JAI HIND COLLEGE
BASANTSING INSTITUTE OF SCIENCE
&
J.T.LALVANI COLLEGE OF COMMERCE
(AUTONOMOUS)

"A" Road, Churchgate, Mumbai - 400 020, India.

Affiliated to
University of Mumbai

Program: M.Sc. in Chemistry

Course: Organic Chemistry II

Semester II

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2021-22

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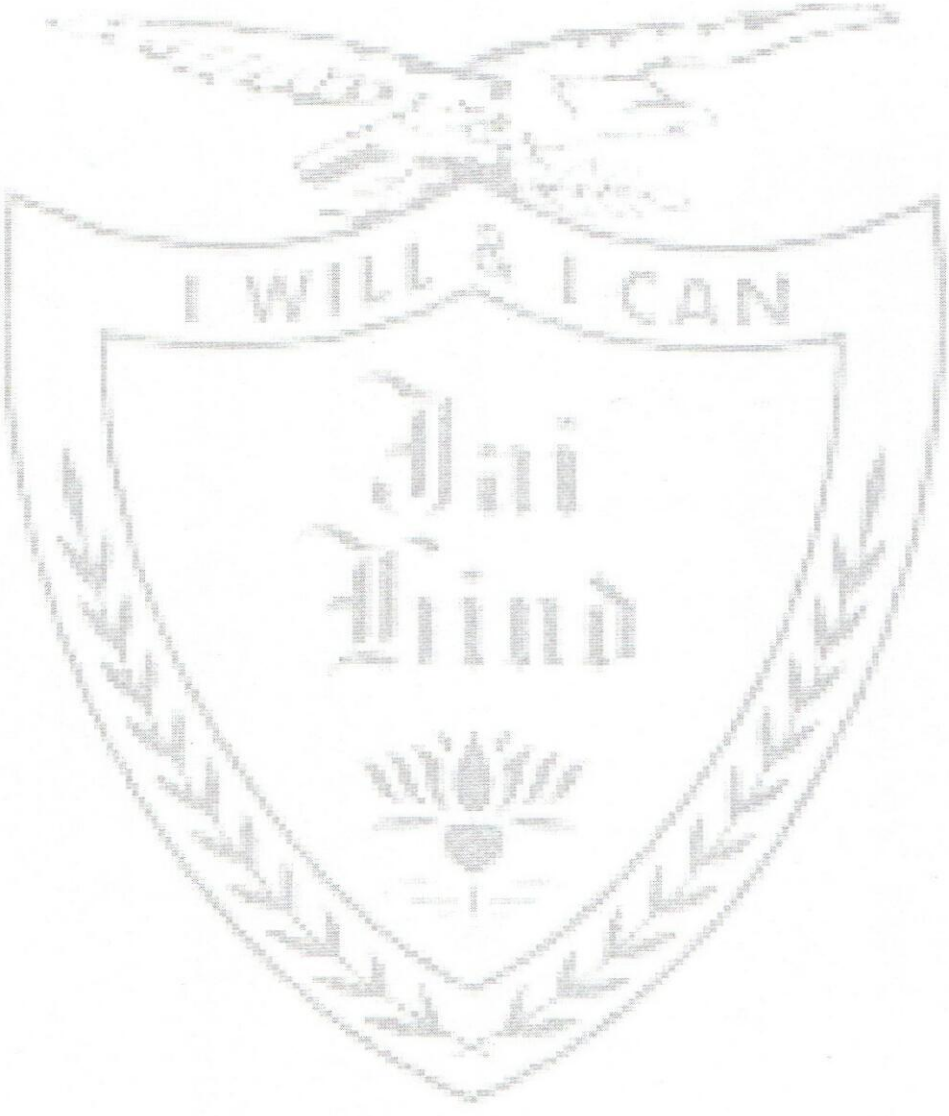
M.Sc. Chemistry Syllabus

Semester II			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHE203	**Organic Chemistry II**	**04**	**04**



