

# NORTH MAHARASHTRA UNIVERSITY, JALGAON DEPARTMENT OF ORGANIC CHEMISTRY

## SYLLABUS FOR

# MASTER OF SCIENCE In ORGANIC CHEMISTRY

## PART- II

(Semester III and IV)

(Choice Based Credit System, 60:40 Pattern)

w. e. f. June 2016

### NORTH MAHARASHTRA UNIVERSITY, JALGAON DEPARTMENT OF ORGANIC CHEMISTRY

#### Syllabus for M.Sc. Part-II Organic Chemistry

(Semester - III & IV) (With Effect from June 2016)

#### **Course Structure for Second Year**

The following will be the structure for revised syllabus from June 2016 for Semester III and Semester IV

#### **SEMESTER - III**

Sub. Code: Title

- OC-301: Organic Reaction Mechanism
- OC-302: Spectroscopic Methods in Structure Determination

OC-303: Organic Stereochemistry

OC-304: Heterocyclic Chemistry

OC-004: Organic Chemistry Practical Course-II

Seminar-I: Audit Course

#### SEMESTER - IV

Sub. Code: Title

- OC-401: Chemistry of Natural Products
- OC-402: Synthetic Methods in Organic Chemistry
- OC-403: Bio-organic and Drug Chemistry
- OC-005: Organic Chemistry Practical Course-III

OC-006: A Short Research Project (Annual)

Seminar-II: Audit Course

#### Important Notes:

1. Each theory course prescribed for M. Sc. should be covered in 4 lectures, each of 60 minutes duration per week per course including lectures, tutorials, seminars, classroom discussions etc. (Total 60 hrs / theory course)

2. Each practical course will require 12 hours of laboratory work per week per semester. The research project will be extended over two semesters (06 hrs/week) and will be examined at the end of the year. (Total 180 hrs / practical course)

3. There should not be more than 10 students in a batch for M. Sc. Practical course.

4. For theory course the question paper (Internal/External) should include numerical, short answer, long answer, MCQ questions to test understanding of the subject.

5. Of the 60 lectures in each course about 10 lectures will include tutorials, student seminars, classroom discussions and tests.

6. The marks for each paper are distributed as external examination 60 marks and internal examination 40 marks. For internal assessment of each theory and practical course, 2 written tests will be taken.

7. Two credits, one each in the III and IV semesters have been allocated for the Seminar. There shall be at least one seminar per student. Seminar is an audit credit.

8. The 80 % attendance of students is compulsory.

9. Students should visit at least five chemical industries in two years of M. Sc. and submit the observations/report to the Department.

10. Department of Organic Chemistry has implemented CGPA system from July 2009 and CBCS from July 2015.

#### **OC-301: Organic Reaction Mechanism**

#### 1. Linear free energy relationship:

Hammett plot, Hammett equation, substituent and reaction constants, physical significance of substituent and reaction constants, substituent constant involving through conjugation. Use of Hammett plot and equation. Deviations from straight line plot. Concave upward deviation. Concave downward deviation. Steric effects, Taft equation, Steric parameters, solvent effects, change of reaction constant. (12 L)

#### 2. Carbocations & Carbanions:

Formation, stability and mechanisms of important reactions. (12 L)

(12 L)

(14 L)

(10 L)

#### 3. Free Radical Reactions:

Formation, stability and detection of long and short-lived radicals. Homolysis and free radical displacement, Fragmentation, substitution, addition, oxidation, reduction, and rearrangements, Radical cyclisation in synthesis.

#### 4. Photochemistry:

General principles, orbital symmetry considerations, photochemistry of carbonyl groups, alkenes and dienes, aromatic compounds.

#### 5. Mechanism in Biological Chemistry:

Nature's NaBH<sub>4</sub> in a nucleotide: NADH or NADPH, reductive amination in nature, Nature's enols-lysine enamines and coenzyme A, Nature's acyl anion equivalent in thiamine pyrophosphate, rearrangements in the biosynthesis of valine and isoleucine, carbon dioxide is carried by biotin, the shikimic acid pathway, haemoglobin carriers oxygen as an iron(II) complex.

