DEPARTMENT OF CHEMISTRY				*CLASS: I M.Sc. Chemistry*				
Sem	Course Type	Course Code	Course Title	Credits	Contact Hours/week	CIA	Ext	**Total**
I	Major Core	21P1CMC1	Organic Chemistry-I	4	5	25	75	**100**

Nature of Course				
Knowledge and skill	✓		Employability oriented	
Skill oriented			Entrepreneurship oriented	

Course Objectives:*Theobjectiveofthiscourseistomakethestudent*

(i) To expand the knowledge of basic concepts in organic chemistry
(ii) To know and prove the mechanism for given organic reaction through various techniques and to examine the intermediates involved in the given conversion
(iii) To explore the knowledge of aromatic electrophilic substitution reactions
(iv) To gain the knowledge of nucleophilic substitution in aliphatic and aromatic systems
(v) To apply knowledge in synthesizing molecules using various substitution reactions.

Unit	Description	Hours	K-Level	CLO
I	**NATURE OF BONDING AND AROMATICITY** *Nature of bonding*: Shapes of simple organic molecules - bond angle, bond length, bond energies, electronegativity, dipole moment in organic molecules – ElectronicEffects: hyperconjucative, inductive and field effects and their influence - rules of resonance – tautomerism - steric effects – Hard and soft acids and bases. *Aromaticity*: Huckel's theory of aromaticity: three-, four-, five-, six-, seven-, and eight-membered rings – other systems with aromatic sextet - concept of homo-aromaticity and anti-aromaticity. *Bonding weaker than covalent*: Addition compounds – Electron donor-acceptor (EDA) complexes – Crown ether complexes – inclusion compounds – Cyclodextrins – Catenanes and Rotaxanes. Self-study: Hydrogen bonding: Inter- and intra- molecular – study of fullerenes.	15	Up to K2	CLO-1
II	**REACTION MECHANISM** Types of reaction and mechanism – Thermodynamic and kinetic requirements of reaction – Kinetic and thermodynamic control – Hammond postulate – Methods of determining mechanisms: Identification of products, determination of the presence of intermediate, study of catalysis, isotopic labelling, kinetic and stereochemical evidence, isotope effects.	15	Up to K4	CLO-2

	Linear Free energy Relationships: First Hammett plots - Hammett equation – physical significance of reaction and substituent constants – uses of Hammett plots - Taft equation – simple problems. Organic reactive intermediates: Generation, stability, structure and reactivity of carbocations, carbanions and free radicals. Self-study: Carbenes and nitrenes.			
III	**AROMATIC ELECTROPHILIC SUBSTITUTION REACTIONS** Arenium ion mechanism – σ and π complex - Mechanism of nitration, sulfonation, Friedel Crafts alkylation, acylation and diazo coupling reactions. Orientation and reactivity in mono substituted benzene ring and benzene ring with more than one substituent – *ortho*/*para* ratio – *ipso* substitutions – Quantitative treatment – Electrophilic substitution of other aromatic species: Naphthalene, Pyridine, Pyrrole, Indole, Quinoline. Study of following reactions: Bischler-Napieralski, Pictet-Spengler, Scholl, Vilsmeier, Gattermann, Reimer-Tiemann, Kolbe-Schmitt, Mannich, Jacobsen and Haworth reactions.	15	Up to K3	CLO-3
IV	**ALIPHATIC NUCLEOPHILIC SUBSTITUTION REACTIONS** Mechanism of nucleophilic substitution reaction: S_N^1 and S_N^2 mechanisms. Stereochemistry of substitution reactions: Steric orientation in S_N^1 and S_N^2 – Neighbouring group participation: NGP by σ and π bonds – Role of following groups in NGP: C=C, cyclopropyl, aromatic rings, C-C, Hydrogen - S_N^imechanism – Factors affecting reactivity: structure of alkyl group, nature of solvent, nature of leaving group, nature of nucleophilic reagent – Phase transfer catalysts in nucleophilic substitution reactions.	15	Up to K4	CLO-4
V	**AROMATIC NUCLEOPHILIC SUBSTITUTION REACTIONS** S_NArmechanism in aryl halides by Meisenheimer complex - S_N^1, $S_{RN}1$ and benzyne mechanism – Reactivity: The effect of substrate structure, leaving group and attacking nucleophile - Ambident nucleophiles and ambident substrates – Study of following name reactions and rearranements: Chichibabin, Schiemann, Meerweinarylation, Gomberg, Bamberger, Heck, Ullmann, Suzuki coupling, Stephens-Castro coupling, Von Richter, Sommelet Hauser and Smiles.	15	Up to K4	CLO-5

Books for study:

1. Clayden, J., Greeves, N. and Warren, S. "Organic Chemistry" Second Edition, Oxford University Press, New York, 2012.
2. Smith, M. B. March, J. "March's Advanced Organic Chemistry: Reactions, mechanisms and Structure" Sixth Edition, Wiley, 2007.
3. Skyes, P., "A Guide Book to Mechanism in Organic Chemistry" Sixth Edition, John Wiley & Sons, Inc. New York, 2011.

