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

Courses:: Organic Chemistry I

Semester I

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

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M.Sc. ChemistrySyllabus

Semester I			
Course Code	Course Title	Credits	Lectures/Week
PSCHE103	**Organic Chemistry I**	04	04

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Semester I – Theory

Course Code: PSCHE103	Course Title: Organic Chemistry I	Credits: 04 Lectures/Week: 04
	Course description: Physical Organic Chemistry, Nucleophilic Substitution, Aromaticity, Stereochemistry & Reagents in organic synthesis	
	Objectives: **1. To understand the concept outlining the feasibility of a reaction and its possible pathway.** **2. To synthesise the desired product with the appropriate reagent.** **3. To analyse the stereochemical arrangement of molecules.** **Outcomes:** **1. To predict the correct stereochemical configuration of molecules.** **2. To justify the formation of products based on the reaction pathway.**	
Unit I	**Physical Organic Chemistry** 1.1 **Thermodynamic and kinetic requirements of a reaction:** rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity *vs* selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic *vs* thermodynamic control of organic reactions. 1.2 **Determining mechanism of a reaction:** Product analysis, kinetic studies, use of isotopes (Kinetic isotope effect – primary and secondary kinetic isotope effect). Detection and trapping of intermediates, crossover experiments and stereochemical evidence. 1.3 **Acids and Bases:** Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pKa values, Leveling effect and non-aqueous solvents. Acid and base catalysis – general and specific catalysis with examples.	**15L**
Unit II	**Nucleophilic substitution reactions and Aromaticity** 2.1 **Nucleophilic substitution reactions: (9 L)** 2.1.1 **Aliphatic nucleophilic substitution:** a. S_N1 (ion pair mechanism), S_N2, S_N^i& $S_NCA$mechanism-evidences & factors governing b. SET mechanism ($S_{RN}1$) c. NGP –introduction & evidences; examples of neighboring group participation by lone pair &aryl rings	**15L**

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	d. Nucleophilic substitution at allylic & propargylic systems (S_N1' and S_N2') e. Nucleophilic substitution at vinylic carbon (addition-elimination & elimination-addition) f. Factors affecting nucleophilic substitution: substrate, nucleophilicity, solvent, steric effect, leaving group 2.1.2 **Aromatic nucleophilic substitution:** S_NAr, S_N1, benzyne mechanisms (ipso & cine substitution). 2.1.3 **Ester hydrolysis:** Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples. 2.2 **Aromaticity: (6L)** 2.2.1 Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity. 2.2.2 HMO theory for conjugated polyenes & aromatic compounds, Frost-Musulin diagrams; Application of HMO theory to monocyclic conjugated systems. 2.2.3 Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (C_{60}).	
Unit III	**Stereochemistry of Organic Compounds** 3.1 **Molecular symmetry & Chirality:** symmetry operations & symmetry elements, point group classification, molecular symmetry & chirality **(3L)** 3.2 **Stereoisomerism & Centre of chirality:** Molecular representation- Flying wedge, Fischer, Sawhorse, Newman projections & interconversions; Configurational nomenclature- DL, RS, R*S*, EZ& syn-anti; molecules with two or more chiral centres- constitutionally unsymmetrical & symmetrical chiral molecules, concepts of stereogenic, chirotopic & pseudoasymmetric centres. **(4L)** 3.3 **Molecular chirality:** Chiral axes & chiral planes as stereogenic units **(4L)** i. **Axial chirality:** stereochemistry of allenes, spiranes & biphenyls, configurational descriptors (R,S), configurational stability & buttressing effect. ii. **Planar chirality:** stereochemistry of cyclophanes, ansa compounds, trans-cycloalkenes, configurational descriptors (R,S)	**15L**