#### References:

- A guide book to mechanism in Organic Chemistry 6<sup>th</sup> edition, By Peter Sykes: Orient Longman
- **2.** Mechanism and structure in Organic Chemistry, Edwin S. Gould, Holt, Rinechart and Winston.
- **3.** Organic Chemistry 5<sup>th</sup> edition, By S. H. Pine. MaGraw-Hill International editions.
- **4.** Advanced Organic Chemistry 3<sup>rd</sup> edition, by R. O. C. Norman and J. M. Coxon 3<sup>rd</sup> edition ELBS.
- **5.** Advanced Organic Chemistry Part A and B 2<sup>nd</sup> edition, by F. A. Carey and R. J. Sundberg. Plenum Press. New York and London.
- 6. Organic Chemistry-Clayden, Greeves, Warren and Wothers, OXFORD.
- **7.** Advance Organic Chemistry: Reactions, Mechanisms and Structure by Jerry March.

#### **OC-302: Spectroscopic Methods in Structure Determination**

# Proton Magnetic Resonance: (10 L) Recapitulation, advanced ideas of chemical shift, chemical exchange, effect of deuteration, stereochemistry, hindered rotation, identification of complex spin system. AB, ABC, ABX and AMX systems. Factors affecting vicinal and germinal coupling, long range coupling. Simplification of complex spectra, nuclear double resonance, nuclear overhauser effect, shift reagents.

#### **2.** Carbon magnetic resonance: (12 L)

Elementry means, instrumentation, chemical shift, chemical shift features of aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon. DEPT, DANTE.

#### **3. Two Dimensional NMR Correlation Spectroscopy:** (10 L)

Two dimensional NMR spectroscopy, 2D-HETCOR, <sup>1</sup>H-<sup>1</sup>H COSY, types of COSY experiments, 2D TOCSY, NOSEY, ROSEY, J resolved 2D NMR spectroscopy, HSQC, HMQC and HMBC.

#### **4. NMR Spectroscopy of some other Nuclei-**<sup>15</sup>N, <sup>19</sup>F, <sup>31</sup>P and D and <sup>11</sup>B. (06 L)

(14 L)

#### 5. Mass Spectroscopy:

Theory, Instrumentation, EI, Chemical Ionization, Field Desorption, FAB, ESI, MALDI, TPSI, TOF, MALDI-TOF, Mass Spectral fragmentation of Organic compounds containing common functional groups, McLafferty rearrangement, Molecular Ion peak, metastable peak, isotope peaks, Examples of Mass spectral fragmentation of Organic compounds with respect of their structure determination.

**6. Problems:** Based on joint application of U.V., I.R., NMR, CMR and Mass spectroscopy (including reaction sequence and spectral analysis). (08 L)

#### **References:**

1. Spectroscopic methods in Organic Chemistry, D. H. William and Ian Flemming-4<sup>th</sup> edition.

2. Spectrometric identification of organic compounds, T. C. Morril, R. S. Silverstein, G. C. Bessler 4<sup>th</sup> edition.

3. Mass Spectroscopy, K.G. Das.

4. Absorption Spectroscopy of Organic Molecules, V. M. Parikh

5. Organic Spectroscopy- S. K. Dewan, CBS Publishers.

6. Nuclear Magnetic resonance-Basic Principles-Atta-Ur-Rehman, Springer-Verlag (1986).

7. One and two dimensional NMR spectroscopy, Atta-Ur-Rehman, Elsevier (1989).

#### **OC-303: Organic Stereochemistry**

**1. Principles of stereochemistry:** Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction. (10 L)

**2. Asymmetric synthesis:** Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution - optical and kinetic.
 Racemic modification and resolution of racemic mixture. (10 L)

**3. Pericyclic reactions:** Electrocyclic, Cycloaddition and Sigmatropic reactions and other related concerted reactions. (16 L)

4. Fused rings and bridged rings. (10 L)

#### 5. Stereoisomerism of allenes, related compounds and biphenyls. (04 L)

**6. ORD & CD** : 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  $\alpha$ -haloketone rule with applications. (10 L)

#### References

- 1. Stereochemistry of carbon compounds. E L. Eliel.
- 2. Conservation of Orbital symmetry. R. B. Woodward and Hofmann.
- 3. Stereochemistry. Nasipuri.
- 4. Orbital Symmetry: Problem Solving Approach. R. E. Lehr and Merchand.
- 5. Frontial orbitals and Organic Chemical Reactions. I N Flaming.
- 6. Organic Chemistry- by Finar
- 7. Organic Chemistry-Clayden, Greeves, Warren and Wothers----OXFORD
- 8. Stereoselective synthesis—Mihaly Nograd VCH, Weinheim, 1995.
- 9. Principles and applications of Asymmetric Synthesis—Gou-Qiang Lin, Yue-Ming Li and S. C. Chan---Wiley-Interscience, John Wiley and Sons, Inc. Publication 2001.

