School: Science	Programme: Master of Science (M.Sc.) in Organic Chemistry
Year : Second Year	**Semester - III**
Course: Spectroscopic Methods in Structure Determination	**Course Code: PCH301**
Theory: 4 Hrs/Week	**Max. University Theory Examination: 50 Marks**
Max. Time for Theory Exam.: 3 Hrs	**Continuous Internal Assessment: 50 Marks**

Objectives		
1	To study ^{1}H NMR, ^{13}C NMR, 2D NMR and Mass Spectrometry.	
2	Applications of spectroscopic techniques for structure determination.	
Unit Number	**Details**	**Hours**
1	**^{1}H NMR Spectroscopy** Chemical shift, factors influencing chemical shift, deshielding, chemical shift values and correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and other nuclei (alcohols, phenols, enols, acids, amides and mercaptans), chemical exchange, effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant "J", classification of spin system like AB, AX, AX_2, ABX, AMX, ABC, A_2B_2. Spin decoupling, factors affecting coupling constant, simplification of complex spectra, nuclear magneticdouble resonance, spin decoupling, contact shift reagents, solvent effects, nuclear overhauser effect (NOE), resonance of other nuclei like 31P, 19F.	**18**
2	**^{13}C NMR spectroscopy** FT NMR, Types of ^{13}C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, Homo nuclear (13C - 13C) and Hetero nuclear (13C - 1H)coupling constants .	**12**
3	**2D NMR Techniques** General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)-Homo COSY (1H-1H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.	**6**
4	**Mass Spectrometry**	**12**

	Instrumentation, various methods of ionization (field ionization, field desorption, SIMS , FAB , MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupoulemass filter, timeof flight (TOF). Rules of fragmentation of different functional groups, factors controlling fragmentation.	
5	Problems based on joint application of UV, IR, PMR, CMR and Mass. (Including reaction sequences)	**12**
	Total	**60**

Resources	
Reference Books	1. Introduction to Spectroscopy by D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers). 2. Spectrometric identification of organic compounds by R. M . Silverstein, F. X. Webster, 6th Ed. John Wiley and Sons. 3. Spectroscopic methods in organic chemistry by D. H. Williams and I. Flemming, Mc Graw Hill. 4. Absorption spectroscopy of organic molecules by V. M . Parikh. 5. Nuclear Magnetic Resonance– Basic Principles by Atta-Ur-Rehman, Springer-Verlag (1986). 6. One and Two dimensional NMR Spectroscopy by Atta-Ur-Rehman, Elsevier (1989). 7. Organic structure Analysis by Phillip Crews , Rodriguez, Jaspars, Oxford University Press (1998). 8. Organic structural Spectroscopy by Joseph B.Lambert, Shurvell, Lightner, Cooks, PrenticeHall (1998). 9. Organic structures from spectra by Field L.D., KalmanJ . R. and Sternhell S. 4th Ed. John Wiley and sons Ltd. 10. Spectroscopic identification of organic compound by R M Silverstein, G C Bassler and T C Morril , John Wiley. 11. Introduction to NMR spectroscopy by R J Abrahm, J Fisher and P loftus Wiley. 12. Organic spectroscopy by William kemp, E L B with McMillan. 13. Spectroscopy of organic molecule by PS Kalsi,Wiley, Esterna, New Delhi. 14. Organic spectroscopy by RT Morrison and RN Boyd. 15. Practical NMR spectroscopy by ML Martin, J JDelpench, and D J Martyin. 16. Spectroscopic methods in organic chemistry by D H Willson, I Fleming. 17. Spectroscopy in organic chemistry by C N R Rao and J R Ferraro. 18. NMR –Basic principle and application by H Guntur. 19. Interpretation of NMR spectra by Roy H Bible. 20. Mass spectrometry organic chemical applications by J H Banyon

School: Science	Programme: Master of Science (M.Sc.) in Organic Chemistry
Year : Second Year	**Semester - III**
Course: Organic Reaction Mechanism, Stereochemistry and Natural Products	**Course Code: PCH302**
Theory: 4 Hrs/Week	**Max. University Theory Examination: 50 Marks**
Max. Time for Theory Exam: 3 Hrs	**Continuous Internal Assessment: 50 Marks**

Course Objectives	
1	To study a stereochemistry of six membered rings
2	To study a circular dichroism (CD) and optical rotatory dispersion (ORD)
3	Determination of stereochemistry organic compounds using NMR.
4	To study a natural product chemistry.

