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

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COURSE TITLE: THEORETICAL ORGANIC CHEMISTRY-II  
SEMESTER-IV  
W.E.F. 2024-2025

**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	:	Four
No. of Credits	:	04
Title of the Course	:	Theoretical Organic Chemistry-II
Course Code	:	S610CHT
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-IV**

**Course Title: Theoretical Organic Chemistry-II**

**Type of Vertical: Compulsory Major**

**Paper No.- I**

**No. of Credits: 04**

**COURSE CODE: S610CHT**

### 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	Study structural effects and reactivity of Linear free energy relationship (LFER) in determination of organic reaction mechanism, principles of supramolecular chemistry, basic concept related to stereochemistry, principles of asymmetric synthesis.
CLO-02	Understand	Discuss structure and properties of crown-ether, cryptands etc. and methods of resolution.
CLO-03	Apply	derive Yukawa-Tsuno equation, Hammett equation, synthesis of L-DOPA, synthesis of crown ethers, cryptands and calixarenes.
CLO-04	Analyze	Explain Dimroth's ET parameter, octant rule and the axial $\alpha$ -haloketone rule, Cotton effect and its applications,

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**Paper No.- I**

**No. of Credits: 04**

**COURSE CODE: S610CHT**

<b>COURSE CONTENT</b>			
<b>Module No.</b>	<b>Content</b>	<b>Credits</b>	<b>No. of Hours</b>
1	<p><b>UNIT-I: Physical organic chemistry</b></p> <ul style="list-style-type: none"> <li>○ Structural effects and reactivity: Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of <math>\sigma</math>-values, reaction constants <math>\rho</math>, Yukawa-Tsuno equation.</li> <li>○ Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, <math>\sigma_I</math> and <math>\sigma_R</math> scales, steric parameters <math>E_s</math> and <math>\beta</math>. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's ET parameter, Solvatochromism Z-scale, Spectroscopic Correlations, Thermodynamic Implications.</li> </ul>	01	15
2	<p><b>UNIT-II: Supramolecular chemistry</b></p> <ul style="list-style-type: none"> <li>○ Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.</li> <li>○ Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.</li> <li>○ Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.</li> <li>○ Molecular recognition and catalysis, molecular self-assembly. Supramolecular Polymers, Gels and Fibres</li> </ul>	01	15

3	<b>UNIT-III : Stereochemistry- II</b> <ul style="list-style-type: none"><li>○ Racemisation and resolution of racemates including conglomerates: Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.</li><li>○ Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR).</li><li>○ Correlative method for configurational assignment: chemical, optical rotation, and NMR spectroscopy.</li><li>○ Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial <math>\alpha</math>- haloketone rule with applications.</li></ul>	01	15
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4	<p><b>Unit-IV: Asymmetric synthesis</b></p> <ul style="list-style-type: none"> <li>○ Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions.</li> <li>○ Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantioselective epoxidation, hydroxylation, aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.</li> <li>○ Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.</li> </ul>	01	15
	<b>Total</b>	<b>04</b>	<b>60</b>

### 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) Organic Chemistry, Part A and B, Fifth edition, 2007, Francis A. Carey and Richard J. Sundberg, Springer.
- 8) Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th. Nelson and Sons Ltd., London 1969.
- 9) Organic reactive intermediates, Samuel P. MacManus, Academic Press.
- 10) Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).
- 11) 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.
- 12) Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
- 13) Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012
- 14) Organic Chemistry, W. G. Solomons, C. B. Fryhle, , 9th Edition, Wiley India Pvt. Ltd., 2009.
- 15) Pericyclic Reactions, S. Sankararaman, Wiley VCH, 2005.
- 16) Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
- 17) Pericyclic reactions, Ian Fleming, Oxford university press, 1999.
- 18) Pericyclic reactions-A mechanistic approach, S. M. Mukherji, Macmillan Co. of India 1979.
- 19) Organic chemistry, 8th edition, John McMurry
- 20) Modern methods of Organic Synthesis, 4th Edition W. Carruthers and Iain Coldham,

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Cambridge University Press 2004

- 21) Modern physical chemistry, Eric V Anslyn, Dennis A. Dougherty, University science books, 2006
- 22) Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman
- 23) Stereochemistry of Carbon Compounds: Principles and Applications, D, Nasipuri, 3rd edition, New Age International Ltd.
- 24) Stereochemistry of Organic Compounds, Ernest L. Eliel and Samuel H. Wilen, Wiley-India edit
- 25) Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
- 26) Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005
- 27) Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
- 28) Supramolecular Chemistry; Concepts and Perspectives, J. M. Lehn, VCH.
- 29) Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
- 30) Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.