# **Cluster Elective –III**

# PAPER – VIII-C-1: ORGANIC SPECTROSCOPIC TECHNIQUES

# 45 hrs (3 h / w)

# NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Nuclear spin, Principles of NMR Magnetic moment and Spin angular momentum. Larmour Frequency. Instrumentation. Relaxation- spin-spin & spin lattice relaxation. Chemical shifts, Shielding and Deshielding mechanism-Factors influencing Chemical shift. Spin-Spin interactions-AX, AX<sub>2</sub> and AB types. Vicinal, Geminal and Long range coupling- Factors influencing coupling constants.

# UNIT – II

**UNIT-I** 

Spin decoupling, Spin tickling, Deuterium exchange, Chemical shift reagents and Nuclear over Hauser effect. Applications in Medical diagnostics, Reaction kinetics and mechanically induced dynamic nuclear polarization. FT NMR and its Advantages.

# UNIT-III

# **UV & VISIBLE SPECTROSCOPY**

Electronic spectra of diatomic molecules. The Born - Oppenheimer approximation. Vibrational coarse structure: Intensity of Vibrational-electronic spectra: The Franck-Condon principle. Rotational fine structure of electronic vibration transitions. Electronic structure of diatomic molecules.

Types of transitions, Chromophores, Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds-Woodward - Fieser rules.

# **UNIT-IV**

Chemical analysis by Electronic Spectroscopy – Beer-Lambert's Law. Deviation from Beer's law. Quantitative determination of metal ions (Mn<sup>+2</sup>, Fe<sup>+2</sup>, NO<sub>2</sub><sup>-</sup>,). Simultaneous determination of Chromium and Manganese in a mixture

#### **UNIT-V**

# **Electron Spin Resonance Spectroscopy**

Basic Principles, Theory of ESR, Comparison of NMR & ESR. Instrumentation, Factors affecting the 'g' value, determination of 'g' value. Hyper fine splitting concept and splitting patterns, Zero field splitting and Kramer degeneracy.

Applications: - Detection of free radicals; ESR spectra of (a) Methyl radical (CH<sub>3</sub>), (b) Benzene anion  $(C_6H_6)$  (c) CH<sub>2</sub>.CH<sub>3</sub> (ETHYL RADICAL)

# 15h

# 5h

10h

10h

# 5h

#### List of Reference Books:

- 1. Electron Spin Resonance Elementary Theory and Practical Applications- John E. Wertz and James R. Bolton, Chapman and Hall, 1986.
- 2. Spectroscopic Identification of organic compounds Silverstein, Basseler and Morril.
- 3. Organic Spectroscopy- William Kemp.
- 4. Fundamentals of Molecular Spectroscopy- C.N.Banwell and E.A. Mc cash 4<sup>th</sup> Edition, Tata Mc Graw Hill Publishing Co., Ltd. 1994
- 5. NMR, NQR, EPR and MÖssbauer Spectroscopy in inorganic chemistry R.V Parish, Ellis, Harwood.
- 6. Instrumental Methods of Chemical Analysis- H.Kaur, Pragathi Prakashan, 2003.
- 7. Analytical spectroscopy Kamlesh Bansal, Campus books, 2008.
- 8. Structural Inorganic Chemistry MÖssbauer Spectroscopy Bhide.
- 9. Principle of MÖssbauer Spectroscopy T.C. Gibb, Chapman, and Hall, Landon 1976.

# P. R. GOVERNMENT COLLEGE, KAKINADA SEMESTER – VI (CHEMISTRY) Paper - VIII : CLUSTER-C-1: ORGANIC SPECTROSCOPIC TECHNIQUES

# Weightage to content

S. No.	Course Content	Essay Questions (10M)	Short Answer Questions (5M)	Total No. Of Questions from each Unit	Total No. of Marks allotted to each Unit
1	Unit -I	2	1	3	25
2	Unit –II	1	1	2	15
3	Unit –III	2	2	4	30
4	Unit –IV	1	2	3	20
5	Unit -V	3	2	5	40
	TOTAL	9	8	17	130

## P. R. GOVERNMENT COLLEGE, KAKINADA MODEL PAPER FOR SEMESTER – VI (CHEMISTRY) Paper - VIII : CLUSTER-C-1: ORGANIC SPECTROSCOPIC TECHNIQUES

