



ADIKAVI NANNAYA UNIVERSITY  
DEPARTMENT OF CHEMISTRY

**THIRD SEMESTER**

**Paper – I- ORGANIC REACTION MECHANISMS-I and  
PERICYCLIC REACTIONS**

(Effective from the 2016-17 Admitted Batch)

UNIT – I

15 Hrs

**A) Aliphatic Nucleophilic Substitution:**

Neighboring group participation by Bromine, Phenyl group, Non-Classical carbocations, NGP by Pi bond, Sigma bond and Cyclopropyl group,  $S_N$  at Allylic carbon (allylic rearrangements),  $S_N$  at Aliphatic trigonal carbon,  $S_N$  at Vinylic carbon, Ambident nucleophiles, Hydrolysis of esters ( $B_{AC}^2$ ,  $A_{AC}2$ ,  $A_{AC}1$ ,  $A_{AL}1$ ,  $B_{AL}1$ ), Mechanism of estrification of carboxylic acid with an alcohol using DCC, Mayers Synthesis of aldehydes, ketones and carboxylic acids Mitsunobu reaction, Von-Braun reaction

**B) Aliphatic Electrophilic Substitution:**

Mechanisms of  $S_E^2$ ,  $S_E^1$ ,  $S_{Ei}$ , *Hydrogen as electrophile*: Hydrogen exchange; Migration of double bonds, *Halogen electrophiles*. Mechanism of Halogenation of aldehydes and ketones; HVZ reaction; Halogenation of Sulphoxides & Sulphones, *Nitrogen Electrophiles*: Aliphatic diazo coupling, Diazo transfer reaction, Insertion of nitrenes, *Metal Electrophiles*: Metallation with Organometallic Compounds (Orthometallation), *Carbon as Leaving groups*: Decarboxylation of Aliphatic Acids; Dakin – West reaction; Haller–Bauer reaction.

UNIT – II

15 Hrs

**Principles of asymmetric synthesis:**

Introduction and terminology: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces, symmetry, substitution and addition criteria. Prochirality nomenclature: Pro-R, Pro-S, Re and Si. Stereoselective reactions: Substrate stereoselectivity, product stereoselectivity, enantioselectivity and diastereoselectivity. Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio and diastereoselectivity. Analytical methods: % Enantiomeric excess, enantiomeric ratio, optical purity, % diastereomeric excess and diastereomeric ratio. Techniques for determination of enantiomeric excess, specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.

UNIT – III

15 Hrs

**Pericyclic Reactions-I**

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3 Butadiene, 1,3,5- Hexatriene, allyl system, classification of pericyclic reactions FMO approach, Woodward- Hoffman correlation diagram method and perturbation of molecular (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions.

Electrocyclic Reactions: Conrotatory and disrotatory motions ( $4n$ ) and ( $4n+2$ ), allyl systems  
Cycloadditions: Antarafacial and suprafacial additions, notation. of cycloadditions, ( $4n$ ) and ( $4n+2$ ) systems with a greater emphasis on ( $2+2$ ) and ( $4+4$ ) - cycloadditions, ( $2+2$ ) - additions of ketenes and chelotropic reactions.



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UNIT-IV

15 Hrs

**Pericyclic Reactions-II**

FMO approach and perturbation of molecular (PMO) approach for the explanation of sigma tropic rearrangements under thermal and photochemical conditions. suprafacial and antarafacial shifts of H Sigmatropic shift involving carbon moieties, retention and inversion of configurations, (3, 3) and (5, 5) sigmatropic rearrangements detailed treatment of Claisen and Cope rearrangements, fluxional tautomerism, aza-Cope rearrangement and Barton reaction.

Text Books and Reference Books:

- 1) Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
- 2) Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.
- 3) Pericyclic reactions by S.N. Mukharji, Mcmilan.
- 4) Mechanisms and Theory in Organic Chemistry by T.H. Lowery and K.S. Rich gardson.
- 5) The modern structural theory in Organic Chemistry by L.N.Ferguson, Pretice Hall
- 6) Physical Organic Chemistry by jack Hine, Mc. Graw Hill
- 7) Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourth edition, Kluwer academic publishers, New York
- 8) Organic Synthesis, Christine Willis and Martin Willis, Oxford Chemistry primers.
- 9) Principles of Organic Synthesis, ROC Norman and JM Coxon, third edition, CBS, Publisher, Delhi.
- 10) Organic Synthesis, M. B. Smith, Mc Graw Hill, International Edition.
- 11) Organic Chemistry, Clayden, Greeves and Stuwart Warren.
- 12) Modern Organic Synthesis-an introduction by George S.Zweifel and Michael H. Nantz, W. H. Freeman & company, New York.
- 13) Pericyclic Reactions — a problem solving approach, Lehr and Merchand.
- 14) Conservation of Orbital Symmetry by Woodward and Hoffmann.