Unit Number	Details	Hours
1	**Carbanions :**Formation, stability and related name reactions.	**9**
2	Stereochemistry of six membered rings.	**14**
3	Fused Bridged and caged rings resolution of racemic modification**.**	**14**
4	**CD and ORD** Determination of stereochemistry organic compounds using NMR.	**9**
5	**Natural Products:** Structure and stereochemistry of Hardwickiic acid, Camptothecin and podophyllotoxin.Synthesis of Taxol	**14**
	Total	**60**

Resources	
Reference Books	1. Mechanism and structure in organic chemistry by E. S. Gould (Holt, Rinehart and Winston). 2. Advanced Organic Chemistry by J. March, 6th edition. 3. Advanced Organic Chemistry by F. A. Carey and R. J. Sundberg, 5th edition, Springer, **2007**. 4. A guidebook to mechanism in organic chemistry by Peter Sykes, 6th edition, Ed. Orient Longman. 5. Organic Chemistry by J .Clayden, N. Greeves, S. Warren and P. Wothers, Oxford UniversityPress, **2001**. 6. Stereochemistry of carbon compounds by E. L. Eliel.

	7. Stereochemistry of organic compounds by Nasipuri. 8. Stereochemistry of organic compounds-Kalsi. 9. Organic stereochemistry by Jagdamba Singh. 10. Principles of organic synthesis by R. O. C. Norman and J. M .Coxon; Chapman and Hall. 11. Classics in organic synthesis – K. C. Nicolaou& E. J. Sorensen. 12. J.IndianInst.Sci. 81,287 (2001). 13. Medicinal Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd Ed.(Wiley). 14. Secondary metabolism - J. Mann, 2nd edition. 10. Chemical aspects of Biosynthesis – J. Mann (1994). 15. i) J.C.S. Perkin Transactions II, 288-292, (1973). ii) J.Am.Chem.Soc. Vol.77.432-437, (1955).

School: Sciences	Programme: Master of Science (M.Sc.) in Organic Chemistry
Year : Second Year	**Semester - III**
Course: Pericyclic Reactions, Photochemistry and Heterocyclic Chemistry	**Course Code: PCH303**
Theory: 4 Hrs/Week	**Max. University Theory Examination: 50 Marks**
Max. Time for Theory Exam.: 3 Hrs	**Continuous Internal Assessment: 50 Marks**

Course Objectives	
1	Introduction, general principles and applications of photochemistry in organic chemistry
2	To study a pericyclic reactions
3	To study a various heterocyclic compounds-Synthesis, reactivity and importance

Unit Number	Details	Hours
1	**Photochemistry** General basic principles, photochemistry of carbonyl compounds, alkenes ,dienes, polyenes and aromatic compounds, photorearrangements, Barton reaction. Application of photochemical reactions in synthesis– Isocomene, Cedrene	**14**
2	**Pericyclic reactions** Electrocyclic, cycloaddition, sigmatropicand ENE reactions, 1,3-dipolar additions, Analysis by correlation diagrams, FMO approach and ATS concept. Application ofpericyclic reactions.	**14**
3	**a) Five and six membered heterocycles with one and two hetero atoms :** Synthesis, reactivity, aromatic character and importance of following heterocyclic rings : Furan, Pyrrole, Thiophene, Pyrazole, Imidazole, Pyridine, Pyrimidine. b) **Condensed five and six membered heterocycles** : Benzofuran, Indole, Benzothiophene, Quinoline	**14**
4	**Condensed five membered heterocycles :** Benzoxazole, Benzthiazole, Benzimidazole	**9**
5	**Five and six membered heterocycles with more than two hetero atoms** : Synthesis, reactivity, aromatic character and importance of following heterocycles: 1,2,3-triazole, 1,2,4-triazole, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, tetrazole,	**9**
	Total	**60**

