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. Chemistry
(Organic)

Course: Theoretical Organic Chemistry II
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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M.Sc. Theoretical Organic Chemistry II Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHE3401	Theoretical Organic Chemistry II	04	04

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Semester IV – Theory

Course: PSCHE3401	**Theoretical Organic Chemistry-II (Credits: 04 Lectures/Week: 04)**	
	Physical Organic Chemistry, Supramolecular Chemistry, Stereochemistry & Asymmetric Synthesis	
	Objectives: 1. **To understand the effect of substituents on rate of reaction through Hammett,Yukawa-Tsuno, Taft equations.** 2. **To introduce the emergence of supramolecular chemistry.** 3. **To understand the separation of stereochemical mixtures** 4. **To explain the principles of asymmetric synthesis of organic molecules.** **Outcomes:** 1. **To describe the effect of substituents on rate of reaction through Hammett, Yukawa-Tsuno, Taft equations.** 2. **To describe novel supramolecular architectures.** 3. **To summarise Cotton effect and its applications** 4. **To synthesize organic molecules by asymmetric aldol condensation.**	
Unit I	**Physical Organic Chemistry** 1.1 Linear Free Energy Relationships (LFERs): General mathematics, conditions to create LFER, isokinetic or iso-equilibrium temperature, enthalpy-entropy compensation **[3L]** 1.2 Hammett equation: derivation, substituent and reaction constant & their physical significance, applications of Hammett plots-calculation of k and K values, deciphering mechanisms of reactions using linear plots & deviations from straight line plots **[4L]** 1.3 Separation of resonance from induction- Yukawa-Tsuno equation; Steric and polar effects- Taft parameters; Solvent effects- Grunwald Winstein equation, Schleyer adaptation; Electrophilic substituent constants- Okamoto Brown equation **[5L]** 1.4 Nucleophilicity and Nucleofugality- Swain Scott equation, Edward & Ritchie correlations; Solvatochromism- Dimroth's E_T Parameter & Z scale **[3L]**	**15L**
Unit II	**Supramolecular Chemistry** 2.1 Definition & emergence of Supramolecular Chemistry; binding constant and its measurement; cooperativity & chelate effect; Molecular recognition & self-assembly; host-guest chemistry; complementarity (lock & key, induced fit) & preorganisation **[5L]** 2.2 Molecular recognition with **[6L]** i. Ion pairing component (salt-bridges)	**15L**

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	ii. Ion-dipole component (crowns, cryptands & spherands, tweezers & clefts) iii. Hydrogen bonding component iv. Hydrophobic component (cyclodextrins, cyclophanes and calixarenes) v. π-component (cation-π, polar-π, π-π& D-A) 2.3 Novel supramolecular architectures- catenanes, rotaxanes and knots, container compounds **[4L]**	
Unit III	**Stereochemistry-II** 3.1 Properties of enantiomers & racemates, classification of racemates; mechanisms of racemisation- through carbocations, carbanions, free radicals, symmetrical intermediates & rotation of bonds. **[2L]** 3.2 Resolution of racemates: **[5L]** i. Not involving transformation: Mechanical separation, preferential crystallization, kinetic resolution, chemical resolution, inclusion compounds/molecular complexes ii. Involving transformation: Equilibrium asymmetric transformation (First & second kind) – CIDR, dynamic kinetic resolution iii. Chromatographic method of resolution: separation of diastereomers using achiral chromatography; separation of enantiomers using chiral chromatography; involving precolumn or on-column racemization. 3.3 Configurational analysis: correlative methods for configurational assignment- chemical, optical, NMR spectroscopy, quasi-racemate formation & asymmetric synthesis **[4L]** 3.4 Chiroptical properties: optical activity & polarimeter; linearly and circularly polarized light;circular birefringence and circular dichroism; ORD and CD curves; Cotton effect and its applications;empirical rules- octant rule and the axial α– haloketone rule with applications.**[4L]**	**15L**
Unit IV	**Dynamic Stereochemistry & Asymmetric Synthesis** 4.1 Enantiomer composition & enantiomer excess: optical purity & Horeau effect; NMR based methods- Chiral Derivatising Agents, Chiral Solvating Agents, Chiral Shift Reagents; Chromatographic methods (HPLC/GC)- indirect method using diastereomers, direct method using chiral chromatography **[4L]** 4.2 Recapitulation of prochirality, Stereoselective & stereospecific reactions; classification of asymmetric reactions- enantioselective, diastereoselective (topos, face, mer differentiating reactions) **[3L]** 4.3 Principles of asymmetric synthesis, kinetic and thermodynamic control, asymmetric induction, chiron approach, single and double	**15L**

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	stereodifferentiation, control of molecular orientation and conformation **[4L]** 4.4 Asymmetric aldol condensation- substrate control, reagent control & double stereo differentiation, Sharpless epoxidation, enantioselective reduction of carbonyls- BINAL-H, chiral borane reagents, chiral oxazaborolidine reagents (CBS) **[4L]**	

Standard References:

Unit I

1. Modern Physical Organic Chemistry, Anslyn, E. V., & Dougherty, D. A. (2005),University Science Books.
2. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi

Unit II

3. Modern Physical Organic Chemistry, Anslyn, E. V., & Dougherty, D. A. (2005),University Science Books.
4. Supramolecular Chemistry: Concepts and Perspectives, J.-M. Lehn, VCH, Weinheim, 1995
5. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, John Wiley & Sons, Chichester, 2009.

Unit III& IV

6. Stereochemistry: A Three Dimensional Insight, Anil V. Karnik, Mohammed Hasan, First edition, 2021, Elsevier Publisher
7. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. 4th Edition, New International Publishers Ltd
8. Stereochemistry of Carbon Compounds, E.L Eliel, S.H Wilen and L.N Manden, Wiley
9. Dynamic Stereochemistry of Chiral Compounds: Principles & Applications, Chirstian Wolf,Cambridge, UK: RSC Publisher, 2008.