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DEPARTMENT OF CHEMISTRY

**THIRD SEMESTER**

**Paper – II- ORGANIC SPECTROSCOPY-I**

**(Effective from the 2016-17 Admitted Batch)**

UNIT-I 15 Hrs

**UV-Visible spectroscopy:**

A) Beer-Lambert's law-Deviations from Beers law-Instrumentation-Mechanics of measurement- Energy transitions-Simple chromophores- Auxochrome, Absorption shifts (Bathochromic, Hypsochromic, Hyper chromic and Hypo chromic shifts) UV absorption of Alkenes-Polyenes unsaturated cyclic systems.

B) UV absorption of carbonyl compounds:  $\alpha,\beta$ -unsaturated carbonyl systems-UV absorption of aromatic systems-solvent effects-geometrical isomerism-acid and base effects-typical examples-calculation of  $\lambda$  max values using Woodward Fieser rules, applications.

UNIT-II 15 Hrs

**Infrared spectroscopy:**

A) Mechanics of measurement-Fundamental modes of vibrations-stretching and bending vibrations-Factors effecting Vibrational frequency-hydrogen bonding.

B) Finger print region and its importance, typical group frequencies for  $-\text{CH}, -\text{OH}, \text{N-H}, \text{CC}, -\text{CO}$  and aromatic systems-Application in structural determination-Examples-simple problems.

UNIT-III 15 Hrs

**Nuclear Magnetic Resonance Spectroscopy ( $^1\text{H}$ NMR):**

A) Introduction: Basic principle of- NMR Nuclear spin- nuclear resonance-saturation-Relaxation-Instrumentation (CW&FT).

B) Shielding and deshielding of magnetic nuclei-chemical shift and its measurements, factors influencing chemical shift – spin-spin interactions- factors influencing –coupling constant J and factors effecting J value.

C)  $^{13}\text{C}$  NMR Spectroscopy: Similarities and Differences between PMR and CMR, general considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbon), coupling constants, typical examples of CMR spectroscopy-simple systems.

UNIT-IV 15 Hrs

**Mass spectrometry**

A) Introduction: Ion production-E1, C1, ES, MALDI and FAB- determination of Molecular weight and formulae-Behavior of organic compounds in mass spectrometer- factors affecting fragmentation, ion analysis, and ion abundance.

B) Mass spectral fragmentation of organic compounds, Common functional groups, molecular ion peak, meta stable peak, Mc Lafferty rearrangement, Nitrogen rule, High resolution mass spectrometry, Examples of mass spectral fragmentation of organic compounds with respect of their structure determination.



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Suggested Books:

- 1) Spectroscopic Methods in Organic Chemistry- Forth Edition, D.H. Williams and I.Fleming  
Tata McGraw Hill, New Delhi, 1990.
- 2) Organic Spectroscopy- Second Edition, W.Kemp, ELBS Macmillan, 1987.
- 3) Applications of absorption spectroscopy of Organic Compounds J.R.Dyer,  
Prentice Hall of India, New Delhi, 1984.
- 4) Spectrometric identification of Organic Compounds-Fourth Edition, R.M.  
Silverstein: G.C.Vassiellr and T.C. Merill, Johne Willey, Singapore, 1981.
- 5) Introduction to spectroscopy-D.L.Pavia, G.M.Lampman, G.S.Kriz, 3rdEd  
(Harcourt college publishers).
- 6) Absorption spectroscopy of organic molecules-V.M.Parkih.
- 7) Nuclear Magnetic Resonance-Basic principles-Atta-Ur-Rehman, Springer-Verlag, 1986.



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DEPARTMENT OF CHEMISTRY

**THIRD SEMESTER**

**Paper – III- MODERN ORGANIC SYNTHESIS-I**  
**(Effective from the 2016-17 Admitted Batch)**

UNIT-I

**Formation of C-C single bonds** 15 Hrs

Alkylations via enolate, Thermodynamic and kinetic enolate, Asymmetric Aldol reaction: a) Chiral enolate and achiral aldehyde b) Achiral enolate and chiral aldehyde – explanation by Zimmerman Traxler model; Stork enamine reaction and its synthetic applications; Organo sulphur chemistry: Umpolung and its synthetic applications (Corey Seebach Reaction), sulphur ylides: dimethyl sulphonium methylide, dimethyloxosulphonium methylide preparations and their synthetic applications; Organo Palladium Chemistry: Heck Reaction, Stille coupling, Suzuki coupling, Sonogashira coupling, Negishi coupling, Wacker Oxidation; Organo copper chemistry: Gilman's reagent and synthetic applications; Synthetic applications of carbenes and carbenoids; Baylis Hilman reaction.

