Semester	AUG 2022
Open to semester	13,21
Course code	**CH6352**
Course title	**Reaction Mechanism**
Credits	/2
Course Coordinator & participating faculty (if any)	Hosahudya N. Gopi* and Ramakrishna G. Bhat
Nature of Course	Lectures
Pre-requisites	Organic chemistry
Objectives (goals, type of students for whom useful, outcome etc)	This course will provide basic understating of the reaction mechanisms of organic reactions. In addition to the basics, this course deals with contemporary examples of various types of organic reactions and applications.
Course contents (details of topics /sections with no. of lectures for each)	• Introduction to organic reactions and reaction mechanisms (1) • Acid-Base chemistry (2) • Solvent properties and Non-covalent binding interactions (3 hrs) Solvent scales, dielectric constant, solubility, 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. • Structural Effects on Stability and reactivity (5) 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, and Marcus theory. • 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, 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. • Organic reaction mechanisms: Substitutions at aliphatic and aromatic centers (3) • Organic reaction mechanisms: Reactions involving additions and eliminations (3) • Organotransition Metal Reaction Mechanisms and Catalysis (6) The basics of organometallic complexes, common organometallic reactions, oxidative addition, reductive elimination, migratory insertions, electrophilic addition to ligands, nucleophilic addition to ligands, combining individual reactions in overall transformations and cycles • Pericyclic reactions (7) Basics of pericyclic reactions and contemporary examples of pericyclic reactions involving cycloadditions, sigmatropic and electrocyclic reactions.
Evaluation /assessment	End-Sem Examination-40% Mid-Sem Examination-45% Others-15%
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. (Primary) 2. Carrol, F. A. Perspectives on Structure and Mechanism in Organic Chemistry. Brooks/Cole Publishing Company, 1998 3. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P. Organic Chemistry. Oxford University Press, 2nd Edition. 4. Sundberg, R. J.; Carey, F. A. Advanced Organic Chemistry, Part A: Structure and Mechanism, 5th Edition, Springer, 2007.

	5. Isaacs, N. Physical Organic Chemistry, 2nd Edition, Addison-Wesley-Longman,1995. 6. Chemistry Journals (JACS, Angew Chem, OL, JOC0