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Semester II – Theory

Course: PSCHE203	Course Title: Organic Chemistry II	Credits: 04 Lectures/Week: 04
	Course description: Enols & Enolates, Name Reactions & Rearrangements, Molecular Orbital Theory & Photochemistry, Organic Spectroscopy.	
	Objectives: **1. To understand the chemistry of enolates and name reactions** **2. To understand the MOT of different molecules** **3. To understand the principles of photochemistry and electronic excitations.** **Outcomes:** **1. To discuss new name reaction and enol enolate chemistry along with its application.** **2. To solve spectral problems merging all spectroscopic technique together.**	
Unit I	**Enols & Enolates** 1.1 Acid & Base catalysed enolisation, enols & enolates from aldehydes, ketones, esters, acids, amides; kinetic & thermodynamically stable enols **[2L]** 1.2 Regioselectivity in formation of enolates- thermodynamic & kinetic control, factors governing regioselectivity **[3L]** 1.3 Reactions of enols & enolates: **[5L]** a. O-alkylation versus C-alkylation of enolates b. Alkylation of enolates from nitriles, nitroalkanes, carboxylic acids, esters, aldehydes & ketones c. Regioselective formation of dianion and alkylation of dianion d. Acid and base catalysed halogenation, iodoform reaction e. Nitrosation of enols f. Conjugate addition of enolates to α,β-unsaturated carbonyls (Michael reaction) 1.4 Acid and base catalysed aldol condensation, mixed aldol condensation with aromatic aldehydes, chemoselectivity in mixed reactions of aliphatic aldehydes and ketones, intramolecular aldol & Robinson's annulation **[2L]** 1.5 Nucleophilic reactions at carbonyl carbon- Mannich reaction, Claisen condensation, Knoevenagel reaction **[3L]**	**15L**

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Unit II	**Name Reactions & Rearrangements** Mechanism, stereochemistry (if applicable) and applications of the following: 2.1 **Reactions:**Baylis-Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction 2.2 **Concerted rearrangements:** Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton- Katritzky 2.3 **Cationic rearrangements:** Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein. 2.4 **Anionic rearrangements:** Brook, Neber, Von Richter, Wittig, Gabriel–Colman, Payne	**15L**
Unit III	**Molecular Orbital Theory & Photochemistry** **Applications of Molecular Orbital Theory in Organic Chemistry:** 3.1.1 **MOT:** Formation of MOs by LCAO, concept of nodal planes and energies of π-MOs; Construction of MO of conjugated systems- ethene, butadiene, hextriene, allyl cation, anion & radical; MO of formaldehyde involving electronegativity perturbation. **(2L)** 3.1.2 **Salem-Klopman equation:** Explanation of terms in the equation, frontier molecular orbitals (HOMO & LUMO) and their significance, Pearson's principle and Hard-soft electrophiles and nucleophiles- examples and identification of hard and soft reactive sites.**(3L)** 3.1.3 **Application of FMO concepts to:** (a)significance of HOMO-LUMO band gap in absorption spectra of polyenes, effect of conjugation on FMOs of alkenes (b) SN^2 reaction, (c) dimerization of ethylene to cyclobutane, (d) Diels-Alder cycloaddition**(4L)** **Photochemistry: (6L)** 3.2.1 Introduction to Photochemistry: General Principles, electronic states and transitions, selection rules, fate of excited molecules (Jablonski diagram) 3.2.2 Photochemistry of alkenes: cis-trans isomerization, dimeriztation, oxidative coupling 3.2.3 Photochemistry of carbonyl compounds: $\pi \rightarrow \pi^*$ & $n \rightarrow \pi^*$ transitions, Norrish type I & II reactions, photoreduction & photosensitization.	**15L**