UNIT-II

**Formation of Carbon-Carbon double bonds** 15 Hrs

Stereochemistry of E1 and E2 reactions (Different examples of acyclic and cyclic molecules, Saytzeff rule, Hofmann rules and Bredt's rule); Pyrolytic Syn eliminations (focus should be given on stereochemistry of syn eliminations of amine oxides, xanthates and esters of acyclic and cyclic molecules); Sulphoxide-Sulphenate rearrangement (Mislow-Evans rearrangement); Wittig reaction, Wadsworth Emmons reaction, Corey-Fuchs reaction, Aza Wittig reaction, Wittig-Horner reaction and stereo chemistry of Wittig reaction; Shapiro reaction, Eschen-Moser Tanabe fragmentation, Claisen rearrangement of allyl vinyl ethers, Julia Lythgoe olefination, Mc Murray coupling, Peterson Olefination, Tebbs reagent and its application, Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, applications, olefination by Nysted reagent.

UNIT-III

**Reactions of unactivated C-H bonds and organoboranes** 15 Hrs

The Hoffmann Loeffler- Freytag reaction, the Barton reaction and Photolysis of organic hypothalites;

Organoboranes: Preparation of Organoboranes



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viz hydroboration with  $\text{BH}_3\text{-THF}$ , dicyclohexyl borane, disiamyl borane, theryl borane, 9-BBN mono isopinacamplyl borane ( $\text{IPC}_2\text{BH}_2$ ) and diisopinacamplyl borane ( $\text{IPC}_2\text{BH}$ ) functional group transformations of Organo boranes-Oxidation, protonolysis and isomerisation. Formation of carbon-carbon-bonds viz organo boranes carbonylation and cyanidation, reactions of alkenyl boranes and trialkyl alkynyl borates.

UNIT-IV

**Protecting groups and simple applications of microwave and ultrasound assisted reactions** 15 Hrs

(A) Protecting Groups

- 1) Protection of **alcohols** as **ethers** [methyl ether ( $\text{RO-Me}$ ), Tertiary butyl ether ( $\text{ROCM}_3$ ), Benzyl ethers ( $\text{RO-Bn}$ ), *p*-methoxybenzylethers ( $\text{RO-PMB}$ )], as **Silyl ethers** [Trimethyl silylether ( $\text{R-OTMS}$ ), tri ethyl silyl ethers ( $\text{RO-TEs}$ ), *t*-butyldimethylsilyl ether ( $\text{R-OTBDMS}$  in the presence of imidazole), tri isopropylsilyl ether ( $\text{RO-TIPS}$ ), *t*-butyl diphenylsilyl ether ( $\text{RO-TBDPS}$ )], as **acetals** [tetrahydropyranyl ethers ( $\text{RO-THP}$ ), methoxymethyl ethers ( $\text{RO-CH}_2\text{-OCH}_3 = \text{RO-MOM}$ ) and **ester formation** (carboxylic acid ester and *p*-toluene sulphonate esters).
- 2) Protection of 1,2-diols by acetal, ketal and carbonate formation.
- 3) Protection of amines by acetylation, benzylation, benzoyloxy carbonyl, Fmoc and triphenyl methyl groups.
- 4) Protection of carbonyl by acetal, ketal and thio acetal (Umpolung) groups.
- 5) Protection of carboxylic acids by esters and ortho ester formation.

(B)

Synthetic applications of PTC and crown ethers

1. Microwave Technology: Microwave equipment, activation-benefits, limitations, microwave effects. Microwave assisted reactions in organic solvents-Esterification reactions, Fries rearrangement, Orthoester Claisen rearrangement, Diels- Alder reaction, decarboxylation.
2. Ultrasound assisted reactions: introduction, substitution reactions, addition, oxidation, reduction reactions.
3. Click chemistry: criterion for click reaction, Sharpless azides cycloadditions



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Textbooks and Books for Reference:

- 1) Some Modern Methods of Organic Synthesis W. Carruthers, Third & Fourth Edition, Cambridge University Press, Cambridge, 1988.
- 2) Modern Organic Synthesis-an introduction by George S.Zweifel and Michael H. Nantz, W. H. Freeman & company, New York.
- 3) Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourth edition, Kluwer academic publishers, New York
- 4) Organic Synthesis, Christine Willis and Martin Willis, Oxford Chemistry primers.
- 5) Principles of Organic Synthesis, ROC Norman and JM Coxon, third edition, CBS, Publisher, Delhi.
- 6) Organic Synthesis, M. B. Smith, McGraw Hill, International Edition.
- 7) Organic Chemistry, Clayden, Greeves and Stuart Warren.
- 8) Guide Book to Organic Synthesis (3<sup>rd</sup> edition), R. Mackie, D. M. Smith and Aitken.
- 9) Organo Boranes and Silanes, Thomson, Oxford Chemistry primers.
- 10) Strategic applications of named reactions in organic synthesis, Laszlo Kurti and Barbara Czako.
- 11) Modern Synthetic Reactions, Herbert O. House, Second Edition, W.A. Benzamine Inc. Menio Park, California, 1972.
- 12) Organic Synthesis viz Boranes, Herbert C. Brown Gray, W. Kramer Alan B. Levy and M. Mark Midland John Wiely & Sons, New York, 1975.
- 13) Organic Synthesis: Special Techniques, V. K. Ahluwalia and Renu Agarwal.
- 14) Organic Synthesis, Jagadamba Singh and Dr. A. Yadav, Pragati Edition.



ADIKAVI NANNAYA UNIVERSITY  
DEPARTMENT OF CHEMISTRY

**THIRD SEMESTER**

**Paper – IV- : CHEMISTRY OF NATURAL PRODUCTS**

**(Effective from the 2016-17 Admitted Batch)**

**UNIT–I: Alkaloids** 15 Hrs

Introduction, isolation, general methods of structure elucidation and physiological action, degradation, classification based on nitrogen heterocyclic ring, structure, stereochemistry, synthesis and biosynthesis of morphine, strychnine, vincristine, colchicine, camptothecin and reserpine.

**UNIT–II: Terpenoids** 15 Hrs

Occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of Farnesol, Zingiberene, Forskolin, Taxol, Azadirachtin and  $\beta$ -amyrin.

**UNIT–III: Steroids** 15 Hrs

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and its stereochemistry. Isolation, structure determination and synthesis of cholesterol (total synthesis not expected), androsterone, testosterone, estrone and progesterone, Biosynthesis of steroids.

**UNIT–IV: Flavonoids and Isoflavonoids** 15 Hrs

Occurrence, nomenclature and general methods of structure determination, Isolation, structure elucidation and synthesis of Kaempferol, Quercetin, Cyanidin, Genestein, Butein and Daidzein. Biosynthesis of flavonoids and Isoflavonoids: Acetate Pathway and Shikimic acid Pathway.

Books Suggested:

1. Natural Products: Chemistry and Biological Significance, J. Mann, R.S.Davidson, J. B. Hobbs, D. V. Banthrope and J. B. Hatrbnome, Longman, Essex.
2. Organic Chemistry, Vol. 2, I. L. Finar, ELBS.
3. Chemistry of Organic Natural Products, O. P. Agrawal, Vols. 1 &2, Goel Pubs.
4. Natural Products Chemistry K. B. G. torsell, John Wiley, 1983
5. New Trends in Natural Products Chemistry, Atta-ur-Rahman and M.I.Choudhary, Harwood Academic Publisher.
6. Chemistry of Natural products P. S. Kalsi, Kalyani Publishers
7. Biosynthesis of steroids, terpenes and acetogenins, J. H. Richards & J. R. Hendrieson
8. The biosynthesis of secondary metabolites, R. D. Herbert, Chapman & Hall
9. The Biosynthesis of Secondary Metabolite, R. D. Herbert, Second edn, Chapman and Hall 1984
10. Chemical aspects of Biosynthesis, John Mann, Oxford University Press, Oxford, 1996.





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FOURTH SEMESTER

Paper – I- ORGANIC REACTION MECHANISMS-II and  
ORGANIC PHOTO CHEMISTRY

(Effective from the 2016-17 Admitted Batch)

UNIT – I 15 Hrs

A) **Free Radical Reactions:**

Free radical substitution mechanisms; Mechanism at an aromatic substrate; Neighboring group assistance in free radical reactions; Reactivity for aliphatic substrates; Reactivity in aromatic substrates; Reactivity at bridge head; Reactivity in the attacking radical; Effect of solvent on reactivity, Allylic halogenations using NBS (Wohl – Ziegler bromination); Hydroxylation at aromatic carbon by Fentons reagent; Oxidation of aldehydes to carboxylic acids; Formation of cyclic ethers using Leadtetraacetate; Formation of hydroperoxides (autooxidation); Coupling of alkynes (Eglinton reaction and Glaser reaction); Arylation of Aromatic compounds by diazonium salts (Gomberg – Bachman reaction); Mechanisms of Sandmeyer reaction, Kolbes reaction, Hunsdiecker reaction, Reed reaction; free radical rearrangements.

