

**DEPARTMENT OF CHEMISTRY
NATIONAL INSTITUTE OF TECHNOLOGY, TIRUCHIRAPPALLI**

COURSE OUTLINE TEMPLATE			
Course Title	Organic Chemistry- Reaction mechanisms and their types		
Course Code	CH 601	No. of Credits	3 (Theory)
Department	Chemistry	Faculty	Dr. S. Velmathi
Programme	M.Sc.(Chemistry)		
Pre-requisites Course Code	NIL		
Course Coordinator	Dr. L.Cindrella		
E-mail	velmathis@nitt.edu	Telephone No.	2503640
Course Type	<input checked="" type="checkbox"/> Core course <input type="checkbox"/> Elective course		
COURSE OVERVIEW			
This course is offered to I year M.Sc.(Chemistry) students. This 3 credit course is for theory. Three theory classes will be conducted per week.			
COURSE OBJECTIVE			
To introduce the basic principles involved in writing reaction mechanisms for aliphatic and aromatic nucleophilic, electrophilic substitution, elimination, addition, oxidation and reduction reactions, Physico chemical aspects of reaction mechanism and theories of aromaticity.			
COURSE OUTCOMES (CO)			
Students would become familiar with the:			
<ul style="list-style-type: none"> ✓ Kinetics and thermodynamic factors involved in the reaction ✓ reaction mechanism of important nucleophilic and electrophilic substitution reactions (Aliphatic and aromatic) ✓ Addition to C=C and C=X bonds, Oxidation and reduction reactions and reagents used ✓ Elimination reaction-mechanism and stereochemistry ✓ Theories of aromaticity 			
COURSE TEACHING AND LEARNING ACTIVITIES			
S.No.	Week	Topic	Mode of Delivery
1	I week of September	<u>Unit-I</u> Reaction mechanism: Definition of reaction mechanism, transition state theory, kinetics, qualitative picture. Basic mechanistic concepts like kinetic vs thermodynamic control	C&T
2	II week of September	Substituent effects, linear free energy relationships, Hammett equation and related modifications.	C&T

3	III & IV week of September	Hammond postulate, Curtin-Hammett principle isotope effects, general and specific acid-base catalysis, and nucleophilic catalysis.	C&T	
4	I week of October	Unit-II Aliphatic Nucleophilic Substitution– reactivity, structural and solvent effects, substitution in S_N1 , S_N2 , S_Ni .	C&T, PPT	
5	II week of October	Neighboring group participation -Norbonyl and bridgehead systems, substitution at allylic and vinylic carbons, substitution by ambident nucleophiles.	C&T, PPT	
6	III week of October	Reactive intermediates–Carbenes, nitrenes, radicals, ylides–Formation, stability and their applications.	C&T, PPT	
7	IV week of October	Unit-III Addition to carbon-carbon multiple bonds. Electrophilic, nucleophilic and free radical addition. Stereochemistry and orientation of the addition.	C&T, PPT	
8	I week of November	Hydrogenation, Halogenation, hydroxylation, hydroboration. Addition to carbonyl compounds- 1,2 and 1,4-addition	C&T, PPT	
9	II week of November	Benzoin, Knoevenagel, Stobbe and Darzen glycidic ester reactions. Stereochemistry of Aldol and Michael addition reactions- Felkin- Ahn Model	C&T, PPT	
10	III week of November	Unit-IV Elimination Reactions: E1, E2, E1CB- mechanism, stereochemistry, orientation of double bonds Hofmann, Zaitsev, Bredts rule- pyrolytic elimination	C&T, PPT	
11	IV week of November	Chugaev reaction. Oxidation and reduction: Swern and Dess-Martin oxidations, Corey-Kim oxidation, PCC, $KMnO_4$ oxidations.	C&T, PPT	
12	I week of December	Reduction using hydride reagents, $LiAlH_4$, $NABH_4$ and other organoboranes: chemo - and stereoselectivity, Catalytic hydrogenation (homogenous and heterogeneous catalysts)	C&T, PPT	
13	II week of December	Unit-V Theories of Aromaticity: Aromaticity and Antiaromaticity, Huckel's rule, annulenes and heteroannulenes, fullerenes (C_{60}). Other conjugated systems, Chichibabin reaction.	C&T, PPT	
14	III week of December	Aromatic electrophilic substitution: Orientation, reactivity, and mechanisms. Substitution in thiophene and pyridine. Aromatic nucleophilic substitution, S_NAr , benzyne, S_N1 . Aromatic Nucleophilic substitution of activated halides	C&T, PPT	
COURSE ASSESSMENT METHODS				
S.No.	Mode of Assessment	Week/Date	Duration	% Weightage

Theory				
1	Assignment/Quiz	II week of October	Depends on the activity	05
2	Test I	III week of October	60 minutes	20
3	Quiz/seminar	III week of November	Depends on the activity	05
4	Test II	IV week of Nov	60 minutes	20
5	Compensation Test	II Week of December		
6	End semester	IV week of December	3 hours	50

Theory = Total (100)

ESSENTIAL READINGS : Textbooks, reference books Website addresses, journals, etc

Text Books:

1. M. B. Smith, J. March, March's Advanced Organic Chemistry, John Wiley & Sons, 6th Edn, 2007
2. R. R. Carey and R. J. Sundburg, Advanced Organic Chemistry, Part A and Part B, Springer, 5th Edn, 2007

References:

1. Peter Sykes, A guide book to mechanism in Organic chemistry, Orient-Longmens, 6th Edn, 1996.
2. E. J. Eliel, Stereochemistry of Carbon Compounds, John Wiley, 1997
3. P. Y. Bruice, Organic Chemistry. Pearson Education, 3rd edition, 2006

COURSE EXIT SURVEY (mention the ways in which the feedback about the course is assessed and indicate the attainment also)

1. Feedback from students during class committee meetings.
2. Anonymous feedback through questionnaire at the end of the semester.

COURSE POLICY (including plagiarism, academic honesty, attendance, etc.)

1. 75% attendance is compulsory for Theory component.
2. Theory:
 - A. For those who missed Test I and Test II due to genuine reasons, retest will be conducted during the II week of December.

ADDITIONAL COURSE INFORMATION

The faculty will be available for consultation at times as per the intimation by the faculty.

Coordinator

[Signature]
15/9/2022

CC-Chairperson

[Signature]
16/9/22

HOD

[Signature]
19/9/2022
Head

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