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Unit IV	**Organic Spectroscopy:** **4.1 Uv Spectroscopy (2L):**Principles of absorption spectroscopy, chromophore, auxochrome; factors affecting position and intensity of uv bands- conjugation, steric factor, pH and solvent polarity Woodward-fieser rules for dienes & enones **4.2 Infrared Spectroscopy (3L):** Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for different functional groups. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides, anhydrides, lactones, lactams and conjugated carbonyl compounds. **4.3 NMR Spectroscopy (7L):** **4.3.1 Proton Magnetic resonance:** Principle, Chemical shift, Factors affecting chemical shift (Electronegativity, H-bonding, Anisotropy effects). Chemical and magnetic equivalence, Chemical shift values and correlation for protons bonded to carbon and other nuclei; Spin-spin coupling, Coupling constant (J), Factors affecting J, geminal, vicinal and long range coupling (allylic and aromatic), Karplus equation **4.3.2 ^{13}C NMR spectroscopy:** Theory and comparison with proton NMR, proton coupled and decoupled spectra, off-resonance decoupling. Factors influencing carbon shifts, correlation of chemical shifts of aliphatic, olefin, alkyne, aromatic and carbonyl carbons. **4.4 Mass Spectrometry (3L):** Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS. Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.	**15L**

References:

Unit I

1. *Organic Chemistry*, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press
2. *Advanced Organic Chemistry*, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.

Unit II

3. *Name Reactions- A collection of Detailed Mechanisms and Synthetic Applications,* Jie

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Jack Li, Fourth Edition, Springer Publisher.
4. *Name Reactions and Reagents in Organic Synthesis*, Bradford P. Mundy, M.G. Ellerd, and F.G. Favaloro, John Wiley & Sons.
5. *Organc Reaction Mechanisms,* V.K. Ahluwalia, R.K. Parasher, Alpha Science International, 2011.

Unit III

6. *Molecular Orbitals and Organic Chemical Reactions,* Ian Fleming, Reference Edition 2010, Wiley & Sons Ltd.
7. *Advanced Organic Chemistry*, F.A. Carey and R.J. Sundberg, Part A, Plenum Press.
8. *Principles of Organic Synthesis*, R.O.C. Norman and J.M Coxon, Third edition, Blackie Academic & Professional Publishers.

Unit IV

9. *Introduction to Spectroscopy,* Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
10. *Organic Spectroscopy- Principles and applications,* Jag Mohan, Narosa Publication
11. *Spectrometric Identification of Organic Compounds,* R. Silverstein, G.C. Bassler and T.C. Morrill, John Wiley and Sons.

Additional References:

12. *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, Michael B. Smith, Jerry March, Wiley.
13. *Organic Chemistry*, R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Pearson Publication (7th Edition)
14. *Advanced Organic Chemistry: Reactions and mechanism*, B. Miller and R. Prasad, Pearson Education.
15. *Advanced Organic Chemistry: Reaction mechanisms*, R. Bruckner, Academic Press.
16. *Understanding Organic Reaction Mechanisms,* Adams Jacobs, Cambridge University Press.
17. *Writing Reaction Mechanism in organic chemistry*, A. Miller, P.H. Solomons, Academic Press.
18. *Advanced Organic Chemistry: Reactions and mechanism,* L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
19. *Mechanism in Organic Chemistry,* Peter Sykes, 6th Edition
20. *Organic Spectroscopy,* William Kemp, W.H. Freeman & Company.
21. *Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.*
22. *Spectroscopy of Organic Compounds,* P.S. Kalsi, New Age International Ltd.