B) **Quantitative relationships between Molecular structure and Chemical reactivity:**

Hammett and Taft Equations

C) **Rearrangements:** Wagner – Meerwein Rearrangement, Demjanov Rearrangement, Wittig Rearrangement and Stevens Rearrangement

Unit – II: 15 Hrs

**Methodologies in asymmetric synthesis**

Strategies in Asymmetric Synthesis: 1. Chiral substrate controlled, 2. Chiral auxiliary controlled, 3. Chiral reagent controlled and 4. Chiral catalyst controlled.

1. **Chiral Substrate controlled asymmetric synthesis:** Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

2. **Chiral auxiliary controlled asymmetric synthesis:**  $\alpha$ -Alkylation of chiral enolates, azaenolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder reaction.

3. **Chiral reagent controlled asymmetric synthesis:** Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2 BH and IPCBH2.

4. **Chiral catalyst controlled asymmetric synthesis:** Sharpless and Jacobsen asymmetric epoxidations. Sharpless asymmetric dihydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysis. Enzyme mediated enantioselective synthesis

5. **Asymmetric aldol reaction:** Diastereoselectivity aldol reaction (chiral enolate & achiral aldehydes and achiral enolate & chiral aldehydes) its explanation by Zimmerman-Traxel model.

UNIT – III 15 Hrs

**Photo Chemistry-I**

Photochemical energy, Frank Condon Principle, Types of Electronic Excitation and Molecular orbital view of excitation, Jablonski Diagram, singlet and triplet states, dissipation of photochemical energy, photosensitization, quenching, quantum efficiency and quantum yield, Determination of Quantum yield

Photo Chemistry of Carbonyl Compounds: Norrish Type I reaction (alpha cleavage reaction), Norrish Type – II reaction, Paterno- Buchi reaction, Photo reduction & photo enolisation; photochemical Oxidations [Backstrom mechanism], Photo oxidation of alkenes with singlet oxygen.



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Unit – IV

**Photochemistry-II**

Di – Pi methane Rearrangement, Aza di – Pi methane rearrangement; Photochemistry of Benzene and substituted benzene, 1, 2 , 1,3 ,& 1, 4-additions; Photo Fries rearrangement of Phenolic acetates and Anilides; Photochemistry of unsaturated systems, Cis- Trans Isomerisation of alkenes (Direct and sensitized) (Photoisomerisation of Stilbene), Photochemistry of Butadiene; Dimerisations of alkenes, Intramolecular dimerisation.

Photochemical rearrangement of Cyclohexadienenones; Photochemistry of alpha, beta Unsaturated ketones (dimerisations and addition across the double bond); Photochemical rearrangement reactions of Cyclohexenone, Photorearrangements of Beta, gamma unsaturated systems (Mechanism of 1,2 & 1,3 – acyl shifts); Photochemistry of Nitrite esters (Barton reaction); Photochemistry of alpha diazoketones; Photo Aromatic Substitutions; Photochemistry of Pyridinium ylides.

Text Books and Reference Books:

- 1) Advanced Organic Chemistry: Reactions Mechanisms and Structure by Jerry March, Mc.Graw Hill and Kogakush.
- 2) Molecular reactions and Photochemistry by Charles Dupey and O. Chapman, Prentice Hall.
- 3) Mechanisms and Theory in Organic Chemistry by T.H. Lowery and K.S. Richardson.
- 4) The modern structural theory in Organic Chemistry by L.N.Ferguson, Prentice Hall
- 5) Physical Organic Chemistry by Jack Hine, Mc. Graw Hill
- 6) Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourth edition, Kluwer academic publishers, New York
- 7) Organic Synthesis, Christine Willis and Martin Willis, Oxford Chemistry primers.
- 8) Principles of Organic Synthesis, R.C. Norman and J.M. Coxon, third edition, CBS, Publisher, Delhi.
- 9) Organic Synthesis, M. B. Smith, Mc Graw Hill, International Edition.
- 10) Organic Chemistry, Clayden, Greeves and Stuart Warren.
- 11) Modern Organic Synthesis-an introduction by George S.Zweifel and Michael H. Nantz, W. H. Freeman & company, New York.
- 12) Organic Photochemistry by D Coyle
- 13) Molecular Photochemistry by Gilbert & Baggo
- 14) Organic Photochemistry by Turro
- 15) Photochemistry by C W J Wells



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**FOURTH SEMESTER**

**Paper – II- ORGANIC SPECTROSCOPY-II**

**(Effective from the 2016-17 Admitted Batch)**

UNIT-I:

A) Optical Rotatory Dispersion: Theory of Optical Rotatory Dispersion-Cotton effect –CD curves-types of ORD and CD curves–similarities and difference between ORD and CD curves

B) The octant rule-application in structural studies- $\alpha$ - halo keto rule.