Resources	
Reference Books	1. Advanced Organic Chemistry, Part A by F. A. Carey and R. J .Sundberg, 5th Ed. Springer (2007). 2. Excited states in Organic Chemistry by J.A. Barltrop and J.D.Coyle, John Wiley & sons. 3. Photochemistry and pericyclic reactions by Jagdamba Singh, Jaya Singh 3rd Ed. 4. Organic photochemistry: A visual approach by Jan Kopecky, VCHpublishers(1992). 5. Conservation of orbital symmetry by R. B. Woodward and R. Hoffmann; VerlagChemie, Academic press (1971). 6. Orbital Symmetry : A problem solving approach by R. E. Lehr and A. P . Marchand;Academic (1972). 7. Organic reactions and orbital symmetry by T. L. Gilchrist and R. C .Storr;2nd edition, Cambridge, University Press. 8. Classics in total synthesisby K. C. Nicolaou and E. J . Sorensen; VHC (1996). 9. P. A. Wender and J . J. Howbert*J. Am. Chem. Soc*. 103, 688-690 (1981) 10. Pericyclic reactions : A text book byS . Sankararaman. 10. Pericyclic reactionsby Gill and Willis7 11. Frontier orbitals and organic chemical reactionsbyIan Fleming, John Wiley & sons. 12. Organic Chemistry byJ. Clayden, N. Greeves , S. Warren and P. Wothers 13. Heterocyclic Chemistry byT. Gilchrist. 14. An introduction to the chemistry of heterocyclic compounds by R M Acheso. 15. Heterocyclic Chemistry by J A Joule and K Mills. 16. Principles of modern heterocyclic chemistry by A Paquette. 17. Heterocyclic ChemistrybyJ A Joule and Smith. 18. Handbook of Heterocyclic Chemistry by A R Katritzky, A F Pozharskii 20. Heterocyclic Chemistry-II- R R Gupta, M Kumar, V Gupta, Springer (India) pvt

School: Sciences	Programme: Master of Science (M.Sc.) in Organic Chemistry
Year : Second Year	**Semester - III**
Course: Designing Organic Synthesis and Asymmetric Synthesis	**Course Code: PCH304**
Theory: 4 Hrs/Week	**Max. University Theory Examination: 50 Marks**
Max. Time for Theory Exam.: 3 Hrs	**Continuous Internal Assessment: 50 Marks**

Course Objectives	
1	To study designing of organic synthesis.
2	To understand the principles and applications of asymmetric synthesis.

Unit Number	Details	Hours
1	**Designing of organic synthesis** : Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions as illustrated in the synthesis of polypeptide and polynucleotide, enamines, Umpolung in organic synthesis, Reterosynthesis.	**30**
2	**Principles and applications of asymmetric synthesis :** Stereoselectivity in cyclic compounds, enantio-selectivity, diastereo-s electivity,enatiomeric and diastereomeric excess, stereo selective aldol reactions. Cram's rule,FelkinAnh rule, Cram's chelate model, Asymmetric synthesis, chiral pool strategy, use of chiral auxiliaries,chiral reagents and catalysts, asymmetric hydrogenation, asymmetric epoxidation andasymmetric hydroxylation. Baker Yeast as chiral catalyst.	**30**
	Total	**60**

Resources	
Reference Books	1. Designing of organic synthesis by S. Warren (Wiley). 2. Some modern methods of organic synthesis by W. Carruthers (Cambridge). 3. Organic chemistry byJ .Clayden, N. Greeves , S. Warren and P. Wothers (Oxford Press). 4. Organic synthesis by Michael B . Smith. 5. Advanced organic chemistry, Part B – F. A Carey and R. J .Sundberg, 5th edition (2007).

	6. Guidebook to organic synthesis byR K Meckie, D M Smith and R A Atkin 7. Organic synthesis by Robert E Ireland. 8. Strategic applications of named reactions in organic synthesisbyLaszlo Kurti and Barbara Czako.

School:Science	Programme: Master of Science (M.Sc.) in Organic Chemistry
Year: Second Year	**Semester-III**
Course: Spectroscopic Methods in Structure Determination and Organic Reaction Mechanism Laboratory	**Course Code: PCH311**
Practical: PG –4 Hrs/Batch (20 Students)	**Practical Examination: 50 Marks**
	Term Work: 50 Marks

Objectives	
1	To learn and practice single stage preparations of organic compounds.
2	To learn various synthetic methods and characterization techniques related to organic synthesis.
3	To learn isolation of natural products.

Sr. No.	Description
1	**Single stage preparations (Any Eight)** 1. 2-Phenyl indole (Fischer indole synthesis). 2. 7-Hydroxy -3-methyl flavone (Baker-Venkatraman reaction). 3. Benzyl alcohol and benzoic acid from benzaldehyde (Cannizzaro reaction). 4. 4-Chlorotoluene from p-toluidine (Sandmeyer reaction). 5. Benzilic acid from benzoin (Benzilic acid rearrangement). 6. Benzopinacol (Photochemical reaction). 7. 7-Hydroxy-4-methyl coumarin (Pechmann Reaction). 8. 4-Methyl benzophenone (Friedal Craft reaction). 9. Benzanilide (Beckmann rearrangement). 10. Vanillyl alcohol from vanillin (NaBH4 reduction). 11. 2- and 4-nitrophenols (nitration and separation by steam distillation). 12. Stilbene from benzyl chloride (Wittig reaction). 13. Ethyl cinnamate from benzaldehyde (Wittig reaction). 14. Triphenylor diphenyl methyl carbinol (Grignard reaction). 15. Benzotriazole. 16. 1-Phenyl-3-methyl pyrazol-5-one. 17. Glucose pentaacetate. 18. 2,4-diethoxycarbonyl-3,4-dimethyl pyrrole from ethyl acetoacetate. 19. Quinoline from aniline Skraup synthesis). 20. Benzimidazole from benzyl 21. Cyclohexanol from cyclohexanone (LAH reduction).
2	**Isolation of Natural products** (Any Two) 1. Caffeine from tea leaves (Soxhlet extraction). 2. Piperine from pepper (Soxhlet extraction).

