## University of Pune
### Revised Syllabus 2014
#### M.Sc. II: Organic Chemistry

**Semester III**

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<td>Organic Reaction Mechanism</td>
<td>48 Lectures, 4 C.</td>
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<td>CHO-351</td>
<td>Spectroscopic Methods in Structure Determination</td>
<td>48 Lectures, 4 C.</td>
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<td>CHO-352</td>
<td>Organic Stereochemistry</td>
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<td>CHO-353</td>
<td>Pericyclic Reactions, Photochemistry and Heterocyclic Chemistry</td>
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### M.Sc. II: Organic Chemistry Practical

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### Equivalence of previous Syllabus

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<td>CH-353 Free Radicals, Photochemistry, Pericyclic Reactions and their Applications</td>
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M.Sc. Organic Chemistry PART-II
REVISED SYLLABUS-2014

CHO-350: Organic Reaction Mechanism [4 credits, 48 Lectures]

1. Carbanions-Formation, stability and related name reactions [14L]
   Ref. 1, 2, 3 Vol.A and 7
2. Enamines –formation and applications, Ref. 3 [4L]
3. NGP :Neighbouring group participation , Ref. 1 [6L]
4. Reactions of carbenes and nitrenes Ref.3 Vol B [4L]
5. Free radicals: [14L]
   Generation of radiacls, Stable free radicals, Nucleophilic and electrophilic radicals,
   Characteristics reactions, -Free radical substitution, addition to multiple bonds,
   Radicals in synthesis: Inter and intra molecular C-C bond formation via mercuric
   hydride, tin hydride, thiol dionors, cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds.
   Oxidative coupling. C-C bond formation in aromatics, SNAr reactions
   Ref. 1, 3 Vol A, 6
6. Mechanisms in Biological Chemistry (Ref. 5) [6L]

References:
1. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and
   Winston)
2. Advanced organic chemistry by J. March, 6th Ed.
   University Press (2001)

CHO-351: Spectroscopic Methods in Structure Determination [4 credits, 48 Lectures]

1H NMR Spectroscopy (14 L)

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, AX2, ABX, AMX, ABC, A2B2. Spin decoupling,
Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic
double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear overhauser effect (NOE), resonance of other nuclei like $^{31}$P, $^{19}$F

$^{13}$C NMR spectroscopy (8 L)

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 ($^{13}$C-$^{13}$C) and Hetero nuclear ($^{13}$C-$^1$H)coupling constants.

2D NMR Techniques (6 L)

General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)- Homo COSY ($^1$H-$^1$H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Mass Spectrometry (10 L)

Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupole mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors controlling fragmentation

Problems based on joint application of UV, IR, PMR, CMR, and Mass. (10 L)
(Including reaction sequences)

References:
4. Absorption spectroscopy of organic molecules – V. M. Parikh
CHO-352: Organic Stereochemistry

[4 credits, 48 Lectures]

1. Stereochemistry of six membered rings. Ref. 1, 4, 5, 6 (12L)
2. Stereochemistry of rings other than six membered Ref. 1, 4, 5, 6 (8L)
3. Fused Bridged and caged rings Ref. 1, 2, 4, 5 (6L)
4. Resolution of racemic modification Ref. 1, 4 (6L)
5. Geometrical Isomerism and Stereochemistry of olefins Ref. 1, 2 (10L)
6. CD and ORD Ref. 1, 2, 4 (2L)
7. Determination of stereochemistry organic compounds using NMR. Ref. 3 Chapters 32 (1st Edition) (4L)

References:

1. Stereochemistry of carbon compounds - E. L. Eliel
2. Stereochemistry of carbon compounds - E. L. Eliel and S. H. Wilen
4. Stereochemistry of organic compounds –Nasipuri
5. Stereochemistry of organic compounds-Kalsi
6. Organic stereochemistry – Jagdamba Singh
1. **Photochemistry** [12L]
   General basic principles, photochemistry of carbonyl compounds, alkenes, dienes, polyenes and aromatic compounds, photorearrangements, Barton reaction
   Ref. 1, 2, 3, 4
   Application of photochemical reactions in synthesis—Isocomene, Cedrene
   Ref. 8, 9
2. **Pericyclic reactions** [12L]
   Electro cyclic, cycloaddition, sigmatropic and ene reactions, 1,3-dipolar additions,
   Analysis by correlation diagrams, FMO approach and ATS concept. Application of
   pericyclic reactions.
   Ref. 1, 3, 5, 6, 7, 13
3. **Heterocyclic Chemistry** (24 L)
   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:
      Benzo furan, Indole, Benzothiophene, Quinoline
   c) Condensed five membered heterocycles:
      Benzoazole, Benzthiazole, Benzimidazole
   d) 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.
      Ref. 14-20