Additional References:

10. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
11. Mechanism and theory in Organic Chemistry, T. H. Lowry and K.C. Richardson, Harper and Row
12. Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
13. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.
14. Organic Chemistry, Part A and B, Fifth edition,2007, Francis A.Carey and Richard J. Sundberg, Springer
15. Organic reactive intermediates, Samuel P. MacManus, Academic Press.
16. Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).
17. Organic Chemistry, Seventh Edition, R.T. Morrison, R. N. Boyd & S. K. Bhattacharjee, Pearson.
18. Advanced Organic Chemistry: Reactions & Mechanisms, second edition, B. Miller and R. Prasad, Pearson.
19. Organic reactions & their mechanisms, third revised edition, P.S. Kalsi, New Age International Publishers.
20. Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012

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21. Organic Chemistry, W. G. Solomons, C. B. Fryhle, , 9th Edition, Wiley India Pvt. Ltd.,2009.
22. Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
23. Pericyclic reactions, Ian Fleming, Oxford university press, 1999
24. Organic chemistry, 8th edition, John McMurry
25. Modern methods of Organic Synthesis, 4th Edition W. Carruthers and Iain Coldham, Cambridge University Press 2004
26. Stereochemistry, P. S. Kalsi, 4th edition, New Age International Ltd
27. Organic Stereochemistry, M. J. T. Robinson, Oxford University Press, New Delhi, India edition, 2005

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

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Program: M.Sc. Chemistry
(Organic)

Course: Organic Syntheses
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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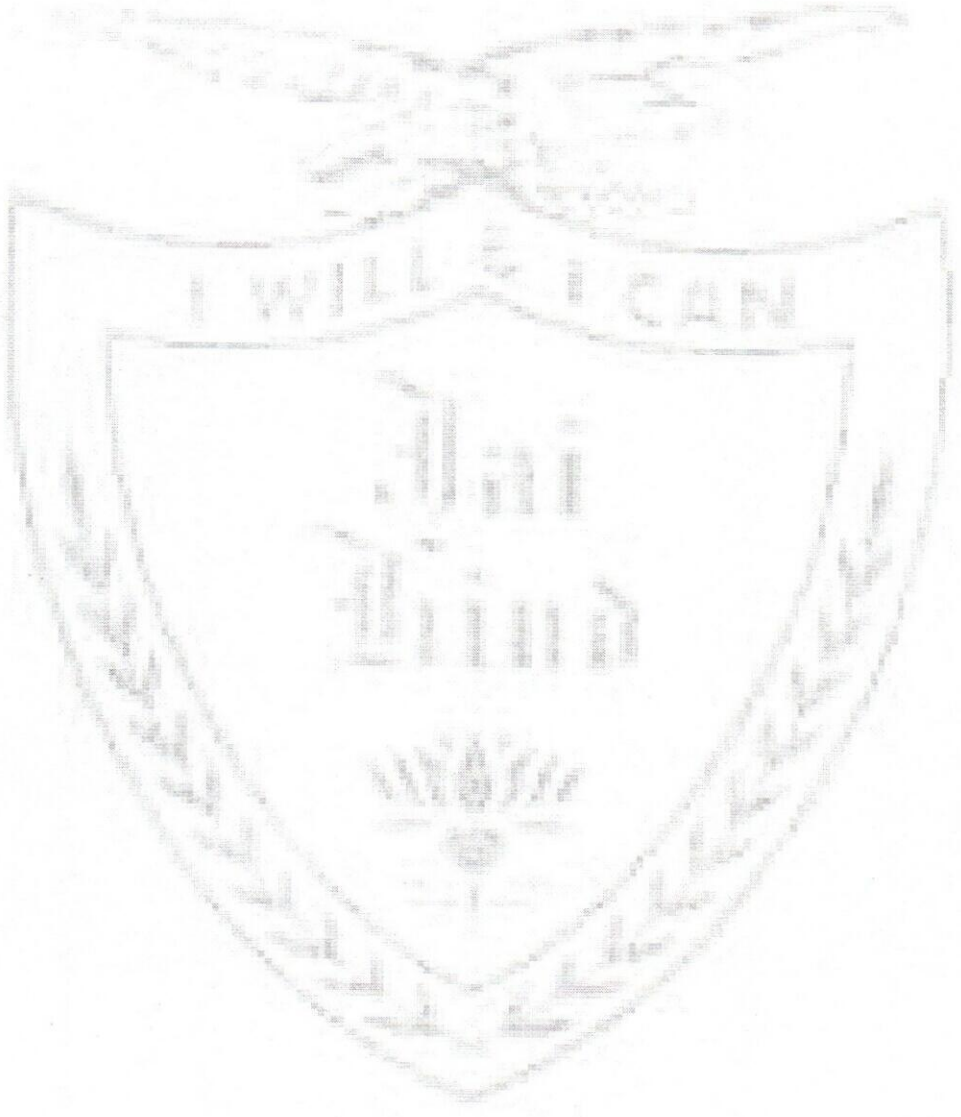
M.Sc. Organic Syntheses Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP3401	Organic Syntheses	02	02



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Semester IV – Practical

Course: PSCHEP3401	**Organic Syntheses** **(Credits: 02, Practicals/Week: 02)**
	Objectives: **To understand the methods of organic synthesis and principles of purification techniques.** **Outcomes:** **To synthesize organic compounds and purify it.**
	PSCHEP3401 **Organic synthesis** 1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography) 2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation) 3. Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography) 4. Preparation of 3-nitroaniline from 1,3-dinitrobenzene. (Purification by column chromatography) 5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation). 6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation). 7. Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation). 8. Preparation of phenyl acetate from phenol. (Purification by vacuum distillation) 9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation) 10. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography) 11. Preparation of fluorenone from fluorene. (Purification by column chromatography) 12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation) **(Minimum 8 experiments)** **NOTE:** 1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS**(ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product. 2. Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