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	iii. **Helical Chirality:** introduction to helical chirality & helical nomenclature (P,M) 3.4 **Topicity & prostereoisomerism:** Prochirality & prostereoisomerism, topicity of ligands & faces, addition-substitution criterion, symmetry criterion, nomenclature of stereoheterotopic ligands & faces.**(4L)**	
Unit IV	**Oxidation and Reduction:** 4.1 **Oxidation:** General mechanism, chemoselectivity, and important applications of the following: 4.1.1 **Oxidation of alcohols to aldehydes and ketones:** Chromium reagents such as $K_2Cr_2O_7/H_2SO_4$ (Jones reagent), CrO_3-pyridine(Collin's reagent) PCC (Corey's reagent) and PDC (Cornforth reagent), Hypervalent iodine reagents (IBX,Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation - advantages over Swern and limitations; and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation. 4.1.2 **Oxidation to carbonyl involving C-C bonds cleavage:** Glycols using HIO_4; cycloalkanones using CrO_3; carbon-carbon double bond using ozone, $KMnO_4$, CrO_3, $NaIO_4$ and OsO_4; aromatic rings using RuO_4 and $NaIO_4$. 4.1.3 **Oxidation of active methylene to carbonyl:** oxidation of CH_2 to CO by SeO_2, oxidation of arylmethanes by CrO_2Cl_2 (Etard oxidation). 4.1.4 **Oxidation of aldehydes and ketones:** with H_2O_2 (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation) 4.1.5 **Dehydrogenation of C-C bonds:** Using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ) include aromatization of six membered rings. 4.2 **Reduction:** General mechanism, chemoselectivity, and important applications of the following reducing reagents: 4.2.1 **Reduction of CO to CH_2 in aldehydes and ketones-** Clemmensen reduction, Wolff- Kishner reduction and Huang-Minlon modification. 4.2.2 Reduction of carbonyl and others functional groups using metals and metal hydride as reducing agents along with chemoselectivity: Boron reagents ($NaBH_4$, $NaCNBH_3$), Aluminium reagents ($LiAlH_4$, DIBAL-H); stereoselectivity of reductions- Cram's rule and Felkin	**15L**

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	Ahn model. 4.2.3 Reduction of symmetric unsaturated compounds: NH_2NH_2 (diimide reduction) and other non-metal based agents. 4.2.4 Reductions of Aromatic ring and acetylenes: Using Li/Na-liquid NH_3 mediated reduction (Birch reduction)	

Standard References:

Unit I

1. *Physical Organic Chemistry*, Neil Isaacs
2. *Modern Physical Organic Chemistry*, Eric V. Anslyn and Dennis A. Dougherty
3. *Mechanism in Organic Chemistry*, Peter sykes, 6th edition onwards.

Unit II

1. *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, Michael B. Smith, Jerry March, Wiley.
2. *Mechanism in Organic Chemistry*, Peter Sykes, 6th edition onwards
3. *Organic Chemistry*, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
4. *Advanced Organic Chemistry*, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.

Unit III

5. *Stereochemistry: A ThreeDimensional Insight*, Anil V. Karnik, Mohammed Hasan, First edition, 2021,Elsevier Publisher
6. *Stereochemistry of Organic Compounds- Principles and Applications*, D. Nasipuri. 4th Edition, New International Publishers Ltd
7. *Stereochemistry of Carbon Compounds*, E.L Eliel, S.H Wilen and L.N Manden, Wiley

Unit IV

8. *Principles of Organic Synthesis*, R.O.C. Norman and J.M Coxon, Nelson Thornes.
9. *Modern Methods of Organic Synthesis*, W. Carruthers and Iain Coldham, Cambridge University Press.
10. *Organic Synthesis*, Jagdamba Singh, L.D.S. Yadav, Pragati Prakashan.
11. *Organic Reaction Mechanisms* V.K.Ahluwalia, Rakesh kumar Prakashan

Additional References:

12. *Comprehensive Organic Chemistry*, Barton and Ollis, Vol 1
13. *Stereochemistry: Conformation and mechamism*, P.S. Kalsi, New Age International, New Delhi.
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.