#### Duration: 2.30hrs.

Max. Marks: 60

Answer any FOUR questions choosing AT LEAST ONE question from each section

#### 4X10=40Marks

#### Section-I

- 1. i. Which type of atoms exhibit nuclear magnetic resonance?
  - ii. Write the principle involved in NMR spectroscopy.
- 2. Define chemical shift. What are the factors influencing chemical shift?
- 3. Discuss in detail the Nuclear Over Hauser effect

#### Section-II

- 4. Write about Born-oppenheimer approximation.
- 5. What are the Woodward-Fieser rules of UV-Visible spectroscopy?
- 6. How is Beer-Lambert's law useful in quantitative determination of Mn(II) and Fe(II)?

# Section-III

- 7. Explain principle and theory of esr spectroscopy
- 8. Explain about the experimental techniques involved in ESR studies.
- 9. Write notes on 'g' value and hyperfine structure.

#### Section-IV

Answer any **FOUR** questions. Each question carries **FIVE** marks. **4** 

4X5=20Marks

- 10. Describe the factors influencing the coupling constant.
- 11. Explain about spin decoupling.
- 12. Write about Franck-Condon principle.
- 13. What are the different types of electronic transitions?
- 14. State and explain Beer-Lambert law.
- 15. Write the quantitative determination of any metal ions.
- 16. How ESR studies are useful to study the structure of free radicals?
- 17. How ESR studies are useful to study the structure of benzene anion?

# III B.SC CHEMISTRY –PAPER VIII-C-1 ORGANIC SPECTROSCOPIC TECHNIQUES. QUESTION BANK

#### ESSAY QUESTIONS: 10M

1. What is the principle of NMR Spectroscopy?

2. Define chemical shift. What are the factors influencing chemical shift.

3. Explain 1) Spin-spin coupling 2) coupling constant-Factors

4. Discuss 1) Born-Oppenheimer approximation 2) Frank- Condon principle.

5. What are the Woodward-fieser rules of UV-Visible Spectroscopy.

6. What is Beer-lamberts law. Write its limitations. How is Beer-Lambert's law useful in quantitative determination of Mn (II) and Fe (II).

7. Give the experimental procedure of simultaneous determination of chromium and manganese in a mixture using Beer-lamberts law.

8. Explain the principle and theory involved ESR Spectroscopy.

9. Write about the experimental techniques involved in ESR Spectroscopy

9. Write about hyperfine splitting and explain the hyperfine splitting pattern of  $CH_3$  radical

10 Explain about the hyperfine splitting lines appear for the following species,

a)  $.C_6H_6^-$  (Benzene anion) b)  $.CH_3CH_2$  (ethyl radical)

11. Write about the following, a). g – Factor b). Hyperfine splitting

#### SHORT ANSWERS

11. Discuss about a) Shielding effect b) de-shielding

12. Write about a) spin- spin relaxation b) spin decoupling

13. Explain about a) Spin tricling b) spin hamiltoniun

14. Write about larmour frequency

15. Write short note on nuclear overhauser effect

16. What are the different types of electronic transitions?

17. What is FT nmr? What are the advantages of FT in NMR?

18. How is Beer-Lambert's law useful in quantitative determination of No2<sup>-</sup>

19. Discuss define Chromophore

20. Write comparisons between NMR & ESR?

21. Explain Zero field splitting in ESR spectroscopy

22. Write about Kramer's degeneracy in ESR spectroscopy

23. Write the Principle involved in esr spectroscopy

24, Write a short note on g factor.

**5M** 

# Cluster Elective –III PAPER – VIII-C-2: ADVANCED ORGANIC REACTIONS.

45 hrs (3 h / w)

## UNIT – I

#### **ORGANIC PHOTOCHEMISTRY**

Organic photochemistry: Molecular orbitals, carbonyl chromophore–triplet states, Jablonski diagram, inter–system crossing. Energy transfer. Energies properties and reaction of singlet and triplet states of and transitions.