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	REFERENCES: 1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000. 2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd 3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications 4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York 5. Vogel's Textbook of Practical Organic Chemistry, 5th Edition, B. S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, Pearson Education 6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall 7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath 8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold 9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold 10. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers 11. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011

Evaluation Scheme

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

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

Affiliated to
University of Mumbai

Program: M.Sc. Chemistry
(Organic)

Course: Synthetic Organic Chemistry II
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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M.Sc. Synthetic Organic Chemistry II Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHE3402	**Synthetic Organic Chemistry II**	**04**	**04**

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Semester IV – Theory

Course: PSCHE3402	**Synthetic Organic Chemistry-II (Credits: 04 Lectures/Week: 04)**	
	Retrosynthetic analysis, use of enamines and ylides in C-C bond forming reactions, CH activation & functionalization and some special techniques in organic synthesis.	
	Objectives: **1. To introduce the concept of Retrosynthesis.** **2. To explain the generation and applications of enamines, ylides in organic synthesis.** **3. To understand the mechanisms of CH activation.** **4. To introduce the special techniques in Organic synthesis.** **Outcomes:** **1. To describe the concept of umpolung (Reversal of polarity).** **2. To discuss the generation and applications of enamines, ylides in organic synthesis.** **3. To exemplify the application of CH activation.** **4. To describe the application of microwave assisted organic synthesis and Sonochemistry.**	
Unit I	**Retrosynthetic Analysis & designing of synthesis:** 1.1 **Protecting groups in Organic Synthesis:** Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications **[3L]** 1.2 **Concept of umpolung (Reversal of polarity)**:Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers **[4L]** 1.3 **Introduction to Retrosynthesis**: An introduction to Target molecule, synthons, synthetic equivalents, alternating polarity disconnection, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR)**[3L]** 1.4 **Strategies for one and two group disconnections**: Order of events in organic synthesis, choosing a disconnection-simplification, symmetry, high yielding steps, recognisable starting material, Use of protecting groups, Chemoselectivity, Regioselectivity, stereoselectivity (with applications). Retrosynthesis of some natural products **[5L]**	**15L**
Unit II	**Enamines, Ylides & α-C-H functionalization** 2.1 **Enamines:** Generation & application in organic synthesis with mechanistic pathways, Stork enamine reaction. Reactivity, comparison between enamines and enolates. Synthetic reactions of	**15L**

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	enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines. **[4L]** 2.2 **Phosphorus, Sulfur and Nitrogen Ylides:** Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination. **[6L]** 2.3 **α-C-H functionalization:** By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth–Gilbert homologation, Steven's rearrangement. **[5L]**	
Unit III	**C-H activation and functionalization** 3.1 **Introduction & challenges in CH activation:**Definitions of CH activation and functionalisation, history of CH activation, CH activation and green chemistry, biomimetic approach; CH bond dissociation energies (BDEs), selectivity in CH activation.**[3L]** 3.2 **Mechanisms of CH activation:** Outer sphere and inner sphere mechanisms for CH activation; outer sphere- metalloradical/rebound mechanism & metal-carbene & metal-nitrene insertions; inner sphere- sigma complex versus agnostic interactions; forward and reverse CT (electrophilic and nucleophilic processes); Electrophilic substitution (S_EAr), Oxidative addition, Sigma bond metathesis, 1,2-Addition**[6L]** 3.3 **Metals and Directing groups (DGs):** Metals used for CH activation, types of DG- strongly and weakly coordinating, mono and bidentate ligands, non-removable/removable/traceless DG **[4L]** 3.4 **Applications of CH activation:** $C(sp^3)$-H, $C(sp^2)$-H, C(sp)-H activation, Arene functionalization, remote CH functionalization, latestage transformations & total synthesis of natural products **[2L]**	**15L**
Unit IV	**Special Techniques in Organic Synthesis** 4.1 **Phase Transfer Quaternary salts:** Definition, types, mechanism, advantages, preparation of PTC, types of phase transfer reactions, applications of PTC in organic synthesis. **[3L]** 4.2 **Crowns:** Introduction, nomenclature, crown ethers, azacrown & cryptands, special features, nature of donor site, general synthesis of crowns, synthetic applications. **[3L]** 4.3 **Microwave assisted organic synthesis:** Introduction, microwave heating, microwave reactor and solvents used, advantages and limitations of microwave synthesis, applications of microwave in organic synthesis.**[3L]** 4.4 **Sonochemistry**: Introduction, generation of ultrasound, cavitation	**15L**

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	effects, localized hotspots and reaction rates, sonochemical reactions- homogenous reactions, heterogeneous liquid-liquid reactions, heterogeneous solid-liquid reactions; applications of ultrasound in organic synthesis. **[3L]** 4.5 **Polymer supported reagents and synthesis**: Introduction to polymer supports, advantages, choice of polymers, applications of polymer supports in synthesis- type 1 (substrate bound to polymer); type 2 (reagent bound to polymer), type 3 (polymer supported catalytic reactions) **[3L]**	

Standard References:

Unit I

1. Warren, S. G., & Wyatt, P. (2008). *Organic synthesis: The disconnection approach*. Oxford: Wiley-Blackwell.
2. Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).

Unit II

3. Organic Chemistry, J. Clayden, S. Warren, N. Greeves, P. Wothers, 1st Edition, Oxford University Press (2001).
4. Carruthers, W. (1978). *Some modern methods of organic synthesis*. Cambridge: Cambridge University Press.

Unit III

5. Goldberg, K. I., & American Chemical Society. (2004). *Activation and functionalization of C-H bonds*. Washington, D.C: American Chemical Society.
6. Li, J. J. (2015). *C-H bond activation in organic synthesis*. CRC Press
7. Maiti, D., & In Guin, S. (2021). *Remote C-H bond functionalizations: Methods and strategies in organic synthesis*. Wiley-VCH

Unit IV

8. Ahluwalia, V. K., & Aggarwal, R. (2006). *Organic synthesis: Special techniques*. Oxford, UK: Alpha Science International.

