T Y B Sc levels so as to have basic knowledge of organic nomenclature and basic principles.	
Course Objectives:	3. Introduction of various concepts based on molecular orbital theory. 4. Introduction of topicity, prostereoisomerism and chemo-, regio- and stereoselectivity in organic reactions. 5. Learning mechanistic aspects of various type of reactions in organic synthesis.	
Course Outcomes:	5. Students should be in a position to evaluate effect of delocalization of electrons & presence or absence of aromaticity in organic compounds. 6. Students should be in a position to apply various concepts in stereochemistry to understand stereochemical output in a reaction. 7. Students shall be in a position to understand/propose plausible mechanism of organic reactions.	
Content:	1. **Molecular orbitals and delocalized chemical bonding**: Qualitative description of Molecular orbitals of simple acyclic and monocyclic Systems, Frontier molecular orbitals, Conjugation, cross conjugation, resonance, hyperconjugation and tautomerism (types and examples), Aromaticity: Origin of Huckel's rule, examples of aromatic, non-aromatic and antiaromatic compounds; concept of Mobius aromaticity. 2. **Structure & Reactivity:** 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, Concept of superacids and superbases, Electrophilicity & Nucleophilicity, Examples of ambident nucleophiles & electrophiles. (Including revision of aromatic electrophilic and nucleophilic substitution) 3. **Stereochemistry**: 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. Conformational analysis of open chain compounds (Butane, 2, 3-butane diol, 2,3-dibromobutane etc.). *Erythro* and *threo* nomenclature. Topicity and Prostereoisomerism: Topicity of ligands and faces-homotopic, enantiotopic and Cram's rule / diastereotopic ligands and faces. Introduction to chemoselective, regioselective and stereoselective reactions. Stereochemistry of *cis*- and *trans*-decalins, conformation and reactivity of cyclohexane and substituted cyclohexanes, cyclohexene / cyclohexanone. 4. **Reaction Mechanism:** Brief revision of carbocations, carbanions, free radicals, carbenes and nitrenes with reference to generation, structure, stability and reactivity; Types of mechanisms, types of reactions, thermodynamic and kinetic control. The Hammond postulate and principle of microscopic reversibility, Methods of determining reaction mechanisms like- 1) Identification of products,	06 hr 06 hr 08 hr 06 hr

	2) Determination of the presence of intermediates (isolation, detection, trapping and addition of suspected intermediate, 3) Isotopic labelling, 4) Stereochemical evidence, 5) Kinetic evidence and 6) Isotope effect (at least two reactions to exemplify each method be studied) 5. **Aliphatic Nucleophilic substitution:** Brief revision of nucleophilic substitutions with respect to Mechanism, Various factors affecting such reactions; 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 non-classical carbocation) 6. **Elimination reactions:** The E2, E1 and E1cB mechanisms. Orientation of the double bond, Saytzeff and Hofmann rule. Effects of changes in the substrate, base, leaving group and medium on 1) overall reactivity, 2) E1 vs. E2 vs. E1cB and 3) elimination vs substitution, Mechanism and orientation in pyrolytic *syn* elimination (various examples involving cyclic and acyclic substrates to be studied).	06 hr 04 hr
Pedagogy:	Mainly Lectures & tutorials. Seminars / assignments / presentations / self-study or a combination of some of these could also be used to some extent.	
References/ **Readings**	1. D. Nassipuri, *Stereochemistry of Organic compounds - Principles and Application*, Wiley Eastern Limited, 2013, 4th Ed. Kent, [England]: New Academic Science Limited, 2013. 2. E.L. Eliel, *Stereochemistry of carbon compounds*, Tata MacGraw Hill Publishing Company Ltd. (1990) 3. J. March, *Advanced Organic Chemistry: Reaction, Mechanism and Structure*, Wiley, 2010, 4th Ed. 4. J. Clayden, N. Greeves, S. Warren & Wothers, *Organic Chemistry*, Oxford University Press, 2012, 2nd Ed. 5. I.L. Finar *Stereochemistry and Chemistry of Natural products*, ELBS, Longmans, 1963, Vol. 2, 3rd Ed. 6. V.M. Potapov, *Stereochemistry*, MIR Publishers, Moscow, 1979 7. E.S. Gould *et al*., Mechanism and structure in Organic Chemistry, 1965 8. F. A. Carey, *Organic Chemistry*, 2000, 4th Ed. 9. S.H. Pine, *Organic Chemistry*, McGraw-Hill International Edn. 2010, 5thEd. 10. F.A. Carey and R.J. Sundberg, *Advanced Organic Chemistry*, Vol. I & II. Plenum Press, 1977 11. J. M. Harris & C.C. Wamser, *Fundamentals of Organic Reaction Mechanisms*, John Wiley & Sons. Inc. 1976 12. F.M. Menger, D.J. Goldsmith & L. Mendell, *Organic Chemistry, A concise approach*, 1975, 2nd Ed.	