Semester	AUG 2022
Open to semester	5,7,11,13,21
Course code	**CH3114/CH6114**
Course title	**Physical Organic Chemistry**
Credits	4 /4
Course Coordinator & participating faculty (if any)	Hosahudya N. Gopi
Nature of Course	Lectures
Pre-requisites	None
Objectives (goals, type of students for whom useful, outcome etc)	Objective: This course is designed to introduce students to the physical basis of organic chemistry, primarily from a qualitative perspective. After completing the course, students will have a firm understanding of the structure and reactivity of organic molecules, methods for designing and interpreting mechanistic studies, and understanding of stereoelectronic concepts of organic reactions.
Course contents (details of topics /sections with no. of lectures for each)	Lecture Topics • A brief introduction to models of bonding, Valance bond theory, and Molecular orbital theory (1) • Solution and solvent properties and Non-covalent binding forces (4) Solvent scales, dielectric constant, surface tension, and wetting, solubility, salvation energy, thermodynamics of solutions, Ion pair interactions, salt bridges, electrostatic interactions, dipole-dipole interactions, Hydrogen bonding (strengths of hydrogen bonds, salvation effects, electronegativity effects, vibrational properties of hydrogen bonds), cation-pi interactions, polar-pi interactions, aromatic-aromatic interactions, induced dipole interactions, hydrophobic effects, ion liquids. • Conformational analysis of acyclic and cyclic systems. (4) Thermochemistry of stable molecules, types of energies, the heat of formation and combustion, stain energy, the relationship between structure and energies, Conformational analysis of acyclic molecules: examples ethane, butane,

	pentane etc, and allylic systems. Conformational analysis of cyclic systems (3-8 membered rings) bicyclic ring systems, Stereoelectronic effects (Anomeric effect, electronic strain, angle strain, hyperconjugation), fused rings. • Molecular Recognitions (3) Thermodynamic analysis of binding phenomena, enthalpy-entropy compensations, binding isotherm, complementarity and pre-organization, molecular recognition with large ion paring component, hydrogen binding component, hydrophobic component, and large pi component. • Aromaticity and electronic effects on structure (3) Interactions involving pi-systems, aromaticity, antiaromaticity and non-aromaticity energy criterion for aromaticity, structural and electronic criteria, destabilizing effects, polycyclic aromatic hydrocarbons, annulenes • Structural Effects on Stability and reactivity (4) Energy surfaces, rate and rate constants, transition state theory, relationship to the Arrhenius rate law, activation parameters, postulates and principles related to kinetic analysis, Kinetic analyses for simple mechanisms, steady-state kinetics, saturation kinetics, Calculating rate constants, reactivity vs. selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic vs. thermodynamic control. Marcus theory, the Bell-Evans-Polanyi principle. • Kinetic Isotope effects and isotopic labeling experiments (4) Isotopic effects, primary isotopic effects, exothermicity and endothermicity, isotopic effects for linear vs. non-linear transition states, secondary isotopic effects, steric isotopic effects, equilibrium isotopic effects, tunneling, solvent isotopic effects • Linear free energy relationships (8) Origin of subsistent effects, field effects, inductive effect, resonance effect, etc., Hammett equation, Hammett plots, Deviation form linearity, Taft equation, solvent effects, Swain-Scott parameters, acid-base related effects, Bronsted relationships, conditions to create LFER, extending LFER to biological and pharmaceutical problems.

	• Catalysis (4) General Principles of catalysis, forms of catalysis, Brønsted acid-base catalysis, The Bronsted catalysis law, acid-base related effects, Brønsted relationships, predicting general acid and general base catalysis, enzymatic catalysis. • Organic Reaction Mechanisms (4) Organic reaction mechanisms: Substitutions at aliphatic and aromatic centers Nucleophilic aliphatic substitution reactions, SN1 and SN2 reactions, stereochemistry and solvent effects, structure-function correlation with nucleophiles, structure-function correlation with leaving group, structure-function-correlations with R groups, SN1 reactions involving non-classical carbocations, Nucleophilic additions of carbonyl compounds, radical aliphatic substitution, electrophilic and nucleophilic aromatic substitution, nucleophilic substitution to olefins. • Organic reaction mechanisms: Reactions involving additions and eliminations Electrophilic addition to alkenes and alkynes, regiochemistry and stereochemistry of addition reactions, hydroboration, and epoxidation. carbene addition and insertions, elimination reactions for aliphatic systems, Kinetic and experimental observations of E2, E1, and E1cb, and experimental observations of elimination from the radical intermediates. Regiochemistry and stereochemistry of eliminations, orbital considerations, thermal eliminations. •Free radical reactions (3) Structural and Stereochemical properties of free Radicals, Characteristics of the reaction involving radical intermediates, free radical substitution reactions, addition reactions, and other types of free radical reactions.
Evaluation /assessment	End-Sem Examination-40% Mid-Sem Examination-35% Others-Quizzes: 20% Assignment: 5% %

Suggested readings (with full list of authors, publisher, year, edn etc.)	1) Anslyn, E.; Dougherty, D. A.; Modern Physical Organic Chemistry, 1st Edition, 2006. University Science Books. 2) Carroll, Felix A. Perspectives on Structure and Mechanism in Organic Chemistry,1st Edition,1998. 3) March, Advanced Organic Chemistry, 4th Edition, 1992, QD251.2.M37 4) Lowry, T. H.; Richardson, K. S. Mechanism and Theory in Organic Chemistry; 3rd ed.; Harper& Row: New York, 1987. 5) Sundberg, R. J.; Carey, F. A. Advanced Organic Chemistry, Part A: Structure and Mechanism, 4th Edition. Kluwer/Plenum Press, 2000. 6) Isaacs, N. Physical Organic Chemistry, 2nd Edition, Addison-Wesley-Longman,1995. 7) Carpenter, B. K. Determination of Organic Reaction Mechanisms. Wiley, 1994 8) J. Clayden, N. Greeves, S. Warren, P. Wothers; Organic Chemistry, Second Edition, Oxford Press.