Additional References:

9. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
10. Mechanism and theory in Organic Chemistry, T. H. Lowry and K.C. Richardson, Harper and Row
11. Organic Reaction Mechanism, 4th edition, V. K. Ahluvalia, R. K. Parashar, Narosa Publication.
12. Reaction Mechanism in Organic Chemistry, S.M. Mukherji, S.P. Singh, Macmillan Publishers, India.
13. Organic Chemistry, Part A and B, Fifth edition,2007, Francis A.
14. Carey and Richard J. Sundberg, Springer
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18. Organic Chemistry: Structure and Function, P. Volhardt and N. Schore, 5th Edition, 2012
19. Organic Chemistry, W. G. Solomons, C. B. Fryhle, 9th Edition, Wiley India Pvt. Ltd.,2009.
20. Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
21. Pericyclic reactions, Ian Fleming, Oxford university press, 1999
22. Organic chemistry, 8th edition, John McMurry

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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. Chemistry
(Organic)

Course: Purification Techniques
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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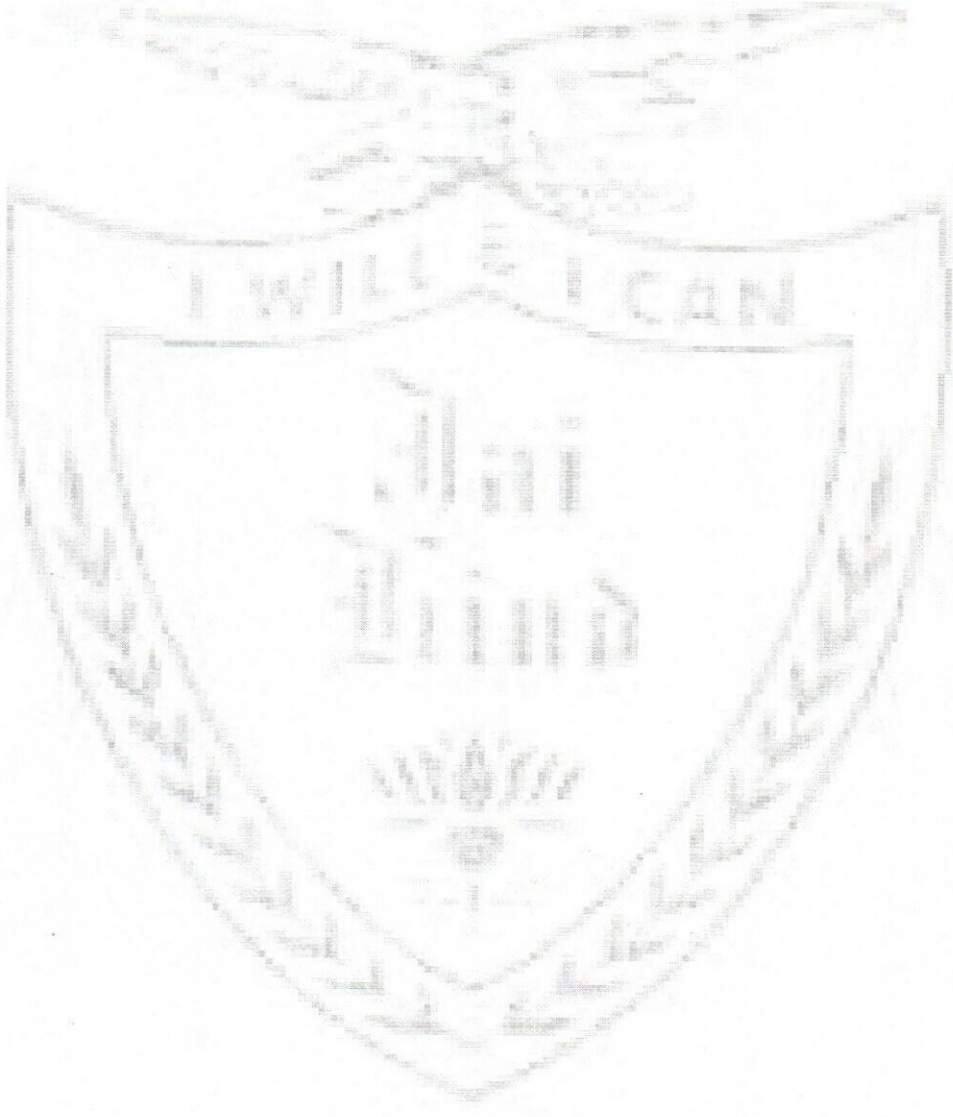
M.Sc. Purification Techniques Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP3402	Purification Techniques	02	02



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Semester IV – Practical

Course: PSCHEP3402	**Purification Techniques** **(Credits: 02, Practical/Week: 02)**
	Objectives: **To understand the methods of organic synthesis and principles of purification techniques.** **Outcomes:** **To synthesize organic compounds and purify it.**
	PSCHEP3402 **Organic synthesis** 1. Preparation of acetanilide from aniline and acetic acid using Zn dust. (Purification by column chromatography) 2. Preparation of 1-nitronaphthalene from naphthalene. (Purification by steam distillation) 3. Preparation of acetyl ferrocene from ferrocene. (Purification by column chromatography) 4. Preparation of 3-nitroaniline from 1,3-dinitrobenzene. (Purification by column chromatography) 5. Preparation of benzyl alcohol from benzaldehyde. (Purification by vacuum distillation). 6. Preparation of methyl salicylate from salicylic acid. (Purification by vacuum distillation). 7. Preparation of 4-methylacetophenone from toluene. (Purification by vacuum distillation). 8. Preparation of phenyl acetate from phenol. (Purification by vacuum distillation) 9. Preparation of 2-chlorotoluene from *o*-toluidine. (Purification by steam distillation) 10. Preparation of 4-nitrophenol from phenol. (Purification by steam distillation/ column chromatography) 11. Preparation of fluorenone from fluorene. (Purification by column chromatography) 12. Preparation of dimethylphthalate from phthalic anhydride. (Purification by vacuum distillation) **(Minimum 8 experiments)** **NOTE:** 1. Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and **safety aspects including MSDS**(ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product. 2. Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