UNIT-II

A) Improving the PMR spectrum: Chemical and Magnetic Equivalence. Chemical exchange, First and Non-First Order Spectra and analysis of AB, AMX and ABX systems.

B) Simplification of complex spectra-: Nuclear Magnetic double resonance, Lanthanide shift reagents, solvent effects, Fourier transforms technique, Nuclear Overhauser Effect (NOE), Deuterium Exchange, spectra at higherfields. Hindered Rotations and Rate processes. Resonance of other nuclei- $^{19}\text{F}$  and  $^{31}\text{P}$

C) 2D NMR spectroscopy: Definitions and importance of COSY, DEPT, HOMCOR, HETCOR, INADEQUATE, INDOR INEPT, NOESY, HOM2DJ, HET2DJ and DQFCOSY.

UNIT-III

Solution of structural problems by joint application of UV, IR, NMR ( $^1\text{H}$ & $^{13}\text{C}$ ) and mass spectrometry.

UNIT-IV

A) Separation Techniques: Solvent extraction chromatography-paper-thin layer partition-column chromatography, Electrophoresis.

B) Instrumentation – Gas Chromatography, High performance Liquid Chromatography, X – Ray diffraction (XRD)

**Suggested Books:**

- 1) Spectroscopic Methods in Organic Chemistry- Forth Edition, D.H. Williams and I. Fleming  
Tata - McGraw Hill, New Delhi, 1990.
- 2) Organic Spectroscopy- Second Edition, W.Kemp, ELBS Macmillan, 1987.
- 3) Spectrometric identification of Organic Compounds-Fourth Edition, R.M. Silverstein: G.C.Vassillr and T.C. Merill, John Willey, Singapore, 1981.
- 4) Introduction to spectroscopy-D.L.Pavia, G.M.Lampman, G.S.Kriz, 3rdEd  
(Harcourt college publishers).
- 5) "Applications of Optical rotation and Circular Dichroism", G.C. Barret, in  
"Elucidation of Organic structures by Physical and Chemical Methods"  
Part I (Eds) K.W. Bentley and G.W.Rirty John Wiley, 1972, Chapter VIII  
(only those aspects mentioned in the syllabus).
- 6) Instrumental methods of chemical analysis by H.Kaur, Pragati Prakasan,meerut.
- 7) Separation Techniques by M.N.Sastri, Himalaya publishing House (HPH), Mumbai.



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**FOURTH SEMESTER**

**Paper – III- MODERN ORGANIC SYNTHESIS-II**

**(Effective from the 2016-17 Admitted Batch)**

UNIT-I

**Organo Silanes**

15 Hrs

Synthetic applications of trimethylsilyl chloride dimethyl-*t*-butylsilyl chloride, trimethylsilyl cyanide, trimethylsilyl iodide and trimethylsilyl triflate, synthetic applications of  $\alpha$ -silyl carbanion and  $\beta$ -silyl carbonium ions. Synthetic applications of silyl enol ethers, Preparation and synthetic applications of alkynyl silanes, aryl silanes, allyl silanes and vinyl silanes, Nazarov cyclization, Synthetic conversion of  $\alpha$ ,  $\beta$ -epoxy silanes, Peterson Olefination, Brook rearrangement and Rubottom oxidation.

UNIT-II

15 Hrs

**Oxidation**

Synthetic applications of the following reagents in the oxidation of functional groups like alkenes, alkynes, alcohols, aldehydes and ketones: 1)  $\text{Pb}(\text{OAc})_4$  2)  $\text{HIO}_4$  3)  $\text{SeO}_2$  4)  $\text{CrO}_3$  (Sodium or potassium dichromate in  $\text{H}_2\text{SO}_4$ , Collins reagent, Jones reagent, Etard reagent,  $\text{CrO}_3$  in acetic anhydride, PCC (Coreys reagent), PDC, Babler oxidation), 4)  $\text{MnO}_2$  5)  $\text{KMnO}_4$  6)  $\text{OsO}_4$  7) Oxidations by using DMSO involving alkoxy sulphonium salts (Kornblum oxidation), DCC- DMSO (Pfitzner-Muffat reagent), Swern oxidation, Corey-Kim oxidation, Albright-Goldman oxidation 8) Oxidations by using IBX, DMP, TPAP, TEMPO, CAN 9) Bayer villager oxidation and Prilezhev epoxidation 10) Oxidation of alkenes using Woodward and Prevost reagents 11) Oxidation by using DDQ 12) Sharpless asymmetric epoxidation and Sharpless asymmetric dihydroxylation 13) Thallium nitrate 14) Oxidative coupling of phenols and alkynes.