**Photochemical reactions:** (a) Photoreduction, mechanism, influence of temperature, solvent, nature of hydrogen donors, structure of substrates on the course of photo reduction,

#### UNIT – II

#### **ORGNAIC PHOTOCHEMISTRY**

Norrish cleavages, type I: Mechanism, acyclic cyclic diones, influence of sensitizer, photo Fries rearrangement. Norrish type II cleavage: Mechanism and stereochemistry, type II reactions of esters: 1: 2 diketones, photo decarboxylation, Di -  $\pi$  methane rearrangement, Decomposition of nitrites – Barton reaction.

## UNIT – III

#### PROTECTING GROUPS AND ORGANIC REACTIONS

Principles of (1) Protection of alcohols – ether formation including silyl ethers – ester formation, (2) Protection of diols – acetal and ,ketal , (3) Protection of carboxylic acids – ester formation, benzyl and t–butyl esters, (4) Protection of amines

- Acetylation, benzoylation, benzyloxy carbonyl, triphenyl methyl groups, (5) Protection of carbonyl groups – acetal, ketal, 1, 2–glycols and 1, 2–dithioglycols formation.

#### $\boldsymbol{UNIT-IV}$

Synthetic reactions: Mannich reaction – Mannich bases – Robinson annulations. The Shapiro reaction, Stork–enamine reaction. Phase transfercatalysis – mechanisms and use of benzyl trialkyl ammonium halides. Witting reaction. **UNIT –V: NEW SYNTHETIC REACTIONS** 

Baylis–Hillman reaction, Mitsunobu reaction, McMurrey reaction, Julia–Lythgoe olefination, and Peterson's stereoselective olefination, Heck reaction, Suziki coupling, Stille coupling and Sonogishira coupling, Buchwald–Hartwig coupling. Ugi reaction, Click reaction.

#### List of Recommended Books

- 1. Molecular reactions and Photochemistry by Charles Dupey and O.L. Chapman.
- 2. Molecular Photochemistry by Turru.
- 3. Importance of antibonding orbitals by Jaffe and Orchin.
- 4. Text Book of Organic Chemistry by Cram, Hammand and Henrickson.
- 5. Some modern methods of organic synthesis by W. Carruthers.
- 6. Guide Book to Organic Synthesis by R.K. Meckie, D.M. Smith and R.A. Atken.
- 7. Organic Synthesis by O.House.
- 8. Organic synthesis by Michael B. Smith.
- 9. Organic Chemistry Claydon and others 2005.
- 10. Name Reactions by Jie Jack Li
- 11. Reagents in Organic synthesis by B.P. Mundy and others.

# P. R. GOVERNMENT COLLEGE, KAKINADA SEMESTER – VI (CHEMISTRY) Paper - VIII : CLUSTER-C-2: ADVANCED ORGANIC REACTIONS

S. No.	Course Content	Essay Questions (10M)	Short Answer Questions (5M)	Total No. Of Questions from each Unit	Total No. of Marks allotted to each Unit
1	Unit -I	2	2	4	30
2	Unit –II	2	1	3	25
3	Unit –III	2	2	4	30
4	Unit –IV	2	2	4	30
5	Unit -V	1	1	2	15
	TOTAL	9	8	17	130

#### Weightage to content

# P. R. GOVERNMENT COLLEGE, KAKINADA MODEL PAPER FOR SEMESTER – VI (CHEMISTRY) Paper - VIII : CLUSTER-C-2: ADVANCED ORGANIC REACTIONS

#### Duration: 2.30 hrs.

#### Max. Marks: 60

Answer any FOUR questions choosing AT LEAST ONE question from each section 4X10=40Marks

#### Section-I

- 1. Write the mechanism of photo reduction reaction? How it is affected by temperature and solvent?
- 2. Explain the following:
  - i) Singlet and triplet states ii) Jablonski diagram
- 3. Discuss the Norrish type-I cleavage with an example.