**References:**

   Springer (2007)
2. Excited states in Organic Chemistry- J.A. Barltrop and J.D. Coyle, John Wiley & sons
   Academic (1972)
7. Organic reactions and orbital symmetry, 2nd Ed. T. L. Gilchrist and R. C. Storr;
   Cambridge, University Press.
11. Pericyclic reactions- Gill and Willis
CHO–450 Chemistry of Natural Products [4 credits, 48 Lectures]

1. Structure and stereochemistry of Hardwickiic acid, Camptothecin and podophyllotoxin
   Ref. 1 to 4 and 11
   (8L)
2. Synthesis of
   i) Taxol
   Ref. 6
   (16L)
   ii) Estrone and Mifepristone
   Ref. 6, 7
   iii) Juvabione (K. Mori and Matsui, Pawson and Cheung Synthesis)
   Ref. 12
   iv) Fredericamycin A
   Ref. 5
3. Biogenesis – The building blocks and construction mechanism of
   Terpenoids – Mono, Sesqui, Di and Triterpenoids and cholesterol
   Alkaloids derived from ornithine, lysine, nicotinic acid, tyrosine and tryptophan.
   The shikimate pathway – cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavonoids and terpenoid quinones.
   Ref. 8, 9, 10

References:
4. Chemistry of Natural products-Kalsi
8. Medicinal Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd Ed.(Wiley)
CHO-451: Advanced Synthetic Organic Chemistry [4 credits, 48 Lectures]


2. C=C formation reactions: Wittig, Horner-Wordworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions, Titanium-carbene mediated olefination: Tebbe, Petasis and Nysted reagent [8L]


4. Ring formation reactions: Pausan-Khand, Bergman and Nazerov cyclization [3L]

5. Click chemistry: criterion for click reaction, Sharpless azides cycloadditions [2L]

6. Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, applications [4L]

7. Use of Boron and Silicon in organic synthesis [8L]

8. Other important reactions: Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction [3L]

References:
1. Organic synthesis using transition metals-Roderick Bates (Wiley)
5. Organic synthesis – Michael B. Smith
8. Guidebook to organic synthesis-R K Meckie, D M Smith and R A Atken
9. Organic synthesis- Robert E Ireland
10. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako

CHO-452: Carbohydrate and Chiron approach, Chiral Drugs and Medicinal Chemistry [4 credits, 48 Lectures]

1. Carbohydrates [4L]
Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of Glucose, conformation and anomic effects in hexoses Ref. 1, 2

2. Chiron approach [8L]
a) Introduction
b) The concept of chiral templates and chirons wherein the carbon skeleton is the chiral precursor.
c) Utilisation of the basic concepts for retrosynthetic strategy and synthesis of the following – (S) Propanediol, (R) and (S) – Epichlorohydrin, L (+)-Alanine,
3. **Chiral Drugs**  
   
   a) Introduction of chiral drugs, Eutomer, Distomer and eudesmic ratio.  
   
   b) Distomers-a) with no side effects b) with undesirable side effects Synthesis and pharmacological activity of S-Ibuprofen, S-Metaprolol, Ininvir sulfate, Dextropropoxyphyn, (+) Ephedrine, Griseofulvin, R-Indacrinone, hydrochloride, S-S-captopril  

References:  
2. Organic Chemistry – I. L. Finar, volume II  
4. Pharmaceutical Chemistry and drug synthesis – Rot and Kleeman  
5. Drug Design – E.J. Arienes

4. **Medicinal Chemistry**

1. Introduction to drugs, their action and discovery Ref. 1,2,3  
2. Relation of Drug structure and its chemical and biological properties Ref. 1,2,3  
3. Structure, activity and quantitative relationship Ref. 1,2,3  
4. Drug targets Ref. 3  
5. Antimicrobial drugs:  
   Antibactaerials: Discovery and development of Penicillins, Cephalosporins, Sulphones and sulphonamides, Tetracyclins, Macrolides, Polypeptides, Chloromycetin  
   Antifungals: Fungal Diseases and Anti-fungal agents  
   Antivirals: Viral diseases and Anti-viral drugs  
   Anti-protozoals: Anti-malarials, Anti-amoebic  

