20MSC501T					Organic Chemistry I					
Teaching Scheme					Examination Scheme					
L	T	P	C	Hrs/Week	Theory			Practical		Total Marks
					MS	ES	IA	LW	LE/Viva	
3	0	3	4.5	6	25	50	25	--	--	100

COURSE OBJECTIVES

- To acquire the basic concepts of reactivity and stability of reactive intermediates.
- To understand and analyze the 3D structures of molecules.
- To demonstrate the basic understanding of chirality.
- To explain the basic knowledge of pericyclic reactions and photochemistry.
- To show the reactivity of different types of heterocycles.

UNIT 1 ORGANIC REACTION MECHANISM AND STUDY OF REACTIVE INTERMEDIATES **10Hrs.**

Aliphatic Nucleophilic Substitution: The SN2, SN1, mixed SN1 and SN2 and SET mechanisms. The SNi mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attaching nucleophile, leaving group and reaction medium. Electrophilic Substitution: Aliphatic: Bimolecular mechanisms: SE1, SE2 and SEi. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. Aromatic: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles.

Aromatic Nucleophile Substitution: The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity; effect of substrate structure, leaving group and attacking nucleophile. Elimination Reactions: The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity; effects of substrate structures, attaching base, the leaving group and the medium.

Generation, structure, stability, and reactions involving Carbocations, Carbanions, Radicals, carbenes, carbenoids and nitrenes. The Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation.

UNIT 2 STEREOCHEMISTRY **10Hrs.**

Configurational and conformational isomerism in acyclic and cyclic compounds. Configuration nomenclature D L, R S and E Z nomenclature. Conformational analysis of cycloalkanes, cyclohexenes, cyclohexanones, halocyclohexanones, decalins, decalols, and decalones; effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge; threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Optical activity in the absence of chiral carbon; Stereochemistry and configuration of allenes, spiranes, alkylidene cycloalkanes, adamantanes, catenanes, biphenyls (atropisomerism), bridged biphenyls, ansa compounds and cyclophanes.

Asymmetric induction: Cram's, Prelog's and Horeau's rule

UNIT 3 INTRODUCTION TO PERICYCLIC AND PHOTOCHEMISTRY **12Hrs.**

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions - conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions - antrafacial and suprafacial additions, 4n and 4n+2 system, 2+2 addition of ketenes, 1, 3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, sigmatrophic shifts involving carbon moieties, 3, 3- and 5, 5- sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Photochemistry: Introduction, Jablonskii diagram, energy pooling, photosensitization, Quantum yields, solvent effects, Stern-Volmer plot, intersystem crossing, delayed fluorescence, photosensitization, and energy transfer reactions.

UNIT 4 FUNDAMENTALS OF HETEROCYCLIC COMPOUNDS **8 Hrs.**

Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S).

Synthesis and reactions of Three membered and four membered Heterocycles i.e. aziridines, oxiranes, thiranes, azetidines, oxitanes and thietanes. Synthesis and reactions of benzopyrroles, benzofurans and benzothiophenes.

Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis.

40 Hrs.

COURSE OUTCOMES

On completion of the course, student will be able to

CO1 – Understand the basic concepts of organic chemistry.
CO2 – Analyse the three-dimensional structure of a molecule
CO3 – Comment upon the stability and reactivity of various organic compounds.
CO4 – Differentiate between various types of reaction intermediates.
CO5 – Acquire knowledge about basic concepts of the photochemistry.
CO6 – Understand the basic concepts of heterocyclic chemistry

TEXT/REFERENCE BOOKS

1. Advanced Organic Chemistry by J. March, John Wiley & Sons, 1992
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill
3. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley, 1994.
4. Organic Chemistry by P.Y. Bruice, Prentice Hall, 1998.
5. Organic Reaction and their Mechanism by P.S. Kalsi, New Age, 1996.
6. Frontier Orbital and Organic Chemical Reactions by I. Fleming, John Wiley, 1976.
7. Heterocyclic Chemistry by T. R. Gilchrist, Longman,1989.

END SEMESTER EXAMINATION QUESTION PAPER PATTERN

Max. Marks: 100 **Exam Duration: 3 Hrs**

Part A/Question: <Details> <> Marks

Part B/Question: <Details> <> Marks