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	REFERENCES: 1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000. 2. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd 3. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications 4. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York 5. Vogel's Textbook of Practical Organic Chemistry, 5th Edition, B. S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, Pearson Education 6. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall 7. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath 8. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold 9. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold 10. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers 11. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011

Evaluation Scheme

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

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

Affiliated to
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Program: M.Sc. Chemistry
(Organic)

Course: Photochemistry and Advanced Spectroscopy
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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M.Sc. Photochemistry and Advanced Spectroscopy Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHE3403	Photochemistry and Advanced Spectroscopy	04	04

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Semester IV – Theory

Course: PSCHE3403	**Photochemistry and Advanced Spectroscopy (Credits:04 Lectures/Week:04)**	
	Photochemistry and photocatalysis, fluorescence phenomenon and its applications, advanced techniques in NMR spectroscopy & mass spectrometry	
	Objectives: **1. To introduce the concept of Photochemistry & Photocatalysis.** **2. To understand the principal and application of fluorescence phenomena.** **3. To describe the principal, instrumentation and applications of advanced Spectroscopic Techniques-I& II.** **Outcomes:** **1. To apply the principles of Photochemistry & Photocatalysis in water splitting, CO_2 reductions etc.** **2. To describe the phenomena and mechanism of fluorescence quenching.** **3. To elucidate the structure of molecules applying advanced Spectroscopic Techniques-I & II.**	
Unit I	**Photochemistry & Photocatalysis** **1.1 Photochemistry [8L]** 1.1.1. **General Introduction:** Laws of photochemistry, selection rules for transitions, shapes of absorption bands and Frank Condon Principle. 1.1.2. **Properties of excited state:** Environmental effect on absorption and emission spectra, solvatochromic shifts, properties of excited state- dipole moment, acidity constant, redox potential. 1.1.3. **Photophysical pathways:** types of photophysical pathways, types of radiationless transitions, fluorescence emission, triplet state and phosphorescence, delayed fluorescence: e-type and p-type. **1.2 Photocatalysis [7L]** 1.1.4. **Photocatalytic activity:** Photocatalytic reactions, mechanism, influence of different parameters on catalytic activity. 1.1.5. **Types of photocatalysts:** SMOs (TiO_2, ZnO), metal chalcogenides (MoS_2, WS_2), quantum dots (C, S), mesoporous materials for photocatalysis and their synthesis (one each) 1.1.6. **Application of photocatalysis:** photodegradation of organic pollutants, CO_2 photoreduction, water splitting.	**15L**
Unit II	**Applications of Fluorescence Phenomena** 2.1. **Introduction & Fluorescence Characteristics:** Fluorescence phenomenon, Characteristics of fluorescence- mirror image rule,	**15L**

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	exceptions, Kasha's Rule; Stokes shift, fluorescence lifetimes and quantum yields, steady state fluorescence and fluorescence anisotropy **[2L]** 2.2. **Structural effects on Fluorescence emission:** π-electron system, substituted aromatic hydrocarbons- internal heavy atom effect, EDG, EWG, Sulfonates, heterocyclic compounds- Nitrogen heterocycles, coumarins, BODIPY; Luminescence of nanostructures- carbon nanostructures, quantum dots. **[2L]** 2.3. **Fluorescence quenching**: mechanism of quenching- static and dynamic; derivation of Stern-Volmer equations for static and collisional quenching, quenching by added substances- charge transfer mechanism (CT) and energy transfer mechanism (RET) **[3L]** 2.4. **Instrumentation and sensing:** instrumentation of a steady state spectrofluorophotometer, modes of measurement- fixed excitation wavelength, fixed emission wavelength, fixed excitation and emission wavelength, variable excitation and emission wavelengths- 3D spectrum, synchronous spectrum; analytical terms associated with sensing- sensitivity, selectivity & ICH guidelines- LOD, LOL, dynamic range **[4L]** 2.5. **Applications of Fluorescence:** Sensing modes and mechanisms, Photoinduced Electron Transfer (PET), Photoinduced Charge Transfer (PCT); design of sensor; miscellaneous applications of fluorescence **[4L]**	
Unit III	**Advanced Spectroscopic Techniques-I** 3.1 **Basic Concepts in NMR:** Nuclear spin states, magnetic moments, absorption of energy, mechanism of absorption, population densities of nuclear spin states, chemical shift and shielding, NMR spectrometer- CW v/s FT NMR **[4L]** 3.2 **Spin-spin coupling:** spin-spin splitting (n+1) rule, origin of spin-spin splitting and Pascal's triangle, coupling constant J, mechanism of coupling, Karplus relationship, long range coupling, magnetic equivalence, first order splitting and complex multiplets- more than one value of J, second order spectra and Pople spin notations; second order effects and field strength of NMR. **[5L]** 3.3 **^{13}C & Heteronuclear NMR:** ^{13}C nucleus, chemical shifts, proton coupled and decoupled ^{13}C NMR, NOE & cross polarization, molecular relaxation processes & integration of spectra, Off-resonance decoupling, solvents used in NMR; ^{19}F, ^{31}P, ^{11}B NMR; heteronuclear coupling of ^{13}C with fluorine and phosphorus. **[4L]** 3.4 **Other topics in 1D NMR:** proton exchange, dynamic NMR, quadrupole broadening of NH protons **[2L]**	**15L**