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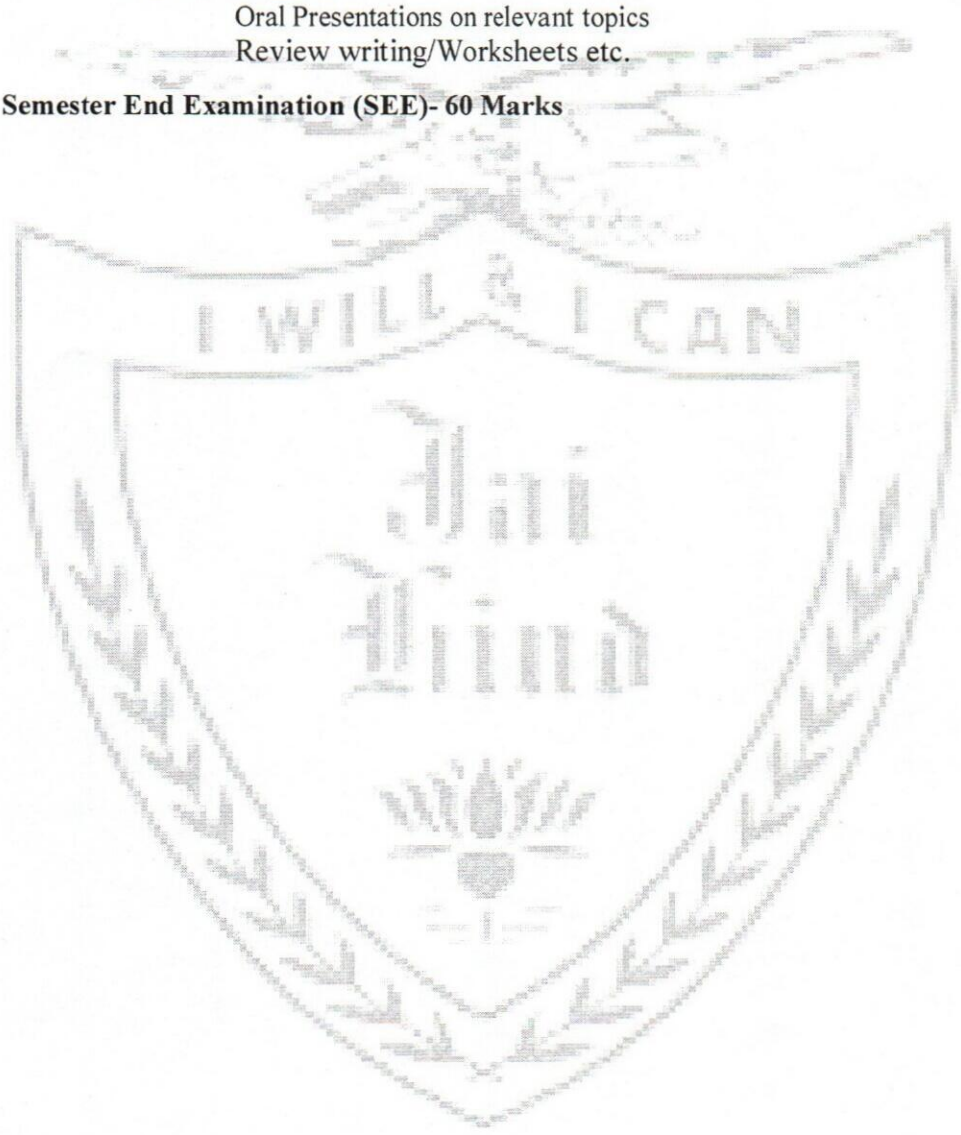
Evaluation Scheme

- **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 I

Semester I

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M.Sc. Chemistry Practical Syllabus

Semester I			
Course Code	**Course Title**	**Credits**	**Practicals/Week**
PSCHEPR103	**Organic Chemistry Practical I**	**02**	**01**

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Semester I – Practical

Course Code: PSCHEPR103	Course Title: Organic Chemistry Practical I	Credits: 02 Practical/Week: 01

Objectives:

1. **To comprehend the planning of a reaction based on stochiomet calculations.**
2. **To apply the theoretical concepts in understanding the reaction conditions.**
3. **To understand the concept of recrystallization.**

Outcomes:

1. **To predict the percentage formation of product based on the re conditions.**
2. **To systemise the correct solvent of recrystallisation based on th solubility of acompound.**

One step organic synthesis:

1. Bromobenzene to p-nitrobromobenzene
2. Anthracene to anthraquinone
3. Benzoin to benzil
4. Anthracene to Anthracene maleic anhydride adduct
5. 2-Naphthol to BINOL
6. p-Benzoquinone to 1,2,4-triacetoxybenzene
7. Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
8. *o*-Phenylenediamine to 2-methylbenzimidazole
9. *o*-Phenylenediamine to 2,3-diphenylqunooxaline
10. Urea and benzil to 5,5-diphenylhydantoin

Learning points:

1. Planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS should be learnt.
2. Purify the product by crystallization. Formation and purity of the product should be checked by TLC
3. Report mass and melting point of the purified product.