#### **OC-304: Heterocyclic Chemistry**

Introduction, Synthetic Approaches & Reactions of following Heterocyclic Compounds:

1.	Three Membered and Four Membered Rings containing One Hetero Atom	
	Aziridine, Oxirane, Thiirane and Azetidine, Oxetane, Thietane	(08 L)
2.	Five Membered Heterocyclic Compounds with One Hetero Atom	
	Pyrrole, Furan, Thiophene	(10 L)
3.	Five Membered Heterocyclic Compounds with Two Hetero Atoms	
	Imidazole, Oxazole, Thiazole	(08 L)
4.	Condensed Five-Membered Heterocycles	
	Indole, Benzofuran, Benzothiophene	(10 L)
5.	Six Membered Heterocyclic Compounds with One Hetero Atom: Pyridine	and
	Bicyclic ring system: Quinoline, Isoquinoline	(16 L)
6.	Six Membered Heterocyclic Compounds with Two Hetero Atoms	
	Pyridazine, Pyrimidine, Pyrazine	(08 L)

#### References

- 1. Heterocyclic Chemistry J. Joule and G. Smith
- 2. Modern Heterocyclic chemistry L. A. Paquette (Benjamin).
- Heterocyclic chemistry 5<sup>th</sup> edition Raj K. Bansal, New Age International (P) Ltd. (2014).

#### **OC-401: Chemistry of Natural Products**

1. Structure, Stereochemistry and Biogenesis of Hardwickiic acid, Camptothecin and Podophyllotoxin. (12 L)

2. Synthesis of Some Natural Products	(14 L)
i) Reserpine (Woodward synthesis)	ii) Taxol
iii) Estrone	iv) Strychnine (Overman's synthesis)
v) Fredericamycin A	vi) Prostaglandin (E. J. Corey synthesis)

3. Secondary Metabolism: Natural Products, Primary and Secondary Metabolism, Enzymes and Coenzymes.

Metabolites Derived from Mevalonates

Metabolites Derived from Shikimic acid

Secondary Metabolism of Amino acids (26 L)

(08 L)

4. Chemistry of Carbohydrates

#### **References:**

- 1. Secondary Metabolism, J. Mann, 2<sup>nd</sup> Edition (Oxford University Press).
- 2. Chemical aspects of Biosynthesis J. Mann (1994).
- 3. Organic Chemistry, Vol. II I. L. Finar.

4. Principles of organic synthesis by R. O. C. Norman and J. M. Coxon; Chapman and Hall.

- 5. Steroids. L. Fieser and Fieser.
- 6. Structure Determination, P. Yates.
- 7. Biosynthesis of Natural Products. P. Manitto.
- 8. Classics in Organic Synthesis K. C. Nicolaou & E. J. Sorensen.

9. Organic Chemistry, Jonathan Clayden, Nick Greeves, Stuart Warren and Peter Wothers, Oxford University Press.

- 10. J. Am Chem. Soc. 88, 3888 (1966).
- 11. Chemistry of Natural Products- Kalsi
- 12. M. C. Wani and M. E. Wall J. Org. Chem. 34, 1364 (1969).

13. (i) Tetrahedron Letters, 3751 (1964).,

- (ii) Tetrahedron Letters, 2861 and 2865 (1968).
- 14. i) J.C.S. Perkin Transactions II, 288-292, (1973).
- ii) J. Am. Chem. Soc. Vol.77.432-437, (1955).
- 15. Organic Chemistry by Morrison and Boyd.

