

CY21205	Fundamentals of Organic Reactions	L-T-P: 3-1-0
<p><u>MO Theory: (8L):</u> Introduction to molecular orbitals, bonding and antibonding interactions, basic idea of σ, σ^*, π, π^*, n-MOs, Frontier MOs (FMO); concept of HOMO, LUMO and SOMO; understanding of chemical reactions by FMO interactions; π-MO diagrams and energy levels of acyclic systems (C=C, conjugated diene, triene, allyl and pentadienyl systems), cyclic systems (neutral systems: [4], [6]-annulenes; charged systems: 3-, 4-, 5-membered ring systems); Hückel's rules for aromaticity up to [10]-annulene (including mononuclear heterocyclic compounds up to 6-membered ring); concept of antiaromaticity and homoaromaticity; non-aromatic molecules; Frost diagram.</p>		
<p><u>Acid base: (6L):</u> Acid–base theory by Arrhenius, Brønsted–Lowry and Lewis. Conjugate acid and base, their comparison. Lewis acids and bases, definition of pKa, pKb, understanding of pKa scale for both acid and base. Comparison of acidity and basicity of aromatic, heteroaromatic compounds containing functional groups like ketone, ester, nitro, nitrile, etc. Hard-soft enolization.</p>		
<p><u>Basic Stereochemistry: (10L):</u> Concept of chirality and symmetry: Symmetry elements, molecular chirality and centre of chirality; asymmetric and dissymmetric molecules; enantiomers and diastereomers; concept of epimers; concept of stereogenicity, chirotopicity and pseudoasymmetry; chiral centres and number of stereoisomerism: systems involving 1/2/3-chiral centre(s) (AA, AB, ABA and ABC types). Chirality arising out of stereoaxis: Stereoisomerism of substituted cumulenes with even and odd number of double bonds; chiral axis in allenes, spiro compounds, alkylidene cycloalkanes and biphenyls; related configurational descriptors (aR/aS and P/M); atropisomerism; racemisation of chiral biphenyls; buttressing effect. Concept of prostereoisomerism: Pro-stereogenic centre; concept of (pro)n-chirality: topicity of ligands and faces (elementary idea); pro-R/pro-S, pro-E/pro-Z and Re/Si descriptors; pro-r and pro-s descriptors of ligands on pro-pseudoasymmetric centre. Stereoselective Reactions: Stereoselectivity: Classifications, terminology and principle. Stereospecific Reactions: Terminology and principle.</p>		
<p><u>Electrophilic & Nucleophilic substitution reactions in aromatic systems (SEAr/SNAr): (6h):</u> Electrophilic attack on benzene and C₆H₅Y-nitration, halogenation, sulfonation, Friedel Crafts reactions, Electronic effect of Y, important reactions of phenols, aromatic amino compounds, Ipso substitution. Nucleophilic attack on aromatic species: substitution of hydrogen, substitution of atoms other than hydrogen, substitution via aryne intermediates. Vicarious mechanism.</p>		
<p><u>Reaction Profile: (4L):</u> Rate constant and free energy of activation; isotope effect: primary and β-secondary kinetic isotopic effect (k_H/k_D); principle of microscopic reversibility; Hammond's postulate. Linear free energy relationships (Hammett, Yukawa-Tsuno equation and Taft equation).</p>		
<p><u>Addition/elimination reactions of carboxylic acid derivatives: (2L):</u> Base and acid catalyzed reactions (different types of saponification mechanism).</p>		
<p>Books:</p> <ol style="list-style-type: none"> 1. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming 2. Modern Physical Organic Chemistry by Dennis A. Dougherty and Eric V. Anslyn 3. Organic Chemistry by J. Clayden, S. Warren, N. Greeves, P. Wothers 4. Stereochemistry of Organic Compounds, D. Nasipuri 5. A Guidebook to Mechanism in Organic Chemistry by Peter Sykes 		