UNIT-III

**Reduction**

15 Hrs

- (1) Catalytic reductions: Homogeneous (Wilkinson's Catalytic reduction) and heterogeneous catalytic reductions and their synthetic applications.
- (2) Reductions by using electrophilic nucleophilic metal hydrides:  $\text{LiAlH}_4$  (Various examples of reductions and Cram's rule), related reagents of LAH,  $\text{NaBH}_4$ ,  $\text{NaBH}_3\text{CN}$ , Trialkyl Borohydrides (Super Hydride and Selectride).
- (3) Reductions by using electrophilic metal hydrides:  $\text{BH}_3$ , DIBAL



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- (4) Reductions by dissolving metals: Clemenson reduction, Acyloin condensation, Bouveault-Blanc reduction, Birch reduction (Various examples should be discussed).
- (5) Reductions by using Diimide and Wolf-Kishner Reduction (6) Hydrogenolysis
- (7) Reductions by using tri n-butyl tin hydride.

UNIT-IV

**Retro Synthetic Analysis**

15 Hrs

1. Basic definitions of the following:
  - a) Retro synthetic analysis
  - b) Disconnection
  - c) Target molecule
  - d) Synthons
  - e) Synthetic equivalent
  - f) Functional Group Inter Conversion (FGI)
  - g) Functional Group Addition (FGA)
2. Guidelines for the order of events: One group C-X disconnections One Group C-X disconnections (Carbonyl derivatives, ethers, sulphides and alcohols); Two group C-X disconnections (1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds), One group C-C disconnections (Alcohols and carbonyl compounds, 1,1-C-C, 1,2-C-C and 1,3-C-C); Synthesis of alkenes (Wittig disconnections and diene synthesis), Two group disconnections (Diels Alder reaction and 1,3-difunctionalised compounds); Linear and convergent synthesis.

Textbooks and Books for Reference:

- 1) Some Modern Methods of Organic Synthesis W. Carothers, Third Edition, Cambridge University Press, Cambridge, 1988.
- 2) Modern Organic Synthesis-an introduction by George S.Zweifel and Michael H. Nantz, W. H. Freeman & company, New York.
- 3) Advanced Organic Synthesis, Part B-Reactions and Synthesis, Francis A. Carey and Richard J. Sudenburg, Fourt edition, Kluwer academic publishers, New York.
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- 7) Organic Chemistry, Clayden, Greeves and Stewart Warren.
- 8) Guide Book to Organic Synthesis (3<sup>rd</sup> edition), R. Mackie, D. M. Smith and Aitken.
- 9) Organo Boranes and Silanes, Thomson, Oxford Chemistry primers.
- 10) Strategic applications of named reactions in organic synthesis, Laszlo Kurti and Barbara Czako.
- 11) Organic Synthesis: The disconnection approach, S. Warrant John Wiley & sons, New York, 1984.
- 12) Modern Synthetic Reactions, Herbet O. Horase, Second Edition, W.A. Benzamine Inc. Menio Park, California, 1972.



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**FOURTH SEMESTER**

**Paper – IV- BIO-ORGANIC CHEMISTRY**  
**(Effective from the 2016-17 Admitted Batch)**

UNIT-I 15 Hours

**Biopolymers and Enzymes**

Peptides:  $\alpha$ -Amino acids, their general properties and synthesis, Synthesis of peptides by Merrified solid phase synthesis. Chemistry of oxytocin and dolastain-10  
Enzymes-Oxidoreductases, hydrolases, transferases, synthesis of ATP, Baker's Yeast.  
Enzyme models-NADH models, Bio transformations, Remotefunctionalization

UNIT-II 15 Hours

**Antimalarials & Antibiotics**

**i. Antimalarials**

Chemotherapy, synthesis and activity of antimalarial drugs- quinoline group-quinine, acridine group-quinacrine and guanidine group-paludrine.

**ii. Antibiotics**

General characteristics, structure- activity relationships, synthesis and activity of antibiotics: Pencillin G, Cephalosporin-C and streptomycin.

UNIT-III 15 Hours

**Vitamins and Prostaglandins**

Definition, occurrence, structural formulae, physiological functions and synthesis of Vitamins.

Vitamins: Structure determination and synthesis of Retinol (A), Thiamine (B<sub>1</sub>), Riboflavin (B<sub>2</sub>), Pyridoxine (B<sub>6</sub>) and Biotins (H), Nicotininc acid.

