FIRST-YEAR OF MASTER OF SCIENCE CHEMISTRY REVISED SYLLABUS ACCORDING TO CBCS NEP2020

COURSE TITLE: THEORETICAL ORGANIC CHEMISTRY-I
SEMESTER-III
W.E.F. 2024-25

RECOMMENDED BY THE BOARD OF STUDIES IN CHEMISTRY
AND
APPROVED BY THE ACADEMIC COUNCIL

Devrukh Shikshan Prasarak Mandal's
Nya. Tatyasaheb Athalye Arts, Ved. S. R. Sapre Commerce, and Vid. Dadasaheb Pitre Science College (Autonomous), Devrukh.
Tal. Sangameshwar, Dist. Ratnagiri-415804, Maharashtra, India

Academic Council Item No:

Name of the Implementing Institute	:	Nya. Tatyasaheb Athalye Arts, Ved. S. R. Sapre Commerce, and Vid. Dadasaheb Pitre Science College (Autonomous), Devrukh. Tal. Sangameshwar, Dist. Ratnagiri-415804,
Name of the Parent University	:	University of Mumbai
Name of the Programme	:	Master of Science
Name of the Department	:	Chemistry
Name of the Class	:	Second Year
Semester	:	Third
No. of Credits	:	04
Title of the Course	:	Theoretical Organic Chemistry-I
Course Code	:	S601CHT
Name of the Vertical in adherence to NEP 2020	:	Compulsory Major
Eligibility for Admission	:	Chemistry Graduate learner seeking Admission to Post Graduate Programme in adherence to Rules and Regulations of the University of Mumbai and Government of Maharashtra
Passing Marks	:	40%
Mode of Assessment	:	Formative and Summative
Level	:	PG
Pattern of Marks Distribution for SEE and CIA	:	60:40
Status	:	NEP-CBCS
To be implemented from Academic Year	:	2024-2025
Ordinances /Regulations (if any)		

Syllabus for Second Year of Master of Science in Chemistry

(With effect from the academic year 2024-2025)

SEMESTER-III **Paper No.- I**

Course Title: Theoretical Organic Chemistry-I **No. of Credits: 04**

Type of Vertical: Compulsory Major **COURSE CODE: S601CHT**

Learning Outcomes Based on BLOOM's Taxonomy:

After completing the course, the learner will be able to…		
Course Learning Outcome No.	Blooms Taxonomy	Course Learning Outcome
CLO-01	Remember	draw mechanisms of pericyclic and photochemical reactions.
CLO-02	Understand	explain method of generation, structure and stability of intermediates, approaches on different pericyclic reaction, symmetry on Frontier Molecular orbital diagrams, effect of conformation on reactivity of cyclohexane derivative.
CLO-03	Apply	predict point group of different organic compounds and stereochemistry of fused ring and bridged ring compounds.
CLO-04	Analyse	differentiate the type of pericyclic reaction.

Syllabus for Second Year of Master of Science in Chemistry

(With effect from the academic year 2024-2025)

SEMESTER-III **Paper No.- I**

Course Title: Theoretical Organic Chemistry-I **No. of Credits: 04**

Type of Vertical: Compulsory Major **COURSE CODE: S601CHT**

COURSE CONTENT			
Module No.	**Content**	**Credits**	**No. of Hours**
1	**UNIT-I: Organic reaction mechanisms** o **Organic reactive intermediates:** Methods of generation, Structure, Stability and Important reactions involving Carbocations, Nitrenes, Carbenes, Arynes and Ketenes. o **Neighbouring group participation:** Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, π-electrons, aromatic rings, σ-bonds with special reference to norbornyl and bicyclo[2.2.2]octyl cation systems (formation of non-classical carbocation) o **Role of FMOs in organic reactivity:** Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, Ambident electrophiles, the α effect. o **Pericyclic reactions:** Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: Evidence for the concertedness of bond making and breaking Symmetry-Allowed and Symmetry-Forbidden Reactions – □ The Woodward-Hoffmann Rules-Class by Class	01	15

	□ The generalised Woodward-Hoffmann Rule Explanations for Woodward-Hoffmann Rules □ The Aromatic Transition structures [Huckel and Mobius] □ Frontier Orbitals □ Correlation Diagrams, FMO and PMO approach ○ **Molecular orbital and symmetry**, Frontier orbital of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system		
2	**UNIT-II: Pericyclic reactions** ○ **Cycloaddition reactions**: Supra and antra facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes. Diels-Alder reactions, 1, 3-Dipolar cycloaddition and cheletropic reactions, ene reaction, retro-Diels-Alder reaction, regioselectivity, periselectivity, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions. Other Cycloaddition Reactions- [4+6] Cycloadditions, Ketene Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. ○ **Electrocyclic reactions:** Conrotatory and disrotatary motions, 4nπ and (4n+2)π electron and allyl systems. ○ **Sigmatropic rearrangements:** H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy Cope and aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A.	01	15

3	**UNIT-III: Stereochemistry-I** o **Classification of point groups**: Based on symmetry elements with examples (nonmathematical treatment). o **Conformational analysis of medium rings:** Eight to ten membered rings and their unusual properties, I-strain, transannular reactions. o **Stereochemistry of fused ring and bridged ring compounds:** Decalins, Hydrindanes, Perhydroanthracenes, Steroids, and Bredt's rule. o **Anancomeric systems, Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism):** Electrophilic addition, Elimination, Molecular rearrangements, of cyclohexanones (with LiAlH4, selectride and MPV reduction) and Oxidation of cyclohexanols.	01	15
4	**Unit-IV: Photochemistry** o **Principles of photochemistry:** Quantum yield, Electronic states and transitions, Selection rules, modes of dissipation of energy (Jablonski diagram), E**lectronic energy transfer:** Photosensitization and Quenching process. o **Photochemistry of carbonyl compounds:** $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Norrish- I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of α, β-unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction. o **Photochemistry of olefins:** cis-trans isomerizations, Dimerization's, Hydrogen abstraction, Addition and Di- π- methane rearrangement including aza-di- π - methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes. o **Photochemistry of arenes:** 1,2-, 1,3- and 1,4-	01	15

	additions. Photocycloadditions of aromatic Rings. o Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions. Chemiluminescence.		
	Total	**04**	**60**

Access to the Course

The course is available for all the students admitted for Second Year of Master of Science.

Methods of Assessment

The assessment pattern would be 60:40, 60% for Semester End Examination (SEE) and 40% for Continuous Internal Assessment (CIA). The structure of the SEE and CIA would be as recommended by the Board of Studies and approved by the Board of Examination and the Academic Council of the college.

References:

1. March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons.
2. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi.
3. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
4. Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
5. Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
6. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.
7. Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th. Nelson and Sons Ltd., London 1969.
8. Organic reactive intermediates, Samuel P. MacManus, Academic Press.
9. Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).

10. Organic Chemistry, Seventh Edition, R.T. Morrison, R. N. Boyd & S. K. Bhattacharjee, Pearson.Advanced Organic Chemistry: Reactions & Mechanisms, second edition, B. Miller and R. Prasad, Pearson.
11. Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
12. Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
13. Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
14. Pericyclic reactions, Ian Fleming, Oxford university press, 1999.
15. Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979.
16. Organic chemistry, 8th edition, John McMurry
17. Modern methods of Organic Synthesis, 4th Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004
18. Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books,2006
19. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
20. Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.
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22. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
23. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
24. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
25. Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
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27. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern
28. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.