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Unit IV	**Advanced Spectroscopic Techniques II:** 4.1 **Pulsed techniques in NMR:** FT-NMR, Attached Proton Test (APT), INEPT & DEPT **[4L]** 4.2 **2D NMR techniques:** Homonuclear 2D NMR- COSY, NOESY; Heteronuclear 2D NMR- HETCOR, HSQC, HMQC, HMBC **[4L]** 4.3 **Mass spectrometer:** Overview, block diagram & sample introduction **[1L]** 4.4 **Ionization methods:** Electron ionization (EI); Chemical ionization (CI); Desorption ionization methods (SIMS, FAB, MALDI); Electron spray ionization (ESI) **[3L]** 4.5 **Mass analyzers:** Magnetic sector, double focusing, Quadrupole, TOF; detection and quantitation; determination of molecular weight & molecular formulae **[3L]** **Spectral problems:** Application of NMR & Mass Spectrometry in structure elucidation.	**15L**

Standard References:

Unit I

1. Rohatgi-Mukherjee, K. K. (1992). Fundamentals of photochemistry. New Delhi: Wiley Eastern Ltd.
2. Photocatalysis- Principles and Applications, Rakshit Ameta, Suresh C.Ameta, CRC Press, Taylor &Francis group, Boca Raton, London, New York, 2017.
3. Zhang, J., Tian, B., Wang, L., Xing, M., Lei, J. - Photocatalysis_ Fundamentals, Materials and Applications-SPRINGER VERLAG, SINGAPORE (2018)

Unit II

4. Lakowicz, J. R. (2006). Principles of fluorescence spectroscopy. New York: Springer.
5. Valeur, B. (2002). Molecular fluorescence: Principles and applications. Weinheim: Wiley-VCH.

Unit III & IV

6. Pavia, D. L., Lampman, G. M., & Kriz, G. S. (1979). Introduction to spectroscopy: A guide for students of organic chemistry. Philadelphia: W.B. Saunders Co
7. Field, L. D., Li, H. L., & Magill, A. M. (2015). Organic structures from 2D NMR spectra.

Additional References:

8. Spectroscopy of Organic compounds, P.S. Kalsi, New Age International Pub. Ltd. And Wiley Eastern Ltd., Second edition, 1995.
9. Applications of Absorption Spectroscopy of Organic compounds, J. R. Dyer, Prentice Hall of India, 1987.
10. Spectrometric Identification of Organic compounds, R.M. Silverstein and others, John Wiley and Sons Inc., 5th ed., 1991
11. Absorption spectroscopy of organic Molecules, V.M. Parikh, 1974.
12. Spectroscopic methods in organic chemistry, Williams and Fleming, Tata McGraw Hill, 4th ed, 1989.
13. Organic spectroscopy, William Kemp, ELBS, 3rd ed., 1987.

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

Affiliated to
University of Mumbai

Program:M.Sc. Chemistry
(Organic)

Course: Spectral Interpretation
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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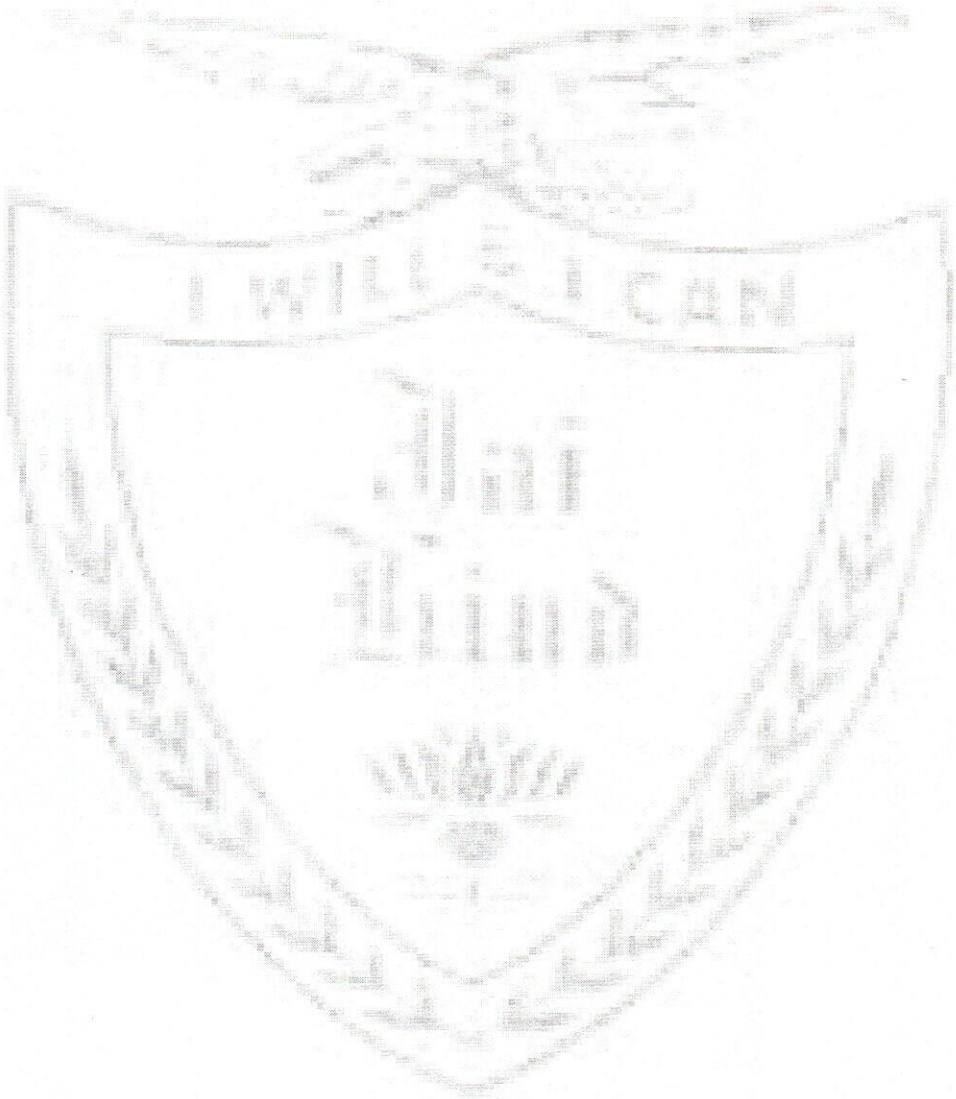
M.Sc. Spectral Interpretation Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP3403	Spectral Interpretation	02	02