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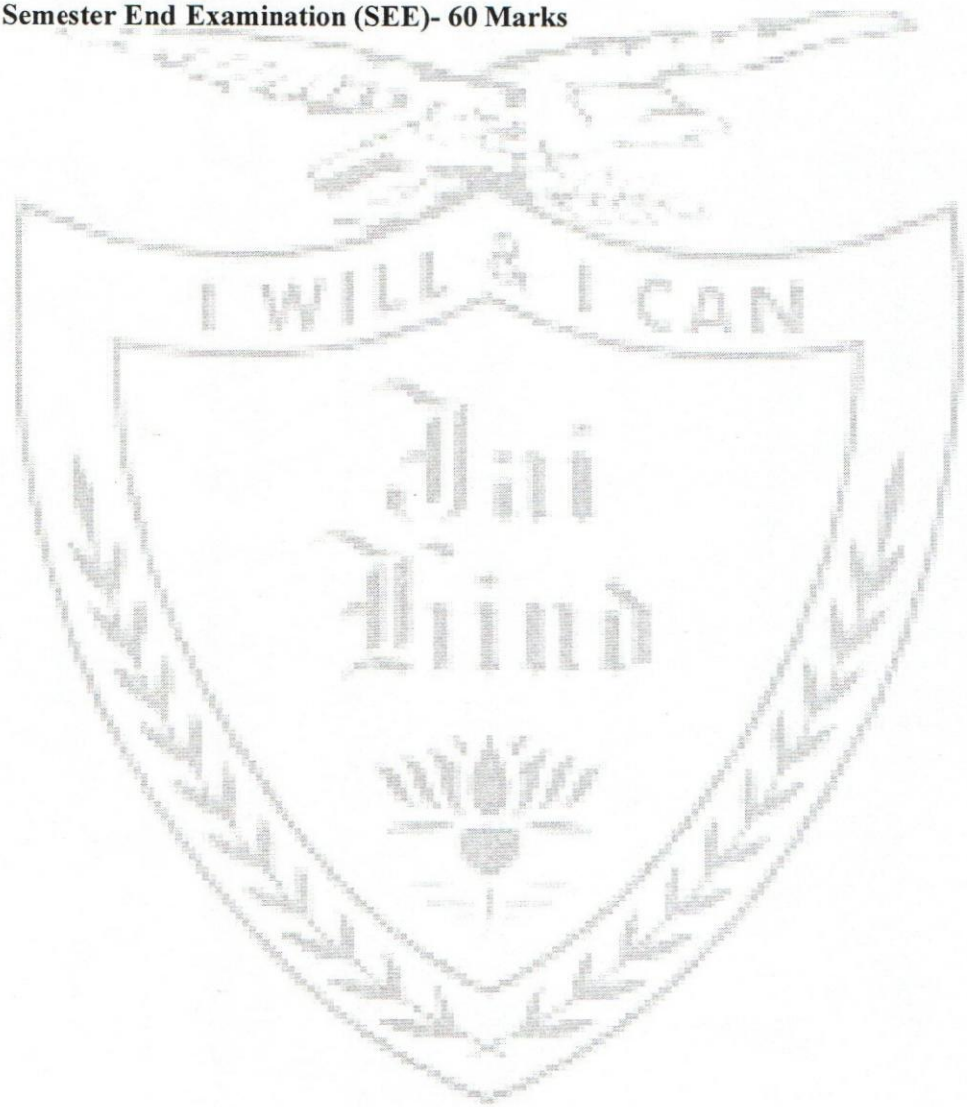
Evaluation Scheme

- **Continuous Assessment (CA) – 40 Marks**
  - Knowledge and Application based: Objective test of 20 Marks
  - Skill based (20 marks): Learner will be assessed on relevant skills pertaining to the course content of a particular paper which could involve but not limited to

    Oral Presentations on relevant topics
    Review writing/Worksheets etc.