Books for reference:

1. Smith, M. B., "Organic Synthesis" Fourth Edition, Elsevier Inc., 2016.
2. Mukherji, S.M., and Singh, S. P., "Reaction Mechanism in Organic Chemistry" Revised edition, Trinity press, 2010.
3. Norman, R. O. C. and Coxon, J. M. "Principles of Organic Synthesis" Third edition, Nelson Thrones, United Kingdom, 2003.
4. Carey, F. A. and Sundberg, R. J. "Advanced Organic Chemistry-Part A: Structure and mechanisms" Fifth edition, Springer, 2007.
5. Carey, F. A. "Organic Chemistry" Fourth edition, Mc Graw Hill, 2000. Mukherji, S.M., and Singh, S. P., "Reaction Mechanism in Organic Chemistry" Third edition, MacMillan India Ltd, 2006.

Web resources:

1. https://onlinecourses.nptel.ac.in/noc21_cy07/preview
2. https://onlinecourses.swayam2.ac.in/cec20_ma20/preview
3. https://www.ntnu.edu/studies/mschem/organic-chemistry
4. https://www.youtube.com/watch?v=SAmLVOKIw28

Rationale for Nature of the course

This course will enable the students to comprehend the basic concepts of organic chemistry, structure of organic molecules, understand the reaction mechanism & the ways to prove it, electrophilic and nucleophilic substitution reactions in both aliphatic and aromatic substrates.

Activities having direct bearing on Skill development/ Employability/Entrepreneurship

The basic knowledge, concepts of reaction mechanism and study of various substitution reactions will help the students to write mechanism for a given conversion and to identify the intermediates involved. They can introduce a new functional group theoretically on the aliphatic and aromatic substrates by applying the techniques of electrophilic and nucleophilic reactions.

Pedagogy:

- Chalk-Talk Class room Activities
- Seminar
- Assignment and Quiz through ICT

Lesson plan:

Unit	Topics	Hours	Mode
I	*Nature of bonding*: Shapes of simple organic molecules - bond angle, bond length, bond energies, electronegativity, dipole moment in organic	3	PPT, Chalk and talk, Group discussion
	Electronic Effects: hyperconjucative, inductive and field effects and their influence - rules of resonance – tautomerism - steric effects	3	
	Hard and soft acids and bases.	1	
	Aromaticity: Huckel's theory of aromaticity: three-, four-, five-, six-, seven-, and eight-membered rings – other systems with aromatic sextet	3	
	Concept of homo-aromaticity and anti-aromaticity.	1	
	Bonding weaker than covalent: Addition compounds – Electron donor-acceptor (EDA) complexes	2	
	Crown ether complexes – inclusion compounds – Cyclodextrins – Catenanes and Rotaxanes.	2	
II	Types of reaction and mechanism – Thermodynamic and kinetic requirements of reaction – Kinetic and thermodynamic control –	4	PPT, Chalk and talk, Assignment
	Methods of determining mechanisms: Identification of products, determination of the presence of intermediate, study of catalysis, isotopic labelling, kinetic and stereochemical evidence, isotope effects.	3	
	Linear Free energy Relationships: First Hammett plots - Hammett equation – physical significance of reaction and substituent constants – uses of Hammett plots - Taft equation – simple problems.	4	
	Organic reactive intermediates: Generation, stability, structure and reactivity of carbocations, carbanions and free radicals.	4	
III	Arenium ion mechanism – σ and π complex	1	PPT, Chalk and talk, Assignment
	Mechanism of nitration, sulfonation, Friedel Crafts alkylation, acylation and diazo coupling reactions.	3	
	Orientation and reactivity in mono substituted benzene ring and benzene ring with more than one substituent	3	
	ortho/*para* ratio – *ipso* substitutions – Quantitative treatment	2	
	Electrophilic substitution of other aromatic species: Naphthalene, Pyridine, Pyrrole, Indole, Quinoline.	3	
	Study of following reactions: Bischler-Napieralski, Pictet-Spengler, Scholl, Vilsmeier, Gattermann, Reimer-Tiemann, Kolbe-Schmitt,	3	
IV	Mechanism of nucleophilic substitution reaction: S_N^1 and S_N^2	3	PPT, Chalk and talk, Group discussion
	Stereochemistry of substitution reactions: Steric orientation in S_N^1 and	2	
	Neighbouring group participation: NGP by σ and π bonds – Role of following groups in NGP: C=C, cyclopropyl, aromatic rings, C-C,	4	
	S_N^1mechanism – Factors affecting reactivity: structure of alkyl group, nature of solvent, nature of leaving group, nature of nucleophilic reagent	4	
	Phase transfer catalysts in nucleophilic substitution reactions.	2	
V	S_NArmechanism in aryl halides by Meisenheimer complex	2	PPT, Chalk and talk, Group discussion
	S_N^1, S_{RN}1 and benzyne mechanism	3	
	Reactivity: The effect of substrate structure, leaving group and attacking	3	
	Ambident nucleophiles and ambident substrates	1	
	Study of following name reactions and rearranements: Chichibabin, Schiemann, Meerweinarylation, Gomberg, Bamberger, Heck, Ullmann	3	
	Suzuki coupling, Stephens-Castro coupling, Von Richter, Sommelet Hauser and Smiles.	3	