**Prostaglandins**

Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE<sub>2</sub> and PGF<sub>2</sub>

UNIT-IV 15 Hours

**Nucleic Acids:**

Nucleic acids: Basic concepts of the structures of RNA and DNA and their hydrolysis products, nucleotides, nucleosides and heterocyclic bases, Genetic Code, Finger Print test.

Application of recombinant DNA technology in production of pharmaceuticals, diagnosis of diseases, insect control, improved biological detergents, gene therapy-examples.



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Reference Books and Material:

1. Chemical Aspects of Biosynthesis, John Man, Oxford University Press, Oxford, 1996.
2. Chemistry of Natural Products: A Unified Approach, N. R. Krishnaswamy, University Press (India) Ltd., Orient Longman Limited, Hyderabad, 1999.
3. Introduction to Organic Chemistry, A Streitwieser, CH Heathcock and E.M./Kosover IV Edition, McMillan, 1992. (For Merrifield synthesis of peptides and also for other aspects of Unit IV)
4. Bio-organic Chemistry, H.Dugas and C. Penney, springer, New York, 1981.
5. Details of Primary literature: Nomenclature: Structure: Dolastatin-10: JACS, 1987, 109, 6883 (structure), ibdi, 1989, 111, 5463, JCS, Parkin I, 1996, 859 (synthesis).



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**III SEMESTER**  
**Laboratory Course-1**

**100 M**

**Multistep Synthesis of Organic Compounds:**

The experiments should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques.

1. Beckmann rearrangement: Benzanilide from Benzophenone  
Benzophenone → Benzophenone oxime → Benzanilide
2. Benzilic acid rearrangement: Benzilic acid from benzoin  
Benzoin → Benzil → Benzilic acid
3. P-Bromo Aniline from Aniline :  
Aniline → Acetanilide → P-Bromo Acetanilide → P-Bromo Aniline
4. Symmetrical Tribromo Benzene from aniline:  
Aniline → Tribromoaniline → Tribromobenzene
5. 2,4,6-trimethylquinoline from p-toluidine  
p-toluidine → 4-(p-tolylamino) pent-3-ene-2-one → 2,4,6-trimethylquinoline
6. Flavone from o-hydroxy acetophenone  
o-hydroxy acetophenone → o-benzoyl acetophenone → o-hydroxy- dibenzoylmethane → Flavone
7. 2-phenylindole from phenylhydrazine  
phenylhydrazine → acetophenone phenylhydrazone → 2-phenylindole

**Laboratory Course-2**

**100 M**

**Spectral Identification of Organic Compounds (UV, IR,  $1^{\text{H}}$ - and  $^{13}\text{C}$ - NMR, MASS).**

A minimum of 40 representative examples should be studied

**Books Suggested**

1. Modern Organic Synthesis in the Laboratory *A Collection of Standard Experimental Procedures*, Jie Jack Li, Chris Limberakis, Derek A. Pflum
2. Practical organic chemistry by Mann & Saunders
3. Text book of practical organic chemistry by Vogel
4. Spectrometric Identification of organic compounds, R.M. Silverstein, F.X. Webster and D.J. Kiemle, 7th Ed., (Wiley)





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**IV – SEMESTER**  
**Laboratory Course-1**

**100 M**

**Chromatographic Separation and Isolation & identification of Natural Products**

1. Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R<sub>f</sub> values of known standards.
2. Isolation and identification of Natural Products
  - (a) Isolation of caffeine from tea leaves
  - (b) Isolation of eugenol from cloves
  - (c) Isolation of casein and lactose from milk
  - (d) Isolation of limonene from lemon peel
  - (e) Isolation of piperines from black pepper
  - (f) Isolation of lycopene from tomatoes
  - (g) Isolation of β-carotene from carrots

**Laboratory Course-2**  
**Estimations and Chromatography**

**100 M**

1. Estimation of (a) Glucose (b) Phenol (c) Aniline (d) Acetone (e) Aspirin (f) Ibuprofen (g) Paracetamol
2. Separation by column chromatography: Separation of a mixture of *ortho* and *para* nitroanilines using silicagel as adsorbent and chloroform as the eluent. The column chromatography should be monitored by TLC.

**Books Suggested:**

1. Ikan, R. *Natural Products, A Laboratory Guide*, 2nd ed.; Academic Press: New York, 1991.
2. Adapted from *Introduction to Organic Laboratory Techniques: A Microscale Approach*. Pavia, Lampman, Kriz and Engel. (1999) Saunders College Publishing.
3. Pharmaceutical drug analysis by Ashutoshkar
4. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
5. Practical pharmaceutical chemistry part-1 and part-2 by A H Beckett and J B Stenlake
6. Practical organic chemistry by Mann & Saunders
7. Text book of practical organic chemistry including qualitative organic analysis by A.I. Vogel (Longman)