	3. Eucalyptus oil from leaves (Steam distillation). 4. Lycopene from tomatoes. 5. Trimyristin from nutmeg. 6. Cinnamaldehyde from cinnamom. 7. Eugenol from clove

Term Work:
Term Work assessment shall be conducted for the Project, Tutorials and Seminar. Term work is continuous assessment based on work done, submission of work in the form of report/journal, timely completion, attendance, and understanding. It should be assessed by subject teacher of the institute. At the end of the semester, the final grade for a Term Work shall be assigned based on the performance of the student and is to be submitted to the University.

Notes	
1	The experiments from the regular practical syllabus will be performed (30 Marks).
2	The regular attendance of students during the syllabus practical course will be monitored and marks will be given accordingly (10 Marks).
3	Good Laboratory Practices (10 Marks)

Practical/Oral/Presentation:
Practical/Oral/Presentation shall be conducted and assessed jointly by internal and external examiners. The performance in the Practical/Oral/Presentation examination shall be assessed by at least a pair of examiners appointed as examiners by the University. The examiners will prepare the mark/grade sheet in the format as specified by the University, authenticate and seal it. Sealed envelope shall be submitted to the head of the department or authorized person.

Notes	
1	Two experiments from the regular practical syllabus will be conducted. (Total 40 Marks).
2	Complete laboratory journal/records (05 Marks).
3	Viva-voce (05 Marks).

School:Science	Programme: Master of Science (M.Sc.) in Organic Chemistry
Year: Second Year	**Semester-III**
Course: Pericyclic Reactions and Designing Organic Synthesis Laboratory	**Course Code: PCH312**
Practical: PG – 3 Hrs/Batch (20 Students)	**Practical Examination: 50 Marks**
	Term Work: 50 Marks

Objectives	
1	To learn and practice organic synthesis: two stage preparations of organic compounds.
2	To learn various synthetic methods and characterization techniques related to organic synthesis.

Sr. No.	Description
1	**Two stage preparations (any Eight)** 1. Benzaldehyde →Benzalacetophenone → Epoxide 2. 4-Nitro toluene → 4-Nitro benzoic acid → 4-Amino benzoic acid 3. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-Methyl-7-acetoxy coumarin. 4. Cyclohexanone → Phenyl hydrazone → 1,2,3,4-Tetrahydrocarbazole. 5. Hydroquinone → Hydroquinone diacetate → 1,2,4-Triacetoxy benzene. 6. Acetanilide → p-Acetamidobenzenesulphonyl chloride → P. Acetamidobenzenesulphonamide. 7. p-Amino phenol → p-Acetyl amino phenol → p-Ethoxy acetanilide. 8. Hippuric acid → Azalactone → 4-Benzylidene 2-phenyl oxazol-5-one. 9. p-Cresol → p-Cresyl benzoate → 2-Hydroxy-5-methyl benzophenone. 10. Phthalimide → N-Benzylphthalimide → Benzylamine 11. o-Nitroaniline → o-Phenylenediamine → Benzimidazole 12. Phthalic acid → Phthalimide → Anthranilic acid 13. Benzyl cyanide→ p-Nitrobenzylcyanide→p-Nitro phenyl acetic acid. 14. Hydroquinone → Hydroquinone diacetate → 2,5-Dihydroxy acetopheneone. 15. Cyclohexanone→ Enamine→2-Acetyl cyclohexanone. 16. α-Pinene→ Disiamylborane→Pinanol

Term Work:
Term Work assessment shall be conducted for the Project, Tutorials and Seminar. Term work is continuous assessment based on work done, submission of work in the form of report/journal, timely completion, attendance, and understanding. It should be assessed by subject teacher of the institute. At the end of the semester, the final grade for a Term Work shall be assigned based on the performance of the student and is to be submitted to the University.

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