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Semester IV – Practical

Course: PSCHEP3403	Spectral Interpretation (Credits: 02, Practical /Week: 02)
	Objectives: **To elucidate structural information about molecules from their spectral data.** **Outcomes:** **Learner will be able to interpret of UV/IR/NMR/Mass/XRD spectra and its analysis.**
	PSCHEP3403: Spectral Interpretation Interpretation of Uv/IR/NMR/Mass/XRD spectra and its analysis. REFERENCES: 1. Jeffery G.H., Bassett J., Mendham J., Denney R.C., Vogel's Textbook of Quantitative Chemical Analysis, 5th Edition, Longman Scientific & Technical John Wiley & Sons Inc., New York, 1989

Evaluation Scheme

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

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Program:M.Sc. Chemistry
(Organic)

Course: Materials, Devices and Computational Chemistry
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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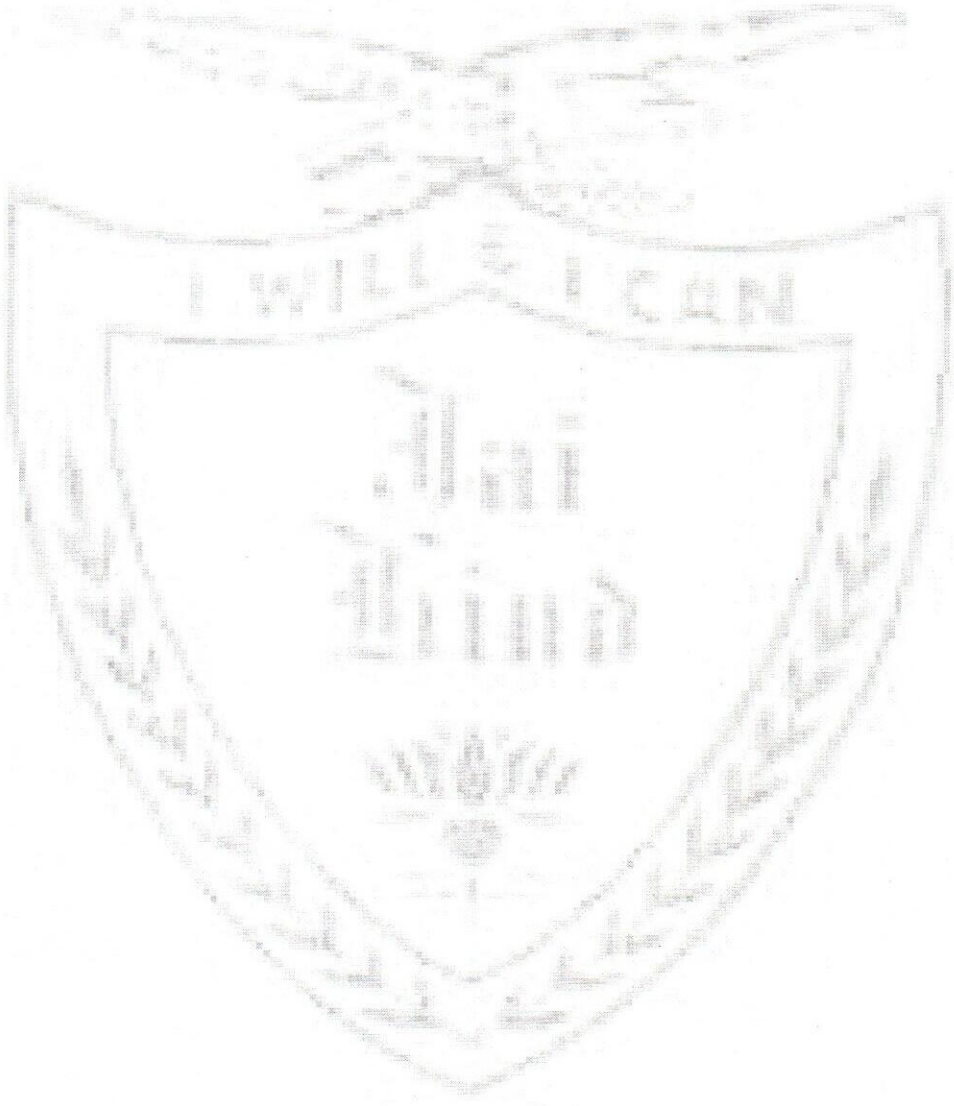
M.Sc. Materials, Devices and Computational Chemistry Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHE3404	**Materials, Devices and Computational Chemistry**	**04**	**04**



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Semester IV – Theory

Course: PSCHE3404	**Materials, Devices and Computational Chemistry (Credits:04 Lectures/Week:04)**	
	Solar photovoltaics, batteries and supercapacitors, organic electronic and photonic materials, Intellectual Property Rights & Cheminformatics	
	Objectives: **1. To describe different photovoltaic cells and its applications in batteries and supercapacitors.** **2. To introduce the concept of organic semiconductors, optoelectronic devices.** **3. To introduce the of Intellectual Property Rights & Cheminformatics.** **Outcomes:** **1. To identify different type photovoltaic cells and its applications in batteries and supercapacitors.** **2. To explain the working of organic semiconductors, optoelectronic devices.** **3. To describe Intellectual Property Rights & Chemoinformatics.**	
Unit I	**Energy Conversion and Storage Devices** 1.1. **Solar Photovoltaics:** P-n junction, light generating current, I-V equation, solar characteristics, effects of various parameters on efficiency, losses in solar cells, Solar cell design, Antireflective coating (ARC), solar simulator, Quantum efficiency. **[5L]** 1.2. **Sensitized and polymer photovoltaics:** DSSC, Quantum dot sensitised solar cells, Perovskite sensitised solar cells, Planar and bulk heterojunction polymer solar cells, Exciton generation and dissociation, Advantages, disadvantages, and types of materials. **[4L]** 1.3. **Batteries and Supercapacitors:** Recapitulation of batteries: primary batteries, rechargeable batteries, electrochemical energy storage: laws, parameters, heat effects. Types of batteries (Lead-acid, Ni/Cd, Ni/metal hybrid), charging methods and techniques, characteristic curves, comparison of supercapacitor and batteries, Energetics, Double layer electrostatic capacitor, Pseudocapacitance, Impedance, materials for supercapacitors. **[6L]**	**15L**
Unit II	**Organic Electronic & Photonic Materials [15L]** 2.1 **Introduction:** Brief history of organic electronics, organic semiconductor materials, electronic states, and transitions **[2L]** 2.2 **Organic semiconductors:** Charge formation- By injection, By absorption, By doping; determining energy levels of charged molecules- cyclic voltammetry, photoemission spectroscopy; difference between electrical and optical gap; **[5L]**	**15L**