#### <u>Section-II</u>

4. What do you know about the following:

i)Di- $\pi$  methane rearrangement ii) Barton reaction

5. Give a detailed account on the protection of carbonyl groups.

6. How amine group is protected by acylation and benzoylation.

#### Section-III

7. Write note on the following:i) Mannich reaction ii) Wittig reaction

8. Write a note on the following:i) use of benzyl trialkyl ammonium halides ii) Phase transfer catalysis

9. Illustrate the following reactions: Baylis-Hillman reaction ii) Heck reaction

#### Section-IV

Answer any FOUR questions. Each question carries FIVE marks. 4X5=20Marks

10. Write notes on inter-system crossing.

11. Explain the nature of hydrogen donars in photochemical reactions

12. Explain about Photo Fries rearrangement.

13. Give a brief account on the protection of carboxylic acids by ester formation.

14. How does carbonate formation protect diols?

15. Write about Robinson annulation.

16. What is Stork-enamine reaction?

17. Write about Buchwald–Hartwig coupling

# Cluster Elective –III PAPER – VIII-C-2 : ADVANCED ORGANIC REACTIONS

#### **Question bank**

# **ESSAYS**

1. Write the mechanism of photo reduction reaction explain the influence of temperature & solvent on photo reduction reaction

2. Explain intersystem crossing energy transfer process by Jablonski diagram

3. Write and Explain the mechanism of Norrish type-I and Norrish type –II reactions

4. Write and explain the mechanism of di-  $\pi$  methane rearrangement and Barton reaction

5. What are protecting groups? Write different methods of preparation of alcohols

6. What are protecting groups write different methods of preparation of amines

7. What are protecting groups? Write different methods of preparation of carbonyl groups

8. Explain the following 1) Mannich reaction 2.) Stork- enamine reaction

9. Explain the following 1) Mcmurrey reaction 2.) Heck reaction

10. Explain the following 1). UGI reaction 2). Click reaction

#### Short answer questions

1.) Write Barton reaction with mechanism

2.) Norrish type-2 reactions of 1, 2 - di ketones

3. Explain Photo decarboxylation reaction.

3.) What are protecting groups explain with one example

4.) Shapiro reaction

5.) Mitsunobu reaction

6.) Photo fries rearrangement

7.) What are phase transfer catalyst? Explain the use of benzyl tri alkyl ammonium halides as phase transfer catalyst

8.) Suzuki coupling reactions

# Cluster Elective –III ORGANIC PAPER – VIII-C-3: PHARMACEUTICAL AND MEDICINAL CHEMISTRY

#### 45 hrs (3 h / w)

Pharmaceutical chemistry Terminology: Pharmacy, Pharmacology, Pharmacophore, Pharmacodynamics, Pharmacokinetics (ADME, Receptors - brief treartment) Metabolites and Anti metabolites.

# UNIT-II

UNIT-I

#### **Drugs:**

Nomenclature: Chemical name, Generic name and trade names with examples Classification: Classification based on structures and therapeutic activity with one example each, Administration of drugs

#### **UNIT-III**

# Synthesis and therapeutic activity of the compounds: 12h

- a) Chemotherapeutic Drugs
  - 1. Sulpha drugs (Sulphamethoxazole) 2. Antibiotics β-Lactam Antibiotics, Macrolide Antibiotics, 3. Anti-malarial Drugs(chloroquine)
- b) Psycho therapeutic Drugs:
  - Anti-pyretics (Paracetamol) 2.Hypnotics, 3.Tranquilizers(Diazepam)
    4.Levodopa

# UNIT-IV

#### **Pharmacodynamics Drugs:**

1. Antiasthma Drugs (Salbutamol) 3. Antianginals (Glycerol Trinitrate)

4. Diuretics (Frusemide)

#### UNIT-V

#### HIV-AIDS:

Immunity - CD-4cells, CD-8cells, Retro virus, Replication in human body, Investigation available, prevention of AIDS, Drugs available - examples with structures: PIS: Indivanir (crixivan), Nelfinavir (Viracept).

#### List of Reference Books:

- 1. Medicinal Chemistry by Dr. B. V. Ramana
- 2. Synthetic Drugs by O. D. Tyagi & M. Yadav
- 3. Medicinal Chemistry by Ashutoshkar
- 4. Medicinal Chemistry by P. Parimoo
- 5. Pharmacology& Pharmaco therapeutics R. S Satoshkar & S. D. Bhandenkar
- 6. Medicinal Chemistry by Kadametal P-I & P II

8h

8h

8h

#### 9h

# P. R. GOVERNMENT COLLEGE, KAKINADA MODEL PAPER FOR SEMESTER – VI (CHEMISTRY) Paper - VIII : CLUSTER-C-3: PHARMACEUTICAL & MEDICINAL CHEMISTRY

**Duration: 2.30hrs.** 

Max. Marks: 60

Answer any FOUR questions choosing AT LEAST ONE question from each section

#### 4X10=40Marks

#### Section-I

- 1. Give a detailed account on pharmacodynamics and pharmacokinetics.
- Explain the following terms with suitable examples.
  i). Metabolites
  ii) Anti-metabolites
- 3. How drugs are classified according to their structure?