#### **OC-402: Synthetic Methods in Organic Chemistry**

1. Use of Boron, Silicon, Thallium and Tin in organic synthesis.	(07 L)		
2. Transition metal complexes in organic synthesis: Cu, Ni, Co, Hg, Pd, Pt, Fe, Rh, Wilkinson Catalyst, Ziegler Natta catalyst			
3. Enamines & Umpolung in Organic Synthesis	(04 L)		
4. Nitrogen, Phosphorous and Sulphur Ylides in Organic synthesis	(03 L)		
5. Protecting groups in Organic Synthesis: Protection & deprotection of Hydroxyl, Carbonyl, amino and carboxylic acid functional groups & its applications			
<ul><li>6. Designing in Organic Synthesis: (</li><li>Retrosynthesis, disconnection, synthons, linear and convergent synthesis</li></ul>			
7. Coupling Reactions and Process: Stills Coupling, Sonogashira reaction, Buchwald reaction, Pusond-Kahn Reaction, Suzuki Coupling, Mitsunobu reaction, Baylis-Hillman reaction, Mukiayama's esterification, Metathesis reaction (08 L)			
8. a) Green Chemistry – Basic Principles, Methods & Reactions b) Supramolecular Chemistry c) Nano Chemistry	(08 L)		
<ul> <li>References <ol> <li>Transition metal intermediates in Organic Synthesis, C. W. Birds.</li> <li>Organometallic in Organic Synthesis, Swan and Black.</li> <li>Designing Organic Synthesis, Stuart Warren.</li> <li>Some Modern methods of organic Synthesis, W. Carruthers.</li> <li>Principles of Organometallic Chemistry, Coats, Green and Wada.</li> <li>Organic Chemistry, By Robert Morrison and Robert N. Boyd. 5<sup>th</sup> Edition.</li> <li>Organic Chemistry, by I. L. Finar, Vol8. 5<sup>th</sup> Edition.</li> <li>Transition Metal Clusters, B. F. G. Johansson - Wiley 1980.</li> <li>Comprehensive Organometallic Chemistry - G. Wilkinson, F.G.A. Stone and E. A Pergamon - 1980.</li> <li>Organometallic Chemistry, G. O. Spessard; G. L. Miessler - Prentice Hall, 1997.</li> <li>Palladium in Organic Synthesis, A. F. Heck.</li> <li>Ring Closing Metathesis, Grubbs, R. H.; Miller, S. J.; Fu, G. C. Acc. Chem. Res. 28, 446.</li> <li>Organic Synthesis: Concepts, methods, starting materials, JH. Fuhrhop and G. VCH-Verlag, Weinheim, 1994.</li> <li>Protective groups in organic synthesis, T. W. Greene and P. G. M. Wuts, 2<sup>nd</sup> Ed. Wiley and Sons, 1991.</li> <li>Green Chemistry - Paul T. Anastas; John C. Warner - Oxford University.</li> </ol></li></ul>	1995, Penzlin,		

- Green Chemistry Paul T. Anastas; John C. Warner Oxford University.
   Supramolecular Chemistry: Concepts and Perspectives, Jean-Marie Lehn, Wiley.

#### OC-403: Bio-organic and Drug Chemistry

**1. A]** Amino acids, peptides-naturally occurring peptides, modern methods of peptide synthesis with protection and deprotection, proteins, primary, secondary, tertiary and quaternary structure, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases etc.

**B]** Lipids: Introduction, classification and biological importance of fatty acids and lipids, chemical synthesis of phospholipids and glycolipids. (16 L)

**2.** Structure, physical and chemical properties of the heterocyclic bases-adenine, guanine, cytosine, uracil and thiamine, chemical and enzymatic hydrolysis of nucleic acid, structure and function of DNA, RNA (m-RNA, t-RNA, r-RNA). (14 L)

#### 3. Classification of drugs

(04 L)

# 4. Synthesis and application of Drugs from each of the following class (26 L)(At least three drugs)

Antibiotics: Introduction, Classification, Structure & Uses of Streptomycin, Penicillin, Tetracycline

Antidiabetics: Introduction & Synthesis of Glibenclamide, Metformin, Insulin Antihistamines: Introduction, Synthesis of Methapyrilene, Chlorpheniramine Antivirals: Introduction, Synthesis of Amantidine and Zidovudine

**Anticancer / Antineoplastic agents:** Introduction, Classification, Causes, Treatment. Synthesis of mechlorethamine, melaphan, uracil mustards.

**Cardiovascular drugs:** Introduction, Classification, Synthesis of amyl nitrite, sorbitrate, atenolol.

**Local Anti-infective agents:** Introduction, Classification, Synthesis of sulphonamides, dapsone, aminosalicylic acid.

**Psychoactive drugs:** Introduction, Classification, Synthesis of diazepam, oxazepam, alprazolam.

#### Anti HIV Drugs

Introduction, Causes, Precautions, Life Cycle, Classification, Synthesis of AZT

#### **Antimalarial Drugs**

Introduction, Treatment, Synthesis.