Course learning outcome:

After successful completion of this course, the student will be able to

CLOs	CLO statement	Knowledge level
CLO 1	Understand the concept of aromaticity and to know the nature of bond, electronic effects and other properties of molecules.	Up to K2
CLO 2	Recognise the type of mechanism & intermediates involved in the given organic reaction and to prove mechanism for the reaction.	Up to K4
CLO 3	Identify the ways to modify aromatic compounds *via* electrophilic substitution reactions.	Up to K3
CLO 4	Analyse chemical transformations based on aliphatic nucleophilic substitution reaction	Up to K4
CLO 5	Organize the techniques of aromatic nucleophilic substitution reactions for synthesizing/transforming molecules	Up to K4

Mapping of CLOs with PLOs

#	PLO–1	PLO–2	PLO–3	PLO–4	PLO–5
CLO–1	2		2		
CLO–2	2		2		
CLO–3	2		2	2	
CLO–4	2		2	2	
CLO–5	2		2	2	

Advance application– 3; Intermediate level–2; Basic level–1

Components of Formative Assessment	Marks	K level
Internal Test	**10**	As per below table
Assignment	**5**	K4
Quiz	**5**	K4
Seminar	**5**	K4
Total	**25**	

Learning Outcome Based Education (LOBE) & Assessment
Formative Examinations I & II – Blue Print
Articulation Mapping-K Levels with Courses Learning Outcomes (CLOs)

Units	CLOs	K- Level	Section A		Section B (Either/or Choice)	Section C (Open Choice)
			Short Answers			
			No. of Questions	K Level		
1	CLO x	Up to K3	2	K2,K3	2 (K3&K3)	2(K2/K3)
2	CLO y	Up to K4	3	K2, K2, K3	2 (K4&K4)	1(K3/K4)
No. of Questions to be asked			5		4	3
No. of Questions to be answered			5		2	2
Marks for each question			2		5	10
Total Marks for each section			10		10	20

K1- Remembering and recalling facts with specific answers
K2- Basic understanding of facts and stating main ideas with general answers
K3- Application oriented- Solving Problems
K4- Examining, analyzing, presentation and make inferences with evidences

Learning Outcome Based Education (LOBE) & Assessment
Summative Examination – Blue Print
Articulation Mapping-K Levels with Courses Learning Outcomes (CLOs)

S. No.	CLOs	K- Level	Section A		Section B		Section C (Either/or Choice)	Section D (Open Choice)
			MCQs		Short Answers			
			No. of Questions	K- Level	No. of Questions	K- Level		
1	CLO 1	Up to K2	2	K1 & K1	1	K1	2 (K1& K1)	1(K2)
2	CLO 2	Up to K4	2	K3 & K4	1	K2	2 (K4 & K4)	1(K4)
3	CLO 3	Up to K3	2	K2 & K3	1	K1	2 (K2& K2)	1(K3)
4	CLO 4	Up to K4	2	K3 & K4	1	K2	2 (K4 & K4)	1(K4)
5	CLO 5	Up to K4	2	K2 & K3	1	K3	2 (K3 & K3)	1(K3)
No. of Questions to be asked			**10**		**5**		**10**	**5**
No. of Questions to be answered			**10**		**5**		**5**	**3**
Marks for each question			**1**		**2**		**5**	**10**
Total Marks for each section			**10**		**10**		**25**	**30**

K1- Remembering and recalling facts with specific answers
K2- Basic understanding of facts and stating main ideas with general answers
K3- Application oriented- Solving Problems
K4- Examining, analyzing, presentation and make inferences with evidences

Distribution of Section-wise Marks with K Levels

K Levels	Section A& B (No Choice)	Section C (Either / or)	Section D (Open Choice)	Total Marks	% of Marks without choice	Consolidated %
K1	6	10	-	16	13.3	35
K2	6	10	10	26	21.7	
K3	6	10	20	36	30	30
K4	2	20	20	42	35	35
Total marks	**20**	**50**	**50**	**120**	**100**	**100**

Name of the course Designers

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