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	2.3 **Semiconductor materials:** Transport in organic materials- electrode contacts, transport regimes & magnetic field effects on transport; preparation of semiconductor materials- synthetic approaches, preparation of thin films & patterning for devices **[3L]** 2.4 **Optoelectronic devices:** Basic processes- photon absorption, spontaneous photon emission, stimulated photon emission; Devices- OFET, OPV, OLED; molecular materials for OLEDs- hole transporting, electron transporting, emitting materials: fluorescent, phosphorescent & TADF. **[5L]**	
Unit III	**Intellectual Property Rights [15L]** 3.1 **Introduction to Intellectual Property:** Definitions and types of IP, importance of protecting IP, economic value of IP- intangible assets and their valuation, licensing, and technology transfer laws. **[2L]** 3.2 **Patents:** Definition, Historical perspective, Basic and associated right, WIPO, PCT system, databases in patent search- google patents, reading and writing patents **[5L]** 3.3 **Industrial Designs:** Definition, how to obtain, features, international design registration **[2L]** 3.4 **Copyrights:** Introduction, how to obtain, differences from Patents **[2L]** 3.5 **Trademarks:** Introduction, how to obtain, different types of marks- collective marks, certification marks, service marks, trade names etc. **[2L]** 3.6 **Geographical indications:** Definition, rules for registration, prevention of illegal exploitation, importance to India. **[2L]**	**15L**
Unit IV	**Cheminformatics [15L]** 4.1 **Introduction to Cheminformatics:** History & evolution of cheminformatics, fundamental questions & learning, major tasks **[2L]** 4.2 **Representation of molecules:** Nomenclature, different types of notations, Line notations- SMILES coding, InChi notation; Graph theory & matrix representations, input and output of chemical structures, standard structure exchange formats, structures of molfiles and sdfiles, Tools- academic programs: Marvin Sketch, ACD labs; commercial tools: ChemDraw, Shrodinger, Accelrys **[5L]** 4.3 **Representation of chemical reactions:** Reaction types, reaction center, chemical reactivity, Hendrickson's scheme **[2L]** 4.4 **Searching Chemical Structures:** Full structure search, sub-structure search, basic ideas, similarity search, basics of computation of physical and chemical data and structure	**15L**

	descriptors, data visualisation **[2L]** 4.5 **Applications:** QSPR, Spectra correlations, Computer aided synthesis design, docking & computer aided drug designing **[4L]**	

Standard References:

Unit I

1. https://www.pveducation.org/pvcdrom/solar-cell-operation
2. Solar photovoltaics, Fundamentals, Technologies and Applications by Chetan Singh Solanki, PHI Learning Private Limited, Delhi-110092.
3. Dye Sensitized Solar Cells by K. Kalyansundaram, EPFL Press, A Swiss academic publisher distributed by CRC press.
4. Battery Technology Handbook by H. A. Kiehne , Marcel Dekker, Inc. , New York, Basel.
5. Electrochemical Supercapacitors, Scientific fundamentals and Technological Applications by B. E. Conway, Kluwer Academic/ Plenum Publishers, New York,Boston, Dordrencht, London, Moscow.

Unit II

6. Kohler, A., & Bassler, H. (2015). *Electronic processes in organic semiconductors: An introduction.*
7. Muller, T. J. J., & Bunz, U. H. F. (2007). *Functional organic materials: Syntheses, strategies and applications*. Weinheim: Wiley-VCH.
8. Ostroverkhova, O. (2019). *Handbook of organic materials for electronic and photonic devices.*
9. Sun, S.-S., & In Dalton, L. R. (2019). *Introduction to organic electronic and optoelectronic materials and devices.*

Unit III

10. Duran, N., Fonseca, L. C., & Seabra, A. B. (2019). *Intellectual property in chemistry: A guide to applying for and obtaining a patent for graduate students and postdoctoral scholars.*

Unit IV

11. Gasteiger, J., & Engel, T. (2008). *Cheminformatics: A textbook*. Weinheim: Wiley-VCH.
12. Andrew R. Leach & Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.
13. Karthikeyan, M., & Vyas, R. (2014). *Practical cheminformatics.*
14. In Engel, T., & In Gasteiger, J. (2018). *Applied cheminformatics: Achievements and future opportunities.*

Evaluation Scheme

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  - 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
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Program:M.Sc. Chemistry
(Organic)

Course: Research Project
Semester IV

Credit Based Semester and Grading System (CBSGS) with effect from the academic year 2022-23

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M.Sc. Research Project Syllabus

Semester IV			
Course Code	**Course Title**	**Credits**	**Lectures/Week**
PSCHEP3404	Research Project	02	02

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Semester IV – Practical

Course: PSCHEP3404	**Research Project (Credits: 02, Practicals/Week: 02)**
	Objectives: **To design a research problem and investigate it experimentally through project.** **Outcomes:** **Learners will be able to understand research workflow- literature review, identification of research problem and investigation.**
	PSCHEP3404: Research Project Short term research project culminating in a dissertation and presentation of the work done.

Evaluation Scheme

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

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