#### Section-II

- 4. Discuss the classification of drugs based on therapeutic activity.
- 5. Write about the synthesis of chloroquin.
- 6. Write about the synthesis and therapeutic activity of Paracetamol.

#### Section-III

- 7. Write about the synthesis of solbutamol.
- 8. What do you know about CD-4 and CD-8 cells?
- 9. What are the drugs available for prevention of AIDS? Give their structures.

#### Section-IV

Answer any **FOUR** questions. Each question carries **FIVE** marks.

4X5=20Marks

10. Define pharmacy and pharmacology.

11. Define pharmacophore and give two examples.

12. Write the clinical, generic and trade names of paracetamol.

- 13. Describe the types of administration of drugs.
- 14. Write about the therapeutic activity of chloroquine.

15. Write the preparation method and uses of antiuritics.

16. Define hypnotics and antipyretics.

17. Write notes on retro virus.

# Paper - VIII : CLUSTER-C-3: PHARMACEUTICAL & MEDICINAL CHEMISTRY Questionbank Essayquestions(10M)

#### 1. Explain metabolites and antimetabolites with an example each

2. Explain ADME in pharmacokinetics.

3. Explain the classification of drugs based on structure.

4. Explain the classification of drugs based on therapeutic activity.

5. Write the synthesis and therapeutic activity of sulphamethoxazole

6. Write the synthesis and therapeutic activity of chloroquine

7. Write the synthesis and therapeutic activity of paracetamol

8. Write the synthesis and therapeutic activity of diazepam

9. Write the synthesis and therapeutic activity of solbutamol

10. Write the synthesis and the rapeutic activity of glycerol tri nitrate.

11. Write the synthesis and therapeutic activity of frusemide.

12. Explain CD-4cells and CD-8 cells.

13. Write the synthesis and the apeutic activity of  $\beta$ - lactum

#### Shortanswerquestions(5M)

1. Explain the terms pharma cyand pharmacology.

2. Explain Pharmacophore with two examples.

3. Explain chemical name, generic name and trade name with examples.

4. Write different types of dosage forms based on a) physical state b) route of admistration

5. Write short note on antibiotics

6. Write short notes on antipyretics

7. What are hypnotics and tranquilizers give examples

8. Write about methods of prevention of AIDS.

9. Write the structures of drugs a) indivanir b) Nelfinavir.

10. Briefly explain pharmacokinetics

11. Write short note on administration on drugs

12. Write the investigations available for HIV-AIDS

13. Write the prevention methods available for HIV-AIDS

# P. R. GOVERNMENT COLLEGE, KAKINADA SEMESTER – VI (CHEMISTRY) Paper - VIII : CLUSTER-C-3: PHARMACEUTICAL & MEDICINAL CHEMISTRY

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5	Unit -V	2	1	4	25
	TOTAL	9	8	17	130

# I. LABORATORY COURSE – VIII Practical Paper – VIII-A-1: (at the end of semester VI) 30 hrs (2 h / W)

- 1. Preparation of Aspirin
- 2. Preparation of Paracetamol
- 3. Preparation of Acetanilide
- 4. Preparation of Barbutiric Acid
- 5. Preparation of Phenyl Azo  $\beta$ -naphthol

# II. LABORATORY COURSE – VIII Practical Paper – VIII-A-2 (at the end of semester VI)

30 hrs (2 h / W)

Green procedure for organic qualitative analysis: Detection of N, S andhalogens 2. Acetylation

of 1<sup>0</sup> amine by green method: Preparation of acetanilide

- 3. Rearrangement reaction in green conditions: Benzil-Benzilic acid rearrangement
- 4. Electrophilic aromatic substitution reaction: Nitration of phenol
- 5. Radical coupling reaction: Preparation of 1,1-bis -2-naphthol
- 6. Green oxidation reaction: Synthesis of adipic acid
- 7. Green procedure for Diels Alder reaction between furan and maleic anhydride

VII-A-3 Practical:- Project Work