Antihypertension Drugs, Antibacterial Drugs, Antitubercular Drugs

#### **References:**

- 1. Biochemistry-by Stryer, L. 4<sup>th</sup> edition---W. H. Freeman and Co. 1995.
- 2. Biochemistry by Zubay, S. Addison-Wesely 1983.
- 3. Natural products: Chemistry and biological significane by J. Mann; R.S. Davidson; J.
- B. Hobbs, D. V. Banthropde and J. B. Harborne, Longman, an, essex.
- 4. Bioorganic Chemistry Frontiers Vol. 2, ed. H. Dugas, Springer-Verlag, 1990.
- 5. Bioorganic Chemistry y Tamlen, E. E. -- Academic Press, 1977.

Peptide chemistry: a practical textbook by Bodansky, M. -- Springer-Verlag 1988.

- 6. Bioorganic Chemistry: A chemical approch to enzyme action-- Springer-Verlag 1989.
- 7. Principles of Nucleic acid structures by Saenger, W. by Springer-Verlag 1984.
- 8. Medicinal Chemistry. G. R. Chatwal.
- 9. Medicinal Chemistry-By A. Kar, Wiley, 2000.
- 10. Strategies for Organic Drug synthesis and design—By D. Lednicer John Wiley 1998.
- 11. Synthetic drugs—G. R. Chatwal—Himalaya, New Delhi 1995.

12. Total synthesis of Natural product: The chiral approch Vol.III, S. Hanessian Pergamon Press 1983.

13. Principles of Medicinal Chemistry (4<sup>th</sup> Edition) W. D. Foye, T. L. Lemke, D. A. Williams.

14. Organic Chemistry of Drug action and Design. R. B. Siwerman, (Academic press, 1993).

#### **OC-004: Organic Chemistry Practical Course-II**

#### Ternary Mixture Separation (Minimum Twelve)

Separation of mixtures containing three components. The mixtures should also involve separation of nitro phenols, amino acids, low boiling substances, water soluble substances. Amines, Phenols and acids used should also contain other elements and functional groups. The mixture separation should be carried out on micro-scale using ether. The purity of the separated compounds should be checked by TLC.

#### Isolation and separation of Natural products: (Minimum Four)

It should involve solvent extraction, chromatographic & distillation techniques.

- 1) Isolation of Hesperdin from orange peel
- 2) Isolation of Eugenol from cloves
- 3) Isolation of Caffeine from tea
- 4) Isolation of Nicotine from tobacco
- 5) Isolation of Piperine from black pepper
- 6) Isolation of Lactose and casein from milk
- 7) Isolation of Cellobiose-octa-acetate from cotton
- 8) Isolation of Stigmasterol from soya bean oil
- 9) Isolation of β-carotene from carrot

#### Interpretation of UV, IR, NMR and Mass Spectra: (Minimum 20 Organic Compounds)

#### **References:**

- 1. Vogel's, Practical Organic Chemistry.
- 2. Practical Organic Chemistry, R. K. Bansal.
- 3. Organic Structures from Spectra, 4<sup>th</sup> Edition, L. D. Field, S. Sternhell, J. R. Kalman, John Wiley & Sons, Ltd.
- 4. Practical Organic Chemistry by Mann & Saunders.

#### **OC-005: Organic Chemistry Practical Course-III**

#### Two Stage Preparations (Minimum Ten)

At least ten two stage preparations should be carried out. The exercise should illustrate the use of organic reagents and may involve the name reactions.

#### Three Stage Preparations (Minimum Four)

Minimum four experiments should be to demonstrate multistep synthesis technique.

#### Multicomponent Reactions (Minimum Eight)

Reactions involving 3, 4, 5 compounds should be carried out on the basis Green Chemistry Principles. The synthesis should be carried out on micro scale.

The progress of reaction should be monitored by TLC.

#### References:

- 1. Vogel's, Practical Organic Chemistry.
- 2. Practical Organic Chemistry, R. K. Bansal.
- 3. Systematic lab experiment in Organic Chemistry by Arun Sethi.

#### **OC-006: A Short Research Project**

Students should carry out a small research project. This should make them familiar with literature survey, research methodologies, identification of products by analytical and spectral methods and familiarity with chromatographic techniques. Students should be present their research work in Avishkar / Conferences.

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