- **Semester End Examination (SEE)- 60 Marks**



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Program: M.Sc. in Chemistry

Course: Organic Chemistry Practical II

Semester II

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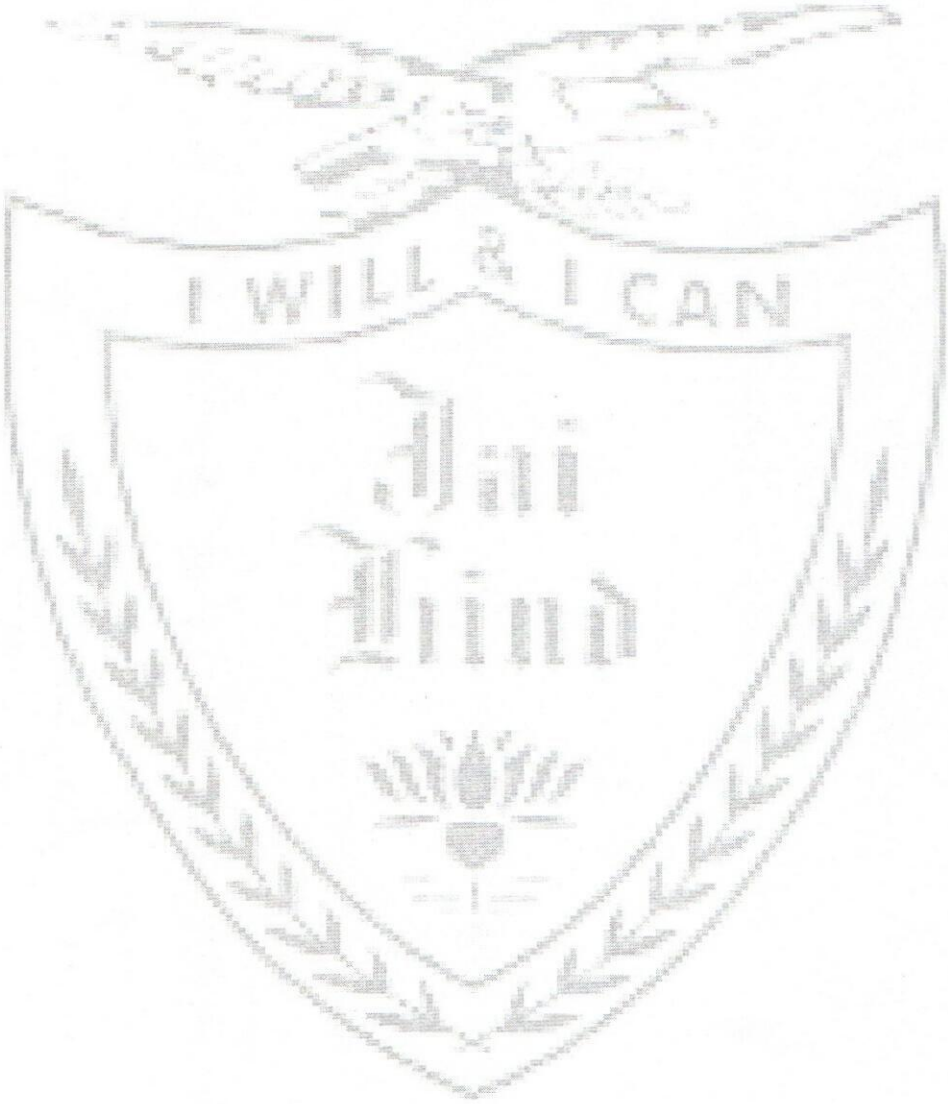
M.Sc. Chemistry Practical Syllabus

Semester II			
Course Code	**Course Title**	**Credits**	**Practicals/Week**
PSCHEPR203	**Organic Chemistry Practical II**	**02**	**01**



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Semester II – Practical

Course: PSCHEPR203	Course Title: Organic Chemistry Practical II	Credits: 02, Practical/Week: 01

Objectives:

1. **To understand the separation of binary mixture using physical and chemical methods.**
2. **To discuss the characterization of one component.**
3. **To describe the purification and determination of mass and physical constant of the second component.**

Outcomes:

1. **To separate binary mixture using physical and chemical methods.**
2. **To determine mass and physical constant of the second component in a mixture.**

Separation of Binary Mixture:

1. Separation of binary mixture using physical and chemical methods.
2. Characterization of one component with the help of chemical analysis and confirmation of the structure with the help of physical constant.
3. Purification and determination of mass and physical constant of the second component. The following types are expected:
   a) Water soluble/water insoluble solid and water insoluble solid,
   b) Non-volatile liquid and Non-volatile liquid (chemical separation)

Minimum three mixtures from each type and a total of ten mixtures are expected.

REFERENCES

1. Organic Analytical Chemistry: Theory and Practice, Jag Mohan, Alpha Science, 2003
2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
3. Vogel's Textbook of Practical Organic Chemistry, Fifth edition,2008, B.S.Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education
4. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
5. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V. K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000

Evaluation Scheme

- **Semester End Examination (SEE)- 50 Marks**

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