REFERENCES:

1. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
2. 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

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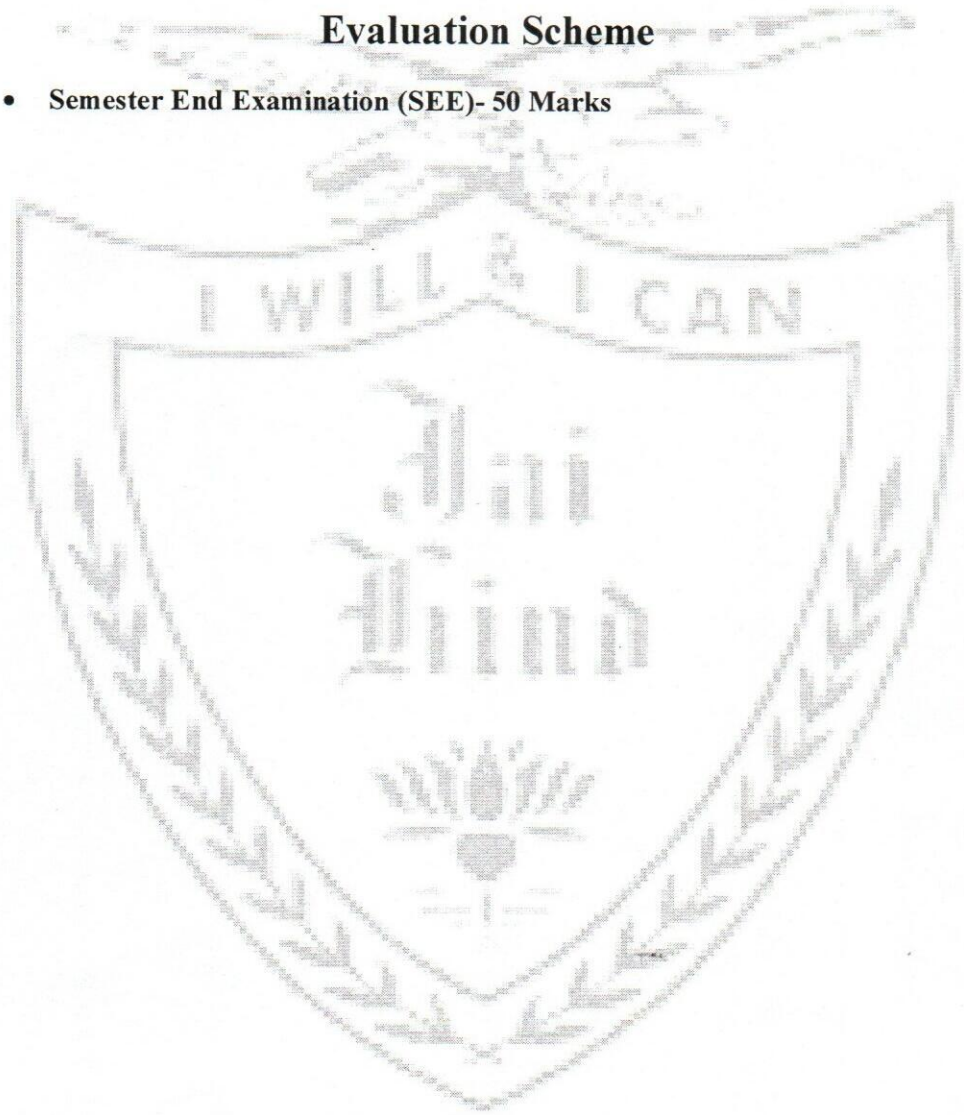
	3. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers. 4. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V. K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000

Evaluation Scheme

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



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