References:  
1. Medicinal Chemistry an Introduction-Gareth Thomas 2nd Ed. Wiley  
3. Introduction to Medicinal Chemistry-Alex Gringauz (Wiley)  
4. Foye’s Medicinal Chemistry  
5. Medicinal Chemistry-A. Burger  
6. Medicinal Chemistry-Ashutosh Karr
CHO-453: Designing Organic Synthesis and Asymmetric Synthesis
[4 credits, 48 Lectures]

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, Retrosynthesis. (24L)

2. Principles and applications of asymmetric synthesis: stereoselectivity in cyclic compounds, enantio-selectivity, diastereo-selectivity, enatiomeric and diastereomeric excess, stereoselective aldol reactions. Cram’s rule, Felkin Anh rule, Cram’s chelate model, Asymmetric synthesis, use of chiral auxiliaries, chiral reagents and catalysts, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation. Ref. 3 chapters 33, 34, 35

1. Designing of organic synthesis – S. Warren (Wiley)
4. Organic synthesis – Michael B. Smith
6. Guidebook to organic synthesis-R K Meckie, D M Smith and R A Atken
7. Organic synthesis- Robert E Ireland
8. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako

M.Sc. II: Organic Chemistry Practical
CHO-347: (A) Single stage preparations [6 Credits]

At least Fourteen single stage and three Isolation of Natural products should carried out. The preparation should be carried out on micro scale.

1. 2-Phenyl indole (Fischer indole synthesis),
2. 7-Hydroxy -3-methyl flavone (Baker-Venkatraman reaction),
3. Benzyl alcohol and benzoic acid from benzaaldehyde (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. Triphenyl or 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)

B) Isolation of Natural products (Any three)

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. Tramyristin from nutmeg
6. Cinnamonaldehyde from cinnamom
7. Eugenol from clove

References:
1. Practical organic chemistry by Mann & Saunders
3. The synthesis, identification of organic compounds –Ralph L. Shriner, Christine K.F. Hermann, Terence C. Morrill and David Y. Curtin

CHO-447 : Two stage preparations (any Ten)  [6 Credits]

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-Acetamidobenzene sulphonyl chloride → P. Acetamidobenzene sulphonamide
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 → Benzyllamine
11. o-Nitroaniline $\rightarrow$ o-Phenylene diamine $\rightarrow$ Benzimidazole
12. Phthalic acid $\rightarrow$ Phthalimide $\rightarrow$ Anthranilic acid
13. Benzyl cyanide $\rightarrow$ p-Nitrobenzyl cyanide $\rightarrow$ p-Nitro phenyl acetic acid
14. Hydroquinone $\rightarrow$ Hydroquinone diacetate $\rightarrow$ 2,5-Dihydroxy acetopheneone
15. Cyclohexanone $\rightarrow$ Enamine $\rightarrow$ 2-Acetyl cyclohexanone
16. $\alpha$-Pinene $\rightarrow$ Disiamyl borane $\rightarrow$ Pinanol

CHO-448: Project/Industrial training/Green Chemistry and Chemical biology experiments (any Twelve) [6 Credits]

1. Preparation of acetanilide from aniline and acetic acid using Zn dust
2. Base catalyzed aldol condensation using LiOH.H₂O as a Catalyst.
3. Bromination of trans-stilbene using sodium bromide and sodium bromate
4. [4+2] cycloaddition reaction in aqueous medium at room temperature
5. Benzil Benzilic acid rearrangement under solvent free condition
6. Thiamine hydrochloride catalyzed synthesis of benzoin from benzaldehyde
7. Clay catalyzed solid state synthesis of 7-hydroxy-4-methylcoumarin
8. Ecofriendly nitration of phenols and its derivatives using Calcium nitrate
9. Bromination of acetanilide using ceric ammonium nitrate in aqueous medium
10. Green approach for preparation of benzopinacolone from bezopinacol using iodine catalyst
11. Preparation of 1, 1-bis-2-naphthol under grinding at room temperature.
12. Solvent free aldol condensation between 3,4-dimethoxybenzaldehyde and 1-indanone
13. Solvent free quantitative solid phase synthesis of azomethines from substituted anilines and substituted benzaldehydes.
14. Sucrose to ethyl alcohol (Baker’s yeast)
15. Asymmetric reduction of EAA by using Baker’s yeast

Note: i) Project/Industrial training students have to perform 6 practical from the above experiments.
ii) 20% students should be given project or industrial training.

Reference:

1. Comprehensive Practical Organic Chemistry by V.K. Ahluwalia and Renu Aggarwal
